Density Functional Theory from Effective Actions

Dick Furnstahl

Department of Physics
Ohio State University

September, 2005

Collaborators: A. Bhattacharyya, S. Bogner, H.-W. Hammer, S. Puglia, S. Ramanan, A. Schwenk, B. Serot

Outline

- Overview: Microscopic DFT
- Effective Actions and DFT
- Issues and Ideas and Open Problems
- Summary

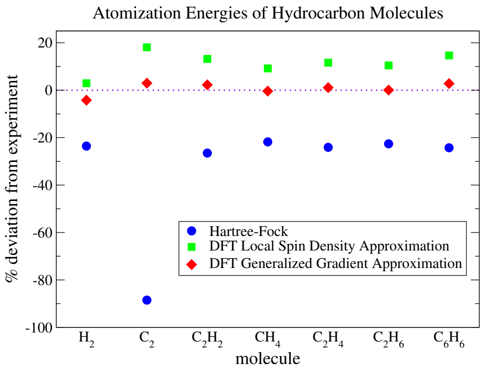
Outline

DFT from Microscopic NN$\cdots$N Interactions

- What?
  - *Constructive* density functional theory (DFT) for nuclei
- Why now?
  - Progress in chiral EFT
  - Application of RG (e.g., low-momentum interactions)
  - Advances in computational tools and methods
- How?
  - Use framework of effective actions with EFT principles
  - EFT interactions and operators evolved to low-momentum
    - Few-body input not enough (?) $\Longrightarrow$ input from many-body
  - Merge with other energy functional developments

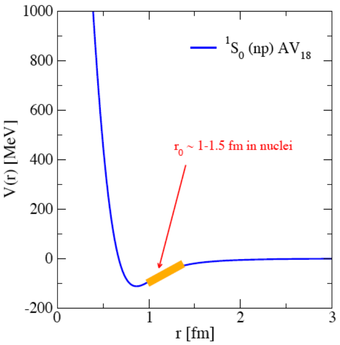
Density Functional Theory (DFT) with Coulomb

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



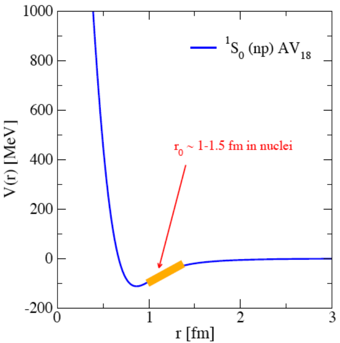
Sources of Nonperturbative Physics for NN

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



Sources of Nonperturbative Physics for NN

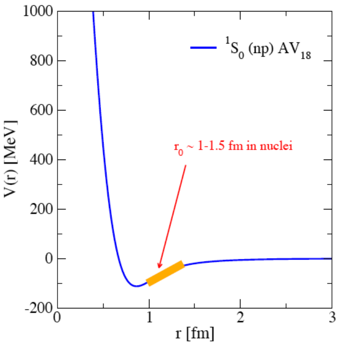
1. Strong short-range repulsion ("hard core")
2. Iterated tensor (S_{12}) interaction
3. Near zero-energy bound states



- 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??

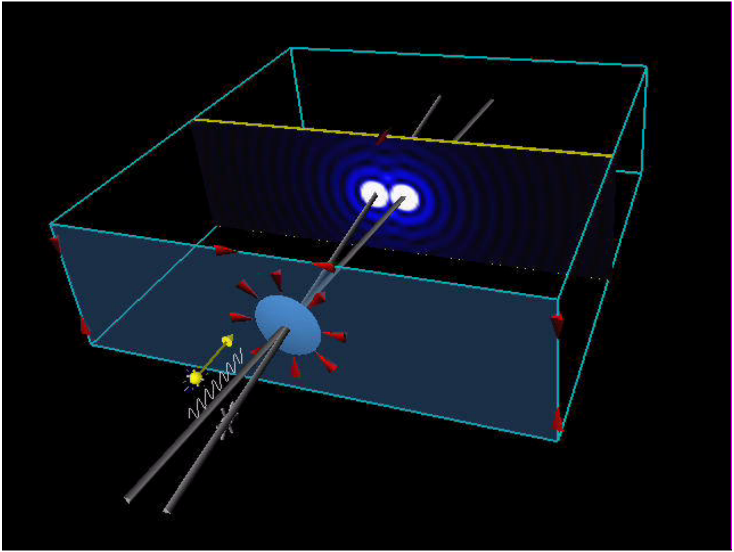
Sources of Nonperturbative Physics for NN

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

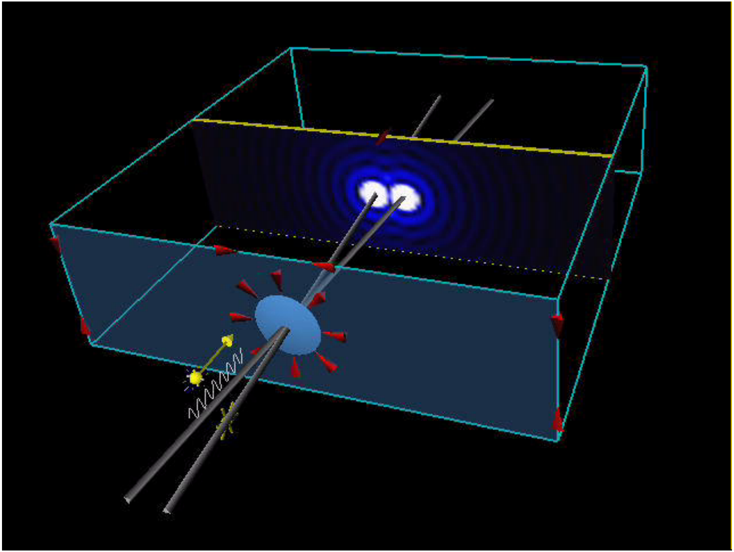


- Consequences:
  - In Coulomb DFT, Hartree-Fock gives dominate contribution $\Longrightarrow$ correlations are small corrections $\Longrightarrow$ DFT works!
  - cf. NN interactions $\Longrightarrow$ correlations $\gg$ HF $\Longrightarrow$ DFT fails??
- However . . .
  - the first two depend on the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

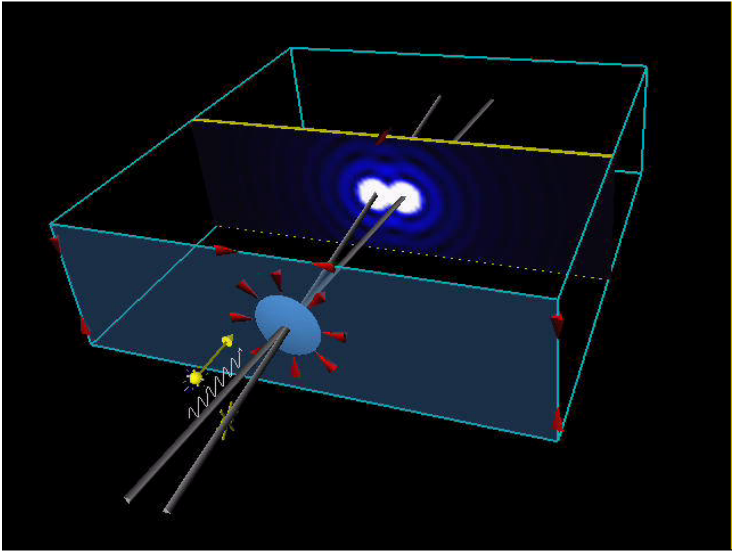
Wavelength and Resolution



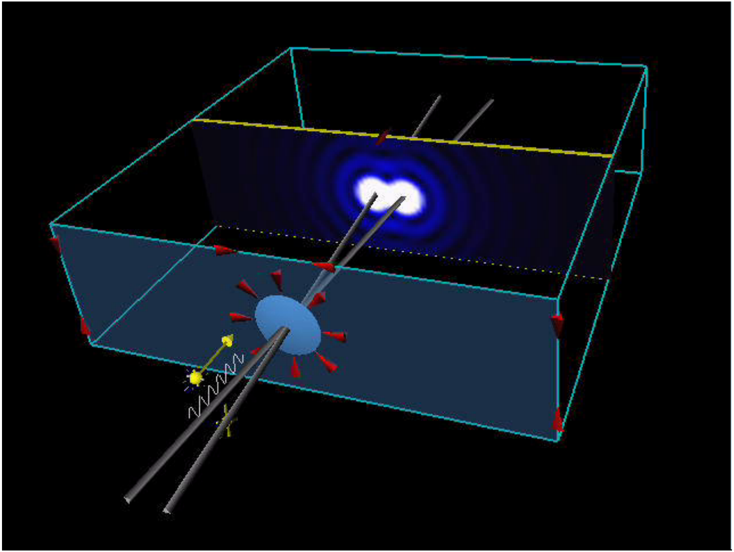
Wavelength and Resolution



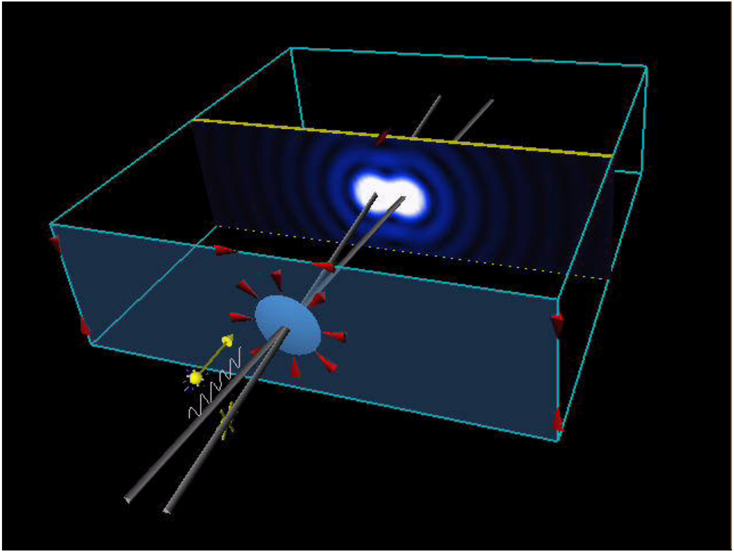
Wavelength and Resolution



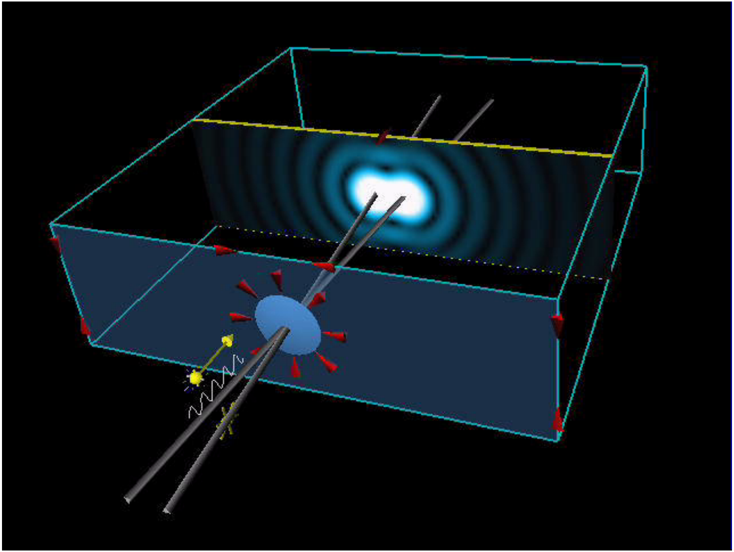
Wavelength and Resolution



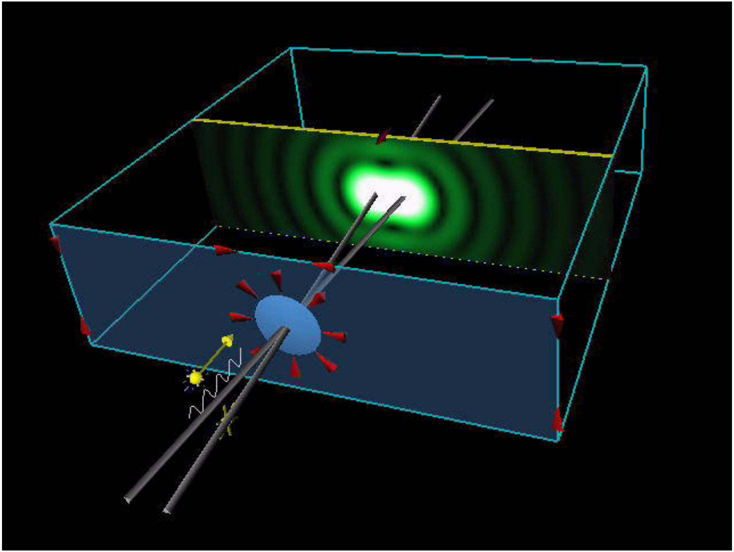
Wavelength and Resolution



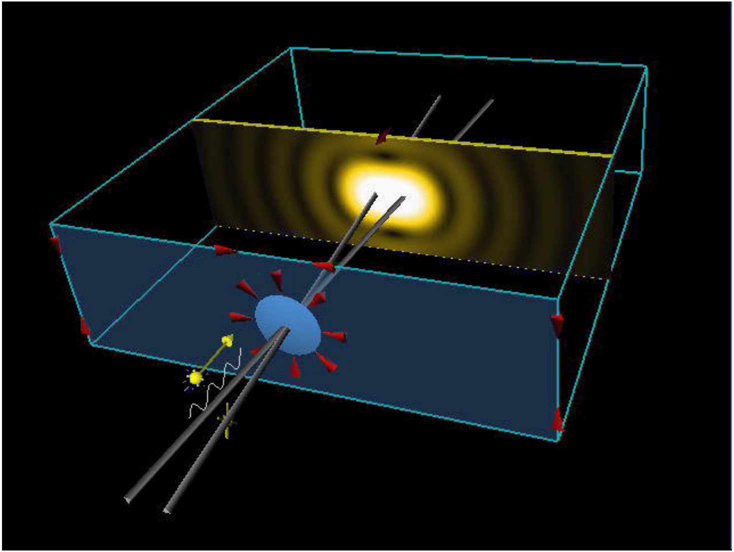
Wavelength and Resolution



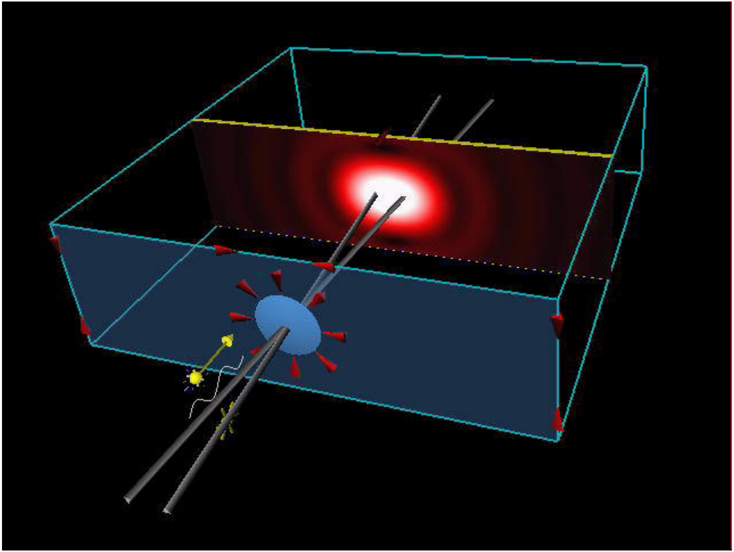
Wavelength and Resolution



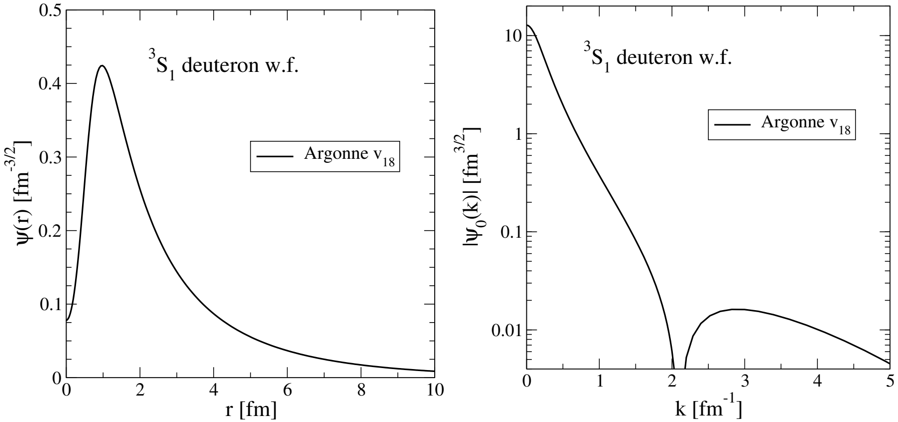
Wavelength and Resolution



Wavelength and Resolution

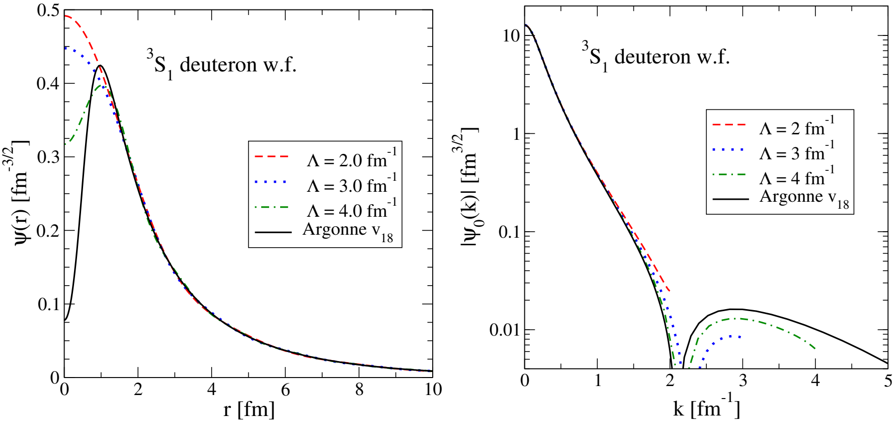


The Deuteron at Different Resolutions



- Repulsive core $\Longrightarrow$ short-distance suppression
  $\Longrightarrow$ high-momentum components

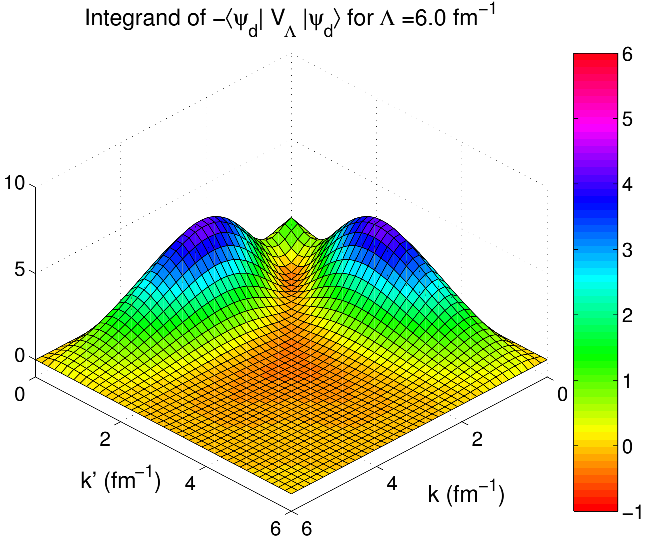
The Deuteron at Different Resolutions



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

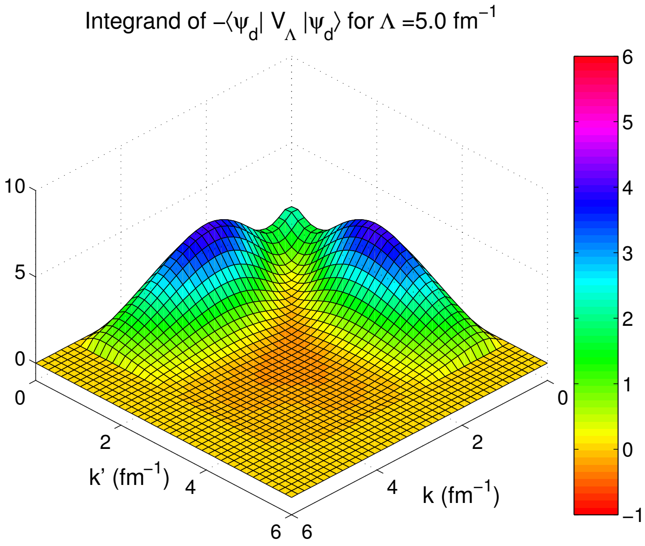
The Deuteron at Different Resolutions

more



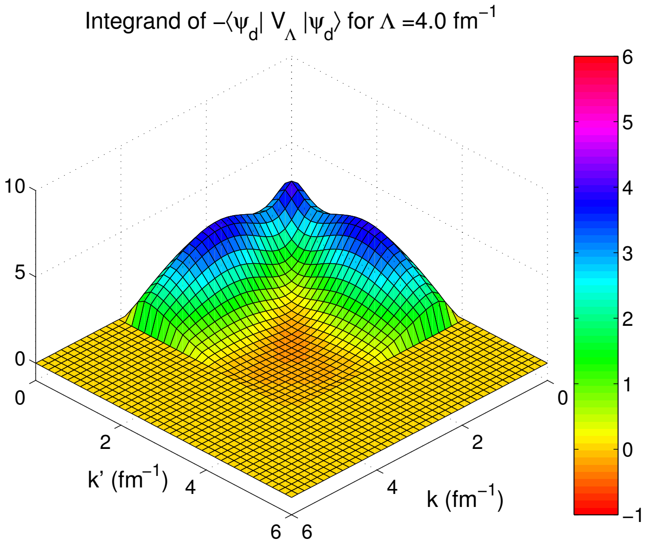
The Deuteron at Different Resolutions

more



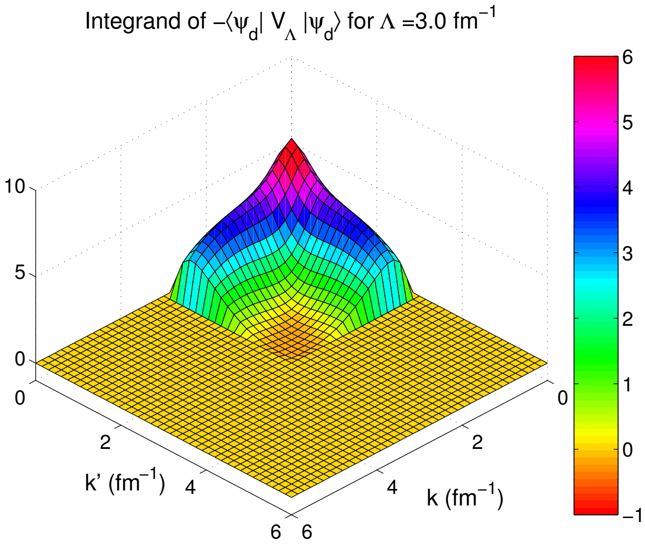
The Deuteron at Different Resolutions

more



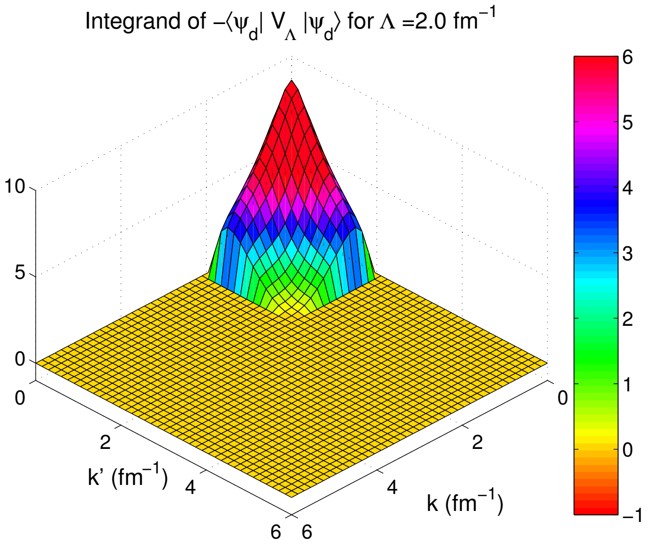
The Deuteron at Different Resolutions

more

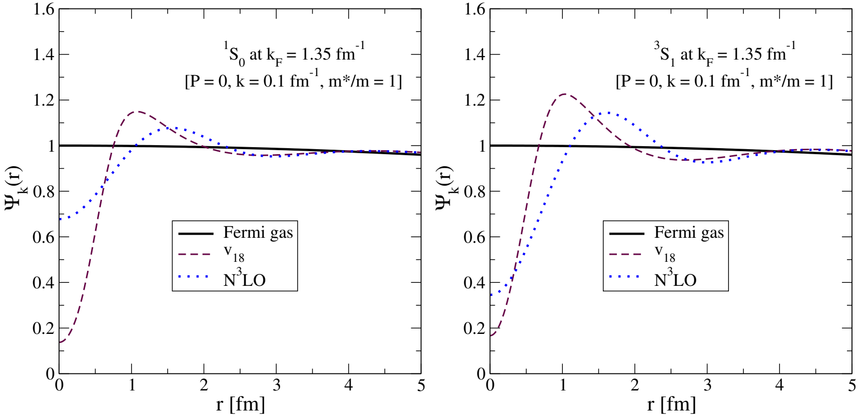


The Deuteron at Different Resolutions

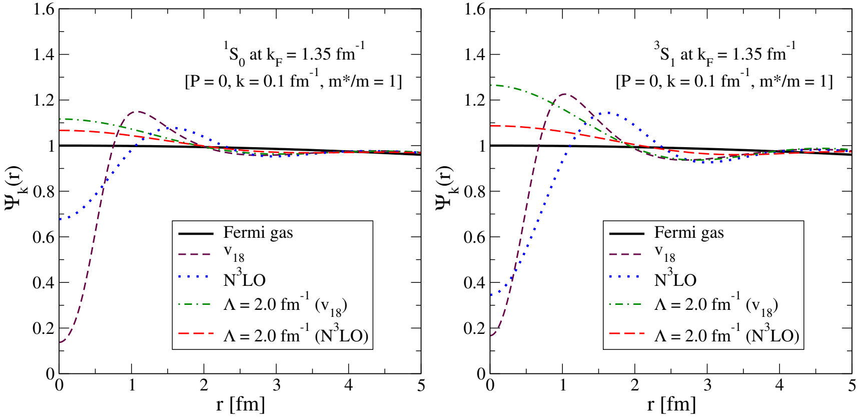
more



In-Medium Wave Functions (NN Only)



In-Medium Wave Functions (NN Only)



Conventional Wisdom on Nuclear Many-Body

- 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)."

Conventional Wisdom on Nuclear Many-Body

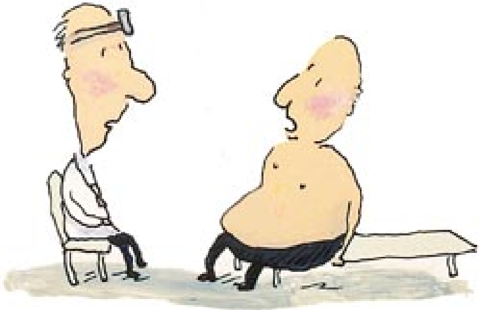
- Hans Bethe in review of nuclear matter (1971):

  "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)."

  "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."

EFT and RG Make Physics Easier

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



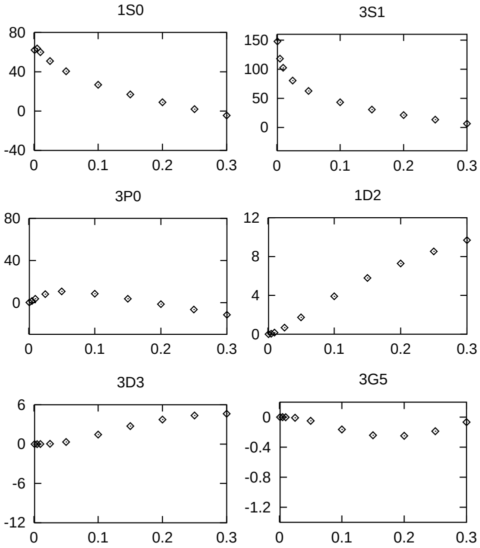
Patient: Doctor, doctor, it hurts when I do this!
Doctor: Then don't do that.

- 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!"

Chiral Effective Field Theory for Two Nucleons

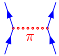
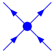
- Epelbaum, Meißner, et al.
- Also Entem, Machleidt
- $\mathcal{L}_{\pi N}$ + match at low energy

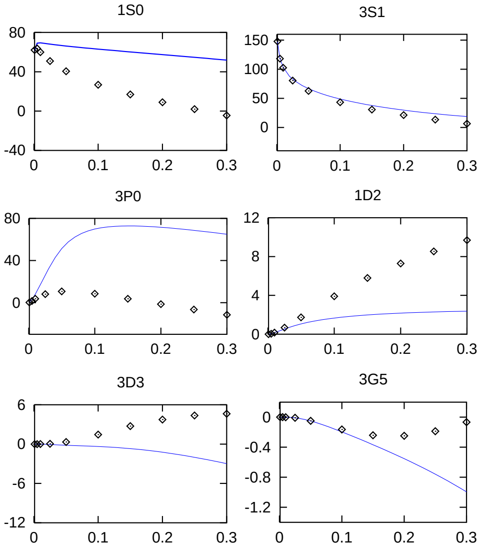
Q^ν	1π	2π	$4N$



Chiral Effective Field Theory for Two Nucleons

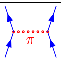
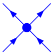
- Epelbaum, Meißner, et al.
- Also Entem, Machleidt
- $\mathcal{L}_{\pi N}$ + match at low energy

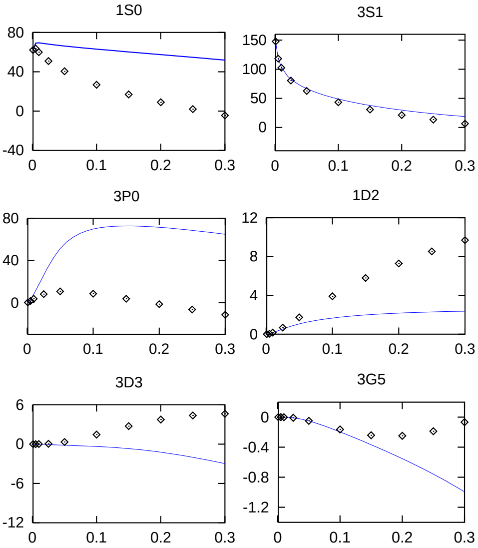
Q^ν	1π	2π	$4N$
Q^0		—	 (2)



Chiral Effective Field Theory for Two Nucleons

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

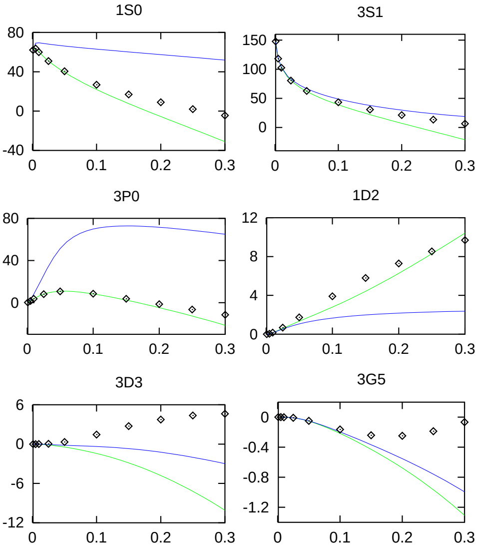
Q^ν	1π	2π	$4N$
Q^0		—	 (2)
Q^1			



Chiral Effective Field Theory for Two Nucleons

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

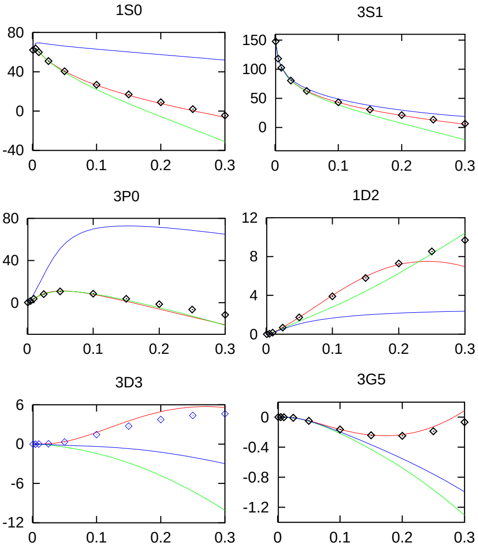
Q^{ν}	1π	2π	$4N$
Q^0	π	—	(2)
Q^1			
Q^2			$\overrightarrow{\nabla}^2$ (7)



Chiral Effective Field Theory for Two Nucleons

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

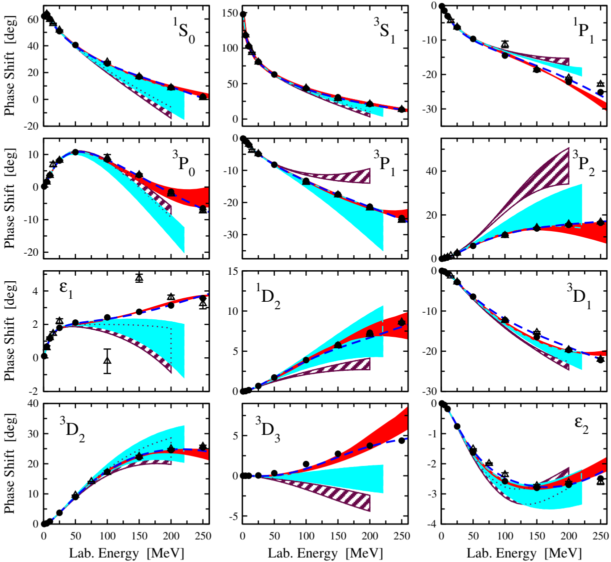
Q^ν	1π	2π	$4N$
Q^0	π	—	(2)
Q^1			
Q^2			$\overrightarrow{\nabla}^2$ (7)
Q^3	$\mathcal{L}_{\pi N}$	$\mathcal{L}_{\pi N}$	



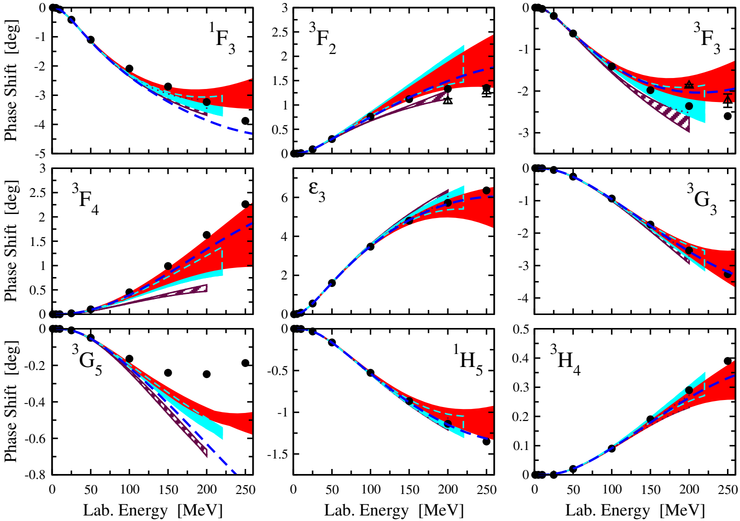
How do you go from Chiral EFT to a Potential?

- E.g., see Evgeny Epelbaum review: nucl-th/0509032
- Method of unitary transformations (e.g., Okubo)
  - *P* space has nucleons only, *Q* space has the pions
  - Use chiral expansion in $\{\mathbf{p}, m_\pi\}/\Lambda$
  - Energy-independent potential
- Consistent operators constructed with power counting

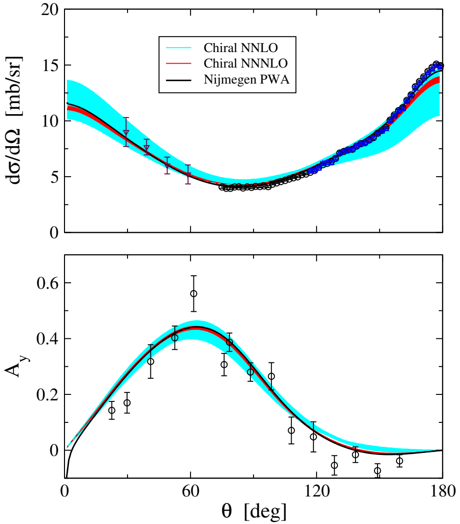
State of the Art: N^{3}LO



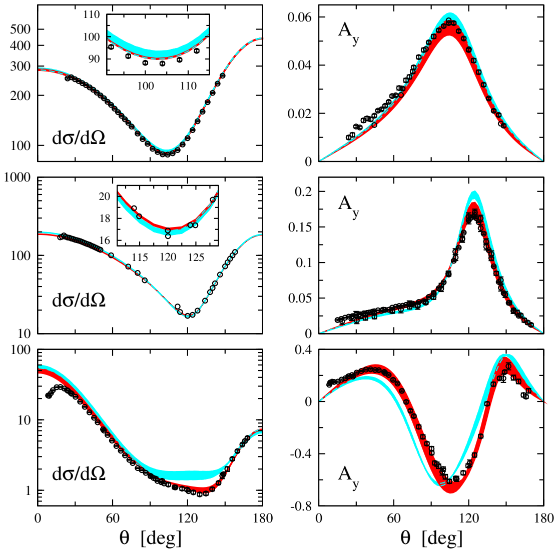
State of the Art: N^{3}LO



State of the Art: N^3LO

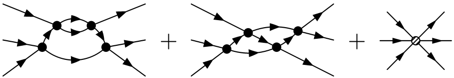


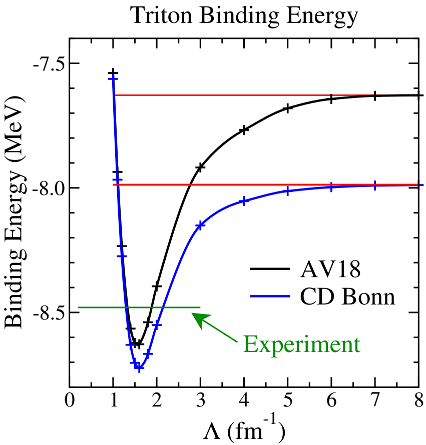
State of the Art: N^{3}LO



Many-Body Forces are Inevitable!

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

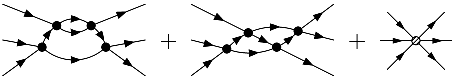




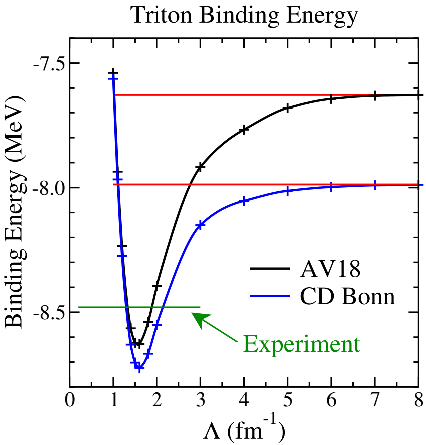
[Bogner, Nogga, Schwenk]

Many-Body Forces are Inevitable!

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



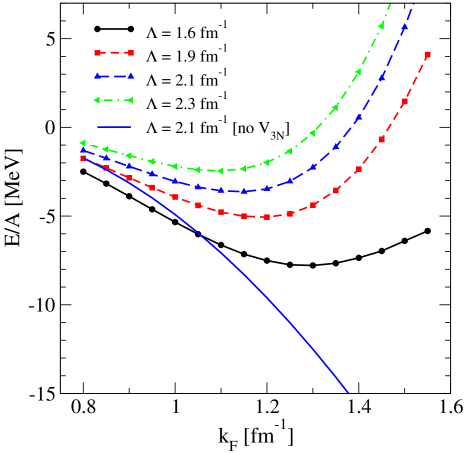
- How do we organize $(3, 4, \cdots)$–body forces? EFT!



[Bogner, Nogga, Schwenk]

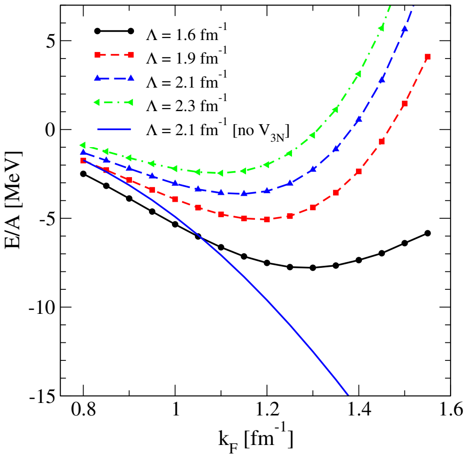
(Approximate) Nuclear Matter with NN and NNN

Hartree-Fock

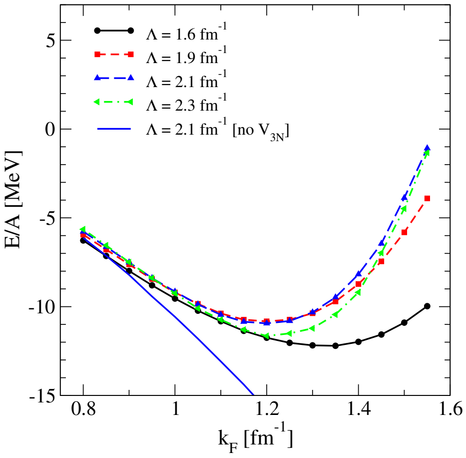


(Approximate) Nuclear Matter with NN and NNN

Hartree-Fock



"≈ 2nd Order"



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

One Hamiltonian for all problems and energy/length scales (not QCD!)	Infinite # of low-energy potentials; different resolutions $\Longrightarrow$ different dof’s and Hamiltonians
Find the “best” potential	There is no best potential $\Longrightarrow$ use a convenient one!
Two-body data may be sufficient; many-body forces as last resort	Many-body data needed and many-body forces inevitable
Avoid (hide) divergences	Exploit divergences (cutoff dependence as tool)
Choose approximations (e.g., diagrams) by “art”	Power counting determines diagrams and truncation error

My Favored Scenario for DFT (Today!)

- Construct a chiral EFT to a given order (N^3LO at present)
  - including many-body forces (N^3LO has leading 4-body)
  - choose cutoff regulator Λ as large as possible up to breakdown scale to minimize truncation error
- Evolve Λ down with RG (to $\Lambda \approx 2\,\mathrm{fm}^{-1}$ for ordinary nuclei)
  - *all* interactions
  - *and* other operators
- Generate density functional in effective action form
  - direct construction (e.g., DME++)
  - *or* match to finite-density EFT expansion

Outline

Overview: Microscopic DFT

Effective Actions and DFT

Issues and Ideas and Open Problems

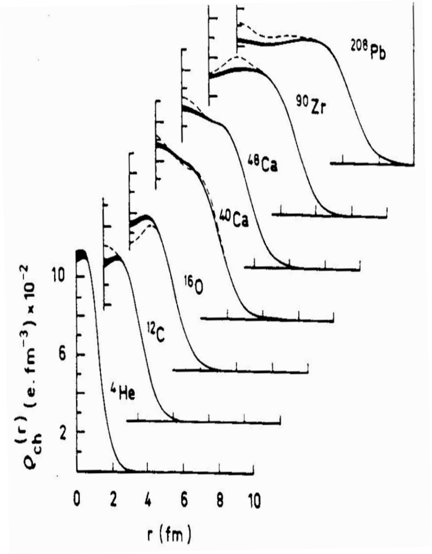
Summary

Density Functional Theory (DFT)

- Hohenberg-Kohn: There exists an energy functional $E_v[\rho]$ ...

$$E_v[\rho] = F_{\mathrm{HK}}[\rho] + \int d^3x\, v(\mathbf{x})\rho(\mathbf{x})$$

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



DFT as Effective Action

- Effective action is generically the Legendre transform of a generating functional with external source
- Partition function in presence of $J(x)$ coupled to density:

$$\mathcal{Z}[J] = e^{-W[J]} \sim \mathrm{Tr}\, e^{-\beta(\widehat{H}+J\,\widehat{\rho})} \longrightarrow \int \mathcal{D}[\psi^\dagger]\mathcal{D}[\psi]\, e^{-\int[\mathcal{L}+J\,\psi^\dagger\psi]}$$

- The density $\rho(x)$ in the presence of $J(x)$ is [we want $J=0$]

$$\rho(x) \equiv \langle\widehat{\rho}(x)\rangle_J = \frac{\delta W[J]}{\delta J(x)}$$

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

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

Partition Function in Zero Temperature Limit

- Consider Hamiltonian with time-independent source $J(\mathbf{x})$:

$$\widehat{H}(J) = \widehat{H} + \int J\,\psi^\dagger\psi$$

- *If* ground state is isolated (and bounded from below),

$$e^{-\beta\widehat{H}} = e^{-\beta E_0}\left[|0\rangle\langle 0| + \mathcal{O}\left(e^{-\beta(E_1-E_0)}\right)\right]$$

- As $\beta\to\infty$, $\mathcal{Z}[J] \Longrightarrow$ ground state of $\widehat{H}(J)$ with energy $E_0(J)$

$$\mathcal{Z}[J] = e^{-W[J]} \sim \mathrm{Tr}\,e^{-\beta(\widehat{H}+J\,\widehat{\rho})} \Longrightarrow E_0(J) = \lim_{\beta\to\infty} -\frac{1}{\beta}\log\mathcal{Z}[J] = \frac{1}{\beta}W[J]$$

Partition Function in Zero Temperature Limit

- Consider Hamiltonian with time-independent source $J(\mathbf{x})$:

$$\widehat{H}(J) = \widehat{H} + \int J\, \psi^\dagger \psi$$

- *If* ground state is isolated (and bounded from below),

$$e^{-\beta \widehat{H}} = e^{-\beta E_0} \left[|0\rangle\langle 0| + \mathcal{O}\left(e^{-\beta(E_1 - E_0)}\right) \right]$$

- As $\beta \to \infty$, $\mathcal{Z}[J] \Longrightarrow$ ground state of $\widehat{H}(J)$ with energy $E_0(J)$

$$\mathcal{Z}[J] = e^{-W[J]} \sim \mathrm{Tr}\, e^{-\beta(\widehat{H} + J\,\widehat{\rho})} \Longrightarrow E_0(J) = \lim_{\beta\to\infty} -\frac{1}{\beta} \log \mathcal{Z}[J] = \frac{1}{\beta} W[J]$$

- Substitute and separate out the pieces:

$$E_0(J) = \langle \widehat{H}(J) \rangle_J = \langle \widehat{H} \rangle_J + \int J \langle \psi^\dagger \psi \rangle_J = \langle \widehat{H} \rangle_J + \int J\, \rho(J)$$

- Expectation value of $\widehat{H}$ in ground state generated by $J[\rho]$

$$\langle \widehat{H} \rangle_J = E_0(J) - \int J\, \rho = \frac{1}{\beta} \Gamma[\rho]$$

Putting it all together ...

$$\frac{1}{\beta}\Gamma[\rho] = \langle \widehat{H} \rangle_J \xrightarrow{J\to 0} E_0 \quad \text{and} \quad J(x) = -\frac{\delta\Gamma[\rho]}{\delta\rho(x)} \xrightarrow{J\to 0} \left.\frac{\delta\Gamma[\rho]}{\delta\rho(x)}\right|_{\rho_{\rm gs}(\mathbf{x})} = 0$$

$\Longrightarrow$ For static $\rho(\mathbf{x})$, $\Gamma[\rho] \propto$ the DFT energy functional $F_{\rm HK}$!

Putting it all together . . .

$$\frac{1}{\beta}\Gamma[\rho] = \langle \widehat{H} \rangle_J \xrightarrow{J\to 0} E_0 \quad \text{and} \quad J(x) = -\frac{\delta\Gamma[\rho]}{\delta\rho(x)} \xrightarrow{J\to 0} \left.\frac{\delta\Gamma[\rho]}{\delta\rho(x)}\right|_{\rho_{\rm gs}(\mathbf{x})} = 0$$

$\Longrightarrow$ For static $\rho(\mathbf{x})$, $\Gamma[\rho] \propto$ the DFT energy functional $F_{\rm HK}$!

- The true ground state (with $J = 0$) is a variational minimum
  - So more sources should be better! (e.g., $\Gamma[\rho, \tau, \mathbf{J}, \cdots]$)

Putting it all together . . .

$$\frac{1}{\beta}\Gamma[\rho] = \langle \widehat{H} \rangle_J \xrightarrow{J\to 0} E_0 \quad \text{and} \quad J(x) = -\frac{\delta\Gamma[\rho]}{\delta\rho(x)} \xrightarrow{J\to 0} \left.\frac{\delta\Gamma[\rho]}{\delta\rho(x)}\right|_{\rho_{gs}(\mathbf{x})} = 0$$

$\Longrightarrow$ For static $\rho(\mathbf{x})$, $\Gamma[\rho] \propto$ the DFT energy functional $F_{\rm HK}$!

- The true ground state (with $J = 0$) is a variational minimum
  - So more sources should be better! (e.g., $\Gamma[\rho, \tau, \mathbf{J}, \cdots]$)
- Universal dependence on external potential is trivial:

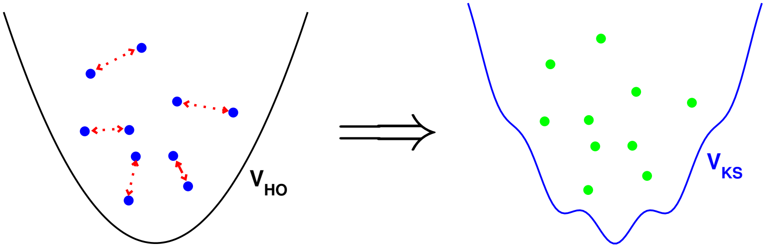
$$\Gamma[\rho] = W[J] - \int J\,\rho = W_{v=0}[J+v] - \int [(J+v) - v]\,\rho = \Gamma_{v=0}[\rho] + \int v\,\rho$$

  - But functionals change with resolution or field redefinitions
    $\Longrightarrow$ only stationary points are observables
- If uniform, find spontaneously broken ground state; if finite . . .
- NOTE: Beware of new UV divergences!
- [For Minkowski-space version of this, see Weinberg Vol. II]

Paths to the Effective Action Density Functional

1. Follow Coulomb Kohn-Sham DFT
   - Calculate asymmetric nuclear matter as function of density
     $\Longrightarrow$ LDA functional + standard Kohn-Sham procedure
   - Add semi-empirical gradient expansion
2. RG approach [Polonyi/Schwenk]
3. Auxiliary field method [Faussurier, Valiev/Fernando]
   - Eliminate $\psi^\dagger\psi$ in favor of auxiliary field φ
   - Loop expansion about expectation value ϕ
   - Kohn-Sham: Use freedom to require density unchanged
4. Inversion method [Fukuda et al., Valiev/Fernando]
   $\Longrightarrow$ systematic Kohn-Sham DFT

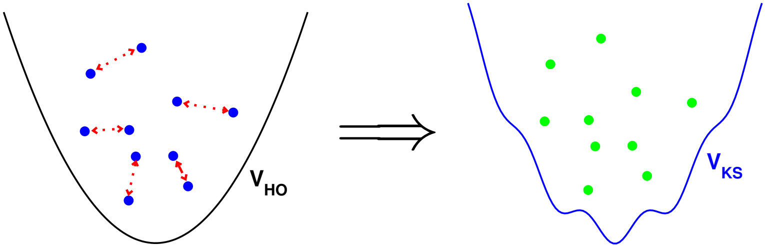
Kohn-Sham DFT



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

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

Kohn-Sham DFT



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

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

- Plan: Make this work by *construction*
  - inversion method (“point-coupling”)
  - auxiliary fields (e.g., “mesons” in covariant DFT)

What can Power Counting do for DFT?

- Given $W[J]$ as an EFT expansion, how do we find $\Gamma[\rho]$?

$$\Gamma[\rho] = W[J] - \int J\rho$$

- Inversion method: order-by-order inversion from $W[J]$ to $\Gamma[\rho]$
  - Decompose $J(x) = J_0(x) + J_{\text{LO}}(x) + J_{\text{NLO}}(x) + \ldots$
  - Two conditions on J_0:

$$\rho(x) = \frac{\delta W_0[J_0]}{\delta J_0(x)} \quad \text{and} \quad J_0(x)\big|_{\rho=\rho_{\text{gs}}} = \left.\frac{\delta \Gamma_{\text{interacting}}[\rho]}{\delta \rho(x)}\right|_{\rho=\rho_{\text{gs}}}$$

What can Power Counting do for DFT?

- Given $W[J]$ as an EFT expansion, how do we find $\Gamma[\rho]$?

$$\Gamma[\rho] = W[J] - \int J\rho$$

- Inversion method: order-by-order inversion from $W[J]$ to $\Gamma[\rho]$
  - Decompose $J(x) = J_0(x) + J_{\rm LO}(x) + J_{\rm NLO}(x) + \ldots$
  - Two conditions on J_0:

$$\rho(x) = \frac{\delta W_0[J_0]}{\delta J_0(x)} \quad \text{and} \quad J_0(x)\big|_{\rho=\rho_{\rm gs}} = \left.\frac{\delta \Gamma_{\rm interacting}[\rho]}{\delta\rho(x)}\right|_{\rho=\rho_{\rm gs}}$$

- Interpretation: J_0 is the external potential that yields for a noninteracting system the exact density
  - This is the Kohn-Sham potential!
  - Two conditions involving $J_0 \Longrightarrow$ Self-consistency

Treat Source $J(\mathbf{x})$ as a Background Field

- Effective action as a path integral $\Longrightarrow$ construct $W[J]$, order-by-order in an expansion (e.g., EFT power counting)
  - Propagators (lines) are in the background field $J(\mathbf{x})$

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

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

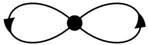
Treat Source $J(\mathbf{x})$ as a Background Field

- Effective action as a path integral $\Longrightarrow$ construct $W[J]$, order-by-order in an expansion (e.g., EFT power counting)
  - Propagators (lines) are in the background field $J(\mathbf{x})$

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

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

- E.g., apply to short-range LO contribution: Hartree-Fock

LO : 

$$W_1[J] = \frac{1}{2}\nu(\nu-1)C_0\int d^3\mathbf{x}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,G_J^0(\mathbf{x},\mathbf{x};\omega)G_J^0(\mathbf{x},\mathbf{x};\omega')$$

$$= -\frac{1}{2}\frac{(\nu-1)}{\nu}C_0\int d^3\mathbf{x}\,[\rho_J(\mathbf{x})]^2 \quad \text{where} \quad \rho_J(\mathbf{x}) \equiv \nu\sum_\alpha^{\epsilon_{\rm F}}|\psi_\alpha(\mathbf{x})|^2$$

Kohn-Sham Via Inversion Method (cf. KLW [1960])

- Inversion method for effective action DFT [Fukuda et al.]
  - order-by-order matching in λ (e.g., EFT expansion)

$$\text{diagrams} \implies W[J,\lambda] = W_0[J] + \lambda W_1[J] + \lambda^2 W_2[J] + \cdots$$

$$\text{assume} \implies J[\rho,\lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots$$

$$\text{derive} \implies \Gamma[\rho,\lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots$$

- Start with exact expressions for Γ and ρ

$$\Gamma[\rho] = W[J] - \int d^4x\, J(x)\rho(x) \quad \implies \quad \rho(x) = \frac{\delta W[J]}{\delta J(x)}$$

$\implies$ plug in expansions with ρ treated as order unity

Kohn-Sham Via Inversion Method (cf. KLW [1960])

- Inversion method for effective action DFT [Fukuda et al.]
  - order-by-order matching in λ (e.g., EFT expansion)

$$\text{diagrams} \Longrightarrow W[J,\lambda] = W_0[J] + \lambda W_1[J] + \lambda^2 W_2[J] + \cdots$$

$$\text{assume} \Longrightarrow J[\rho,\lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots$$

$$\text{derive} \Longrightarrow \Gamma[\rho,\lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots$$

- Zeroth order is noninteracting system with potential $J_0(x)$

$$\Gamma_0[\rho] = W_0[J_0] - \int d^4x\, J_0(x)\rho(x) \quad \Longrightarrow \quad \rho(x) = \frac{\delta W_0[J_0]}{\delta J_0(x)}$$

$\Longrightarrow$ Kohn-Sham system with the exact density! $J_0 \equiv V_{\rm KS}$

Kohn-Sham Via Inversion Method (cf. KLW [1960])

- Inversion method for effective action DFT [Fukuda et al.]
  - order-by-order matching in λ (e.g., EFT expansion)

$$\begin{aligned}
\text{diagrams} &\implies W[J,\lambda] = W_0[J] + \lambda W_1[J] + \lambda^2 W_2[J] + \cdots \\
\text{assume} &\implies J[\rho,\lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots \\
\text{derive} &\implies \Gamma[\rho,\lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots
\end{aligned}$$

- Zeroth order is noninteracting system with potential $J_0(x)$

$$\Gamma_0[\rho] = W_0[J_0] - \int d^4x \, J_0(x)\rho(x) \quad \implies \quad \rho(x) = \frac{\delta W_0[J_0]}{\delta J_0(x)}$$

$\implies$ Kohn-Sham system with the exact density! $J_0 \equiv V_{\rm KS}$

- Diagonalize $W_0[J_0]$ by introducing KS orbitals $\implies$ sum of ε_i's

Kohn-Sham Via Inversion Method (cf. KLW [1960])

- Inversion method for effective action DFT [Fukuda et al.]
  - order-by-order matching in λ (e.g., EFT expansion)

$$\text{diagrams} \Longrightarrow W[J,\lambda] = W_0[J] + \lambda W_1[J] + \lambda^2 W_2[J] + \cdots$$

$$\text{assume} \Longrightarrow J[\rho,\lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots$$

$$\text{derive} \Longrightarrow \Gamma[\rho,\lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots$$

- Zeroth order is noninteracting system with potential $J_0(x)$

$$\Gamma_0[\rho] = W_0[J_0] - \int d^4x\, J_0(x)\rho(x) \quad \Longrightarrow \quad \rho(x) = \frac{\delta W_0[J_0]}{\delta J_0(x)}$$

$\Longrightarrow$ Kohn-Sham system with the exact density! $J_0 \equiv V_{\text{KS}}$

- Diagonalize $W_0[J_0]$ by introducing KS orbitals $\Longrightarrow$ sum of ε_i's
- Find J_0 for the ground state via self-consistency loop:

$$J_0 \to W_1 \to \Gamma_1 \to J_1 \to W_2 \to \Gamma_2 \to \cdots \Longrightarrow J_0(x) = \sum_{i>0} \frac{\delta \Gamma_i[\rho]}{\delta \rho(x)}$$

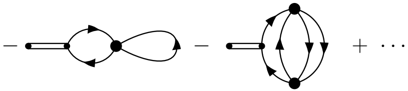
Kohn-Sham Potential

- Local $J_0(\mathbf{x})$ [cf. non-local, state-dependent $\Sigma^*(\mathbf{x},\mathbf{x}';\omega)$]

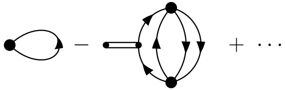
$$\text{e.g.,}\quad J_0(\mathbf{x}) = \frac{\delta\Gamma_{\rm int}[\rho,\tau]}{\delta\rho(\mathbf{x})} \quad \text{and} \quad \eta_0(\mathbf{x}) = \frac{\delta\Gamma_{\rm int}[\rho,\tau]}{\delta\tau(\mathbf{x})}$$

- Direct derivatives (e.g., DME++) are easiest,
  or use "inverse density-density correlator"

$$J_0(\mathbf{x}) = \frac{\delta\Gamma_{\rm int}[\rho]}{\delta\rho(\mathbf{x})} = \int \left(\frac{\delta\rho(\mathbf{x})}{\delta J_0(\mathbf{y})}\right)^{-1} \frac{\delta\Gamma_{\rm int}[\rho]}{\delta J_0(\mathbf{y})} =$$

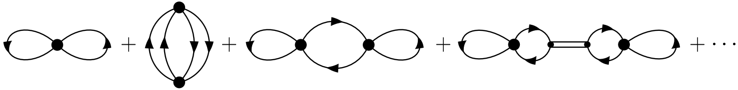


$=$



- New Feynman rules for $\Gamma_{\rm int} \Longrightarrow$ anomalous diagrams

$\Gamma_{\rm int} =$

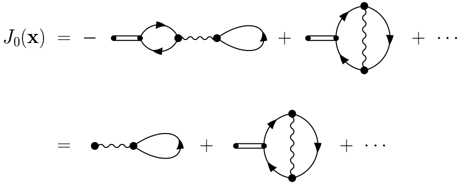


Kohn-Sham Potential

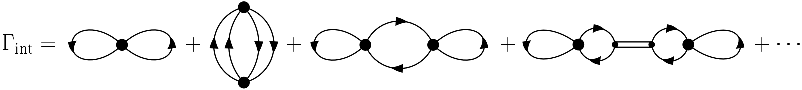
- Local $J_0(\mathbf{x})$ [cf. non-local, state-dependent $\Sigma^*(\mathbf{x},\mathbf{x}';\omega)$]

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

- Direct derivatives (e.g., DME++) are easiest,
  or use “inverse density-density correlator”



- New Feynman rules for $\Gamma_{\rm int} \Longrightarrow$ anomalous diagrams

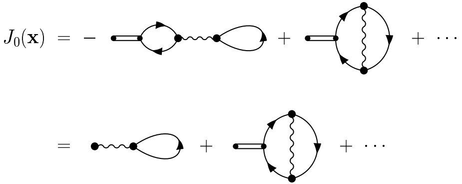


Kohn-Sham Potential

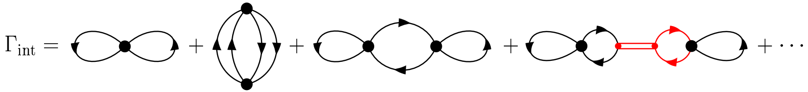
- Local $J_0(\mathbf{x})$ [cf. non-local, state-dependent $\Sigma^*(\mathbf{x},\mathbf{x}';\omega)$]

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

- Direct derivatives (e.g., DME++) are easiest,
  or use “inverse density-density correlator”



- New Feynman rules for $\Gamma_{\rm int} \Longrightarrow$ anomalous diagrams

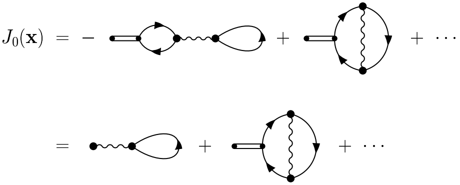


Kohn-Sham Potential

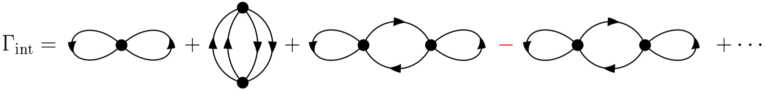
- Local $J_0(\mathbf{x})$ [cf. non-local, state-dependent $\Sigma^*(\mathbf{x},\mathbf{x}';\omega)$]

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

- Direct derivatives (e.g., DME++) are easiest, or use "inverse density-density correlator"



- New Feynman rules for $\Gamma_{\rm int} \Longrightarrow$ anomalous diagrams



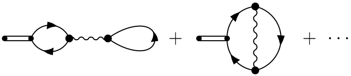
Kohn-Sham Potential

- Local $J_0(\mathbf{x})$ [cf. non-local, state-dependent $\Sigma^*(\mathbf{x},\mathbf{x}';\omega)$]

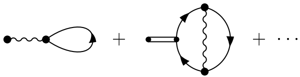
$$\text{e.g.,} \quad J_0(\mathbf{x}) = \frac{\delta\Gamma_{\rm int}[\rho,\tau]}{\delta\rho(\mathbf{x})} \quad \text{and} \quad \eta_0(\mathbf{x}) = \frac{\delta\Gamma_{\rm int}[\rho,\tau]}{\delta\tau(\mathbf{x})}$$

- Direct derivatives (e.g., DME++) are easiest, or use “inverse density-density correlator”

$J_0(\mathbf{x}) = -$

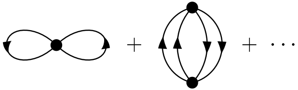


$=$



- New Feynman rules for $\Gamma_{\rm int} \Longrightarrow$ anomalous diagrams

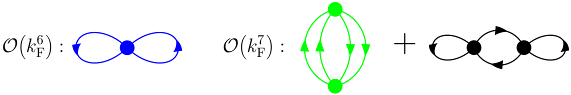
$\Gamma_{\rm int} =$



Example: Dilute EFT Ingredients

See “Crossing the Border” [nucl-th/0008064]

1. Use the most general $\mathcal{L}$ with low-energy dof’s consistent with global and local symmetries of underlying theory
   - $\mathcal{L}_{\rm eft} = \psi^\dagger \left[i\frac{\partial}{\partial t} + \frac{\nabla^2}{2M} \right] \psi - \frac{C_0}{2}(\psi^\dagger\psi)^2 - \frac{D_0}{6}(\psi^\dagger\psi)^3 + \ldots$
2. Declaration of regularization and renormalization scheme
   - natural $a_0 \Longrightarrow$ dimensional regularization and min. subtraction
3. Well-defined power counting $\Longrightarrow$ small expansion parameters
   - use the separation of scales $\Longrightarrow \frac{k_{\rm F}}{\Lambda}$ with $\Lambda \sim 1/R \Longrightarrow k_{\rm F} a_0$, etc.



$$\mathcal{E} = \rho \frac{k_{\rm F}^2}{2M} \left[\frac{3}{5} + \frac{2}{3\pi}(k_{\rm F} a_0) + \frac{4}{35\pi^2}(11 - 2\ln 2)(k_{\rm F} a_0)^2 + \cdots \right]$$

Comparing Skyrme and Dilute Functionals

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

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

- Dilute $\rho\tau$ energy density functional for $\nu = 4$ ($V_{\text{external}} = 0$)

$$E[\rho,\tau,\mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8}C_0\rho^2 + \frac{1}{16}(3C_2 + 5C_2')\rho\tau + \frac{1}{64}(9C_2 - 5C_2')(\boldsymbol{\nabla}\rho)^2 - \frac{3}{4}C_2''\rho\boldsymbol{\nabla}\cdot\mathbf{J} + \frac{c_1}{2M}C_0^2\rho^{7/3} + \frac{c_2}{2M}C_0^3\rho^{8/3} + \frac{1}{16}D_0\rho^3 + \cdots \right\}$$

Comparing Skyrme and Dilute Functionals

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

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

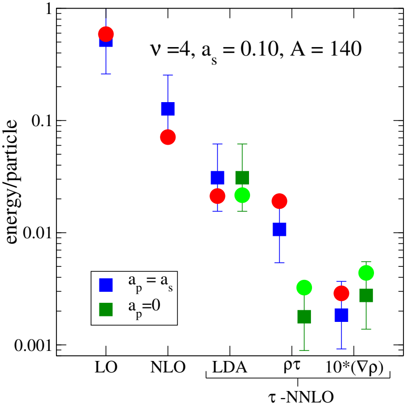
- Dilute $\rho\tau$ energy density functional for $\nu = 4$ ($V_{\mathrm{external}} = 0$)

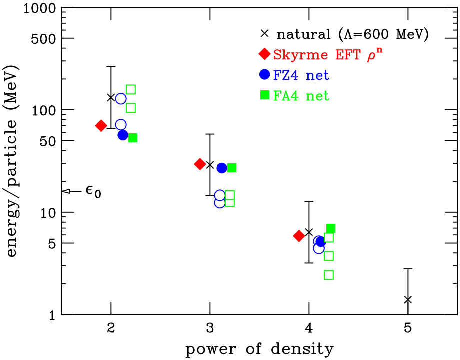
$$E[\rho,\tau,\mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8}C_0\rho^2 + \frac{1}{16}(3C_2 + 5C_2')\rho\tau + \frac{1}{64}(9C_2 - 5C_2')(\nabla\rho)^2 - \frac{3}{4}C_2''\rho\nabla\cdot\mathbf{J} + \frac{c_1}{2M}C_0^2\rho^{7/3} + \frac{c_2}{2M}C_0^3\rho^{8/3} + \frac{1}{16}D_0\rho^3 + \cdots \right\}$$

- Same functional as dilute Fermi gas with $t_i \leftrightarrow C_i$
  - equivalent $a_0 \approx -2$–3 fm but $|k_{\mathrm{F}}a_p|$, $|k_{\mathrm{F}}r_0| < 1$ (with $a_p < 0$)
  - missing non-analytic terms, NNN, . . .

Power Counting Terms in Energy Functionals

- Scale contributions according to average density or $\langle k_F \rangle$





- Reasonable estimates $\Longrightarrow$ truncation errors understood
- Where to truncate for nuclei?

Covariant DFT as Legendre Transformation

- To probe the system, add a source $V^\mu(x)$ coupled to current operator $\widehat{j}^\mu(x) \equiv \overline{\psi}(x)\gamma^\mu\psi(x)$ to the partition function:

$$\mathcal{Z}[V] = e^{-W[V]} \sim \mathrm{Tr}\, e^{-\beta(\widehat{H}+V\cdot\widehat{j})} \longrightarrow \int \mathcal{D}[\psi^\dagger]\mathcal{D}[\psi]\, e^{-\int[\mathcal{L}+V_\mu\,\overline{\psi}\gamma^\mu\psi]}$$

- The (time-dependent) current $j^\mu(x)$ in presence of $V^\mu(x)$ is

$$j^\mu(x) = (\rho_V(x), \mathbf{j}_V(x)) \equiv \langle\overline{\psi}(x)\gamma^\mu\psi(x)\rangle_V = \frac{\delta W[V]}{\delta V_\mu(x)}$$

- Invert to find $V^\mu[j]$ and Legendre transform from V^μ to j^μ:

$$\Gamma[j] = -W[V] + \int V\cdot j \quad \text{with} \quad V^\mu(x) = \frac{\delta\Gamma[j]}{\delta j_\mu(x)} \longrightarrow \left.\frac{\delta\Gamma[j]}{\delta j_\mu(x)}\right|_{j_{\mathrm{gs}}(\mathbf{x})} = 0$$

$\Longrightarrow$ For static $j^\mu(\mathbf{x})$, $\Gamma[j] \propto$ the DFT energy functional $E[\rho_V]$

What About the Scalar Density?

- Can add additional sources and Legendre transformations
- In nonrelativistic DFT, add to Lagrangian $+\,\eta(x)\,\nabla\psi^\dagger\nabla\psi$

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

$\Longrightarrow$ Skyrme HF energy functional $E[\rho,\tau,\mathbf{J}]$ of density *and* kinetic energy density (see A. Bhattacharyya talk)

- In covariant DFT, add to Lagrangian $+\,S(x)\,\overline{\psi}\psi$

$$\Gamma[j^\mu,\rho_s] = W[V^\mu,S] - \int V(x)\cdot j(x) - \int S(x)\rho_s(x)$$

$\Longrightarrow$ RMF energy functional $E[\rho_v,\rho_s]$ [with $j^\mu = (\rho_v,\mathbf{0})$]

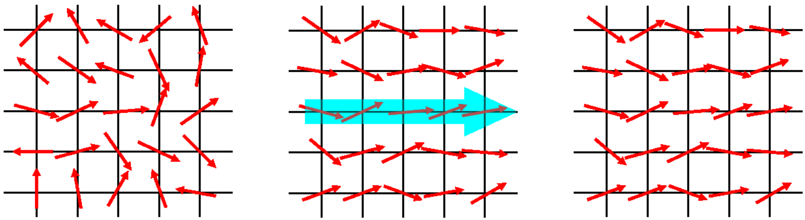
- Generates *point-coupling* functional

Pairing in DFT/EFT from Effective Action

- Natural framework for spontaneous symmetry breaking
  - e.g., test for zero-field magnetization M in a spin system
  - introduce an external field H to break rotational symmetry
  - Legendre transform Helmholtz free energy $F(H)$:

$$\text{invert} \quad M = -\partial F(H)/\partial H \quad \Longrightarrow \quad \Gamma[M] = F[H(M)] + MH(M)$$

  - since $H = \partial\Gamma/\partial M$, minimize Γ to find ground state



Generalizing Effective Action to Include Pairing

- Generating functional with sources J, j coupled to densities:

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

- Densities found by functional derivatives wrt J, j:

$$\rho(x) \equiv \langle\psi^\dagger(x)\psi(x)\rangle_{J,j} = \left.\frac{\delta W[J,j]}{\delta J(x)}\right|_j$$

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

Generalizing Effective Action to Include Pairing

- Generating functional with sources J, j coupled to densities:

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

- Densities found by functional derivatives wrt J, j:

$$\rho(x) \equiv \langle\psi^\dagger(x)\psi(x)\rangle_{J,j} = \left.\frac{\delta W[J,j]}{\delta J(x)}\right|_j$$

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

- Effective action $\Gamma[\rho,\phi]$ by functional Legendre transformation:

$$\Gamma[\rho,\phi] = W[J,j] - \int d^4x\, J(x)\rho(x) - \int d^4x\, j(x)\phi(x)$$

- $\Gamma[\rho,\phi] \propto$ ground-state (free) energy functional $E[\rho,\phi]$
  - at finite temperature, the proportionality constant is β
- The sources are given by functional derivatives wrt ρ and ϕ

$$\frac{\delta E[\rho,\phi]}{\delta\rho(\mathbf{x})} = J(\mathbf{x}) \qquad \text{and} \qquad \frac{\delta E[\rho,\phi]}{\delta\phi(\mathbf{x})} = j(\mathbf{x})$$

  - but the sources are zero in the ground state
  - $\Longrightarrow$ determine ground-state $\rho(\mathbf{x})$ and $\phi(\mathbf{x})$ by stationarity:

$$\left.\frac{\delta E[\rho,\phi]}{\delta\rho(\mathbf{x})}\right|_{\rho=\rho_{\rm gs},\phi=\phi_{\rm gs}} = \left.\frac{\delta E[\rho,\phi]}{\delta\phi(\mathbf{x})}\right|_{\rho=\rho_{\rm gs},\phi=\phi_{\rm gs}} = 0$$

- This is Hohenberg-Kohn DFT extended to pairing!

- $\Gamma[\rho,\phi] \propto$ ground-state (free) energy functional $E[\rho,\phi]$
  - at finite temperature, the proportionality constant is β
- The sources are given by functional derivatives wrt ρ and ϕ

$$\frac{\delta E[\rho,\phi]}{\delta\rho(\mathbf{x})} = J(\mathbf{x}) \qquad \text{and} \qquad \frac{\delta E[\rho,\phi]}{\delta\phi(\mathbf{x})} = j(\mathbf{x})$$

  - but the sources are zero in the ground state
  - $\Longrightarrow$ determine ground-state $\rho(\mathbf{x})$ and $\phi(\mathbf{x})$ by stationarity:

$$\left.\frac{\delta E[\rho,\phi]}{\delta\rho(\mathbf{x})}\right|_{\rho=\rho_{\rm gs},\phi=\phi_{\rm gs}} = \left.\frac{\delta E[\rho,\phi]}{\delta\phi(\mathbf{x})}\right|_{\rho=\rho_{\rm gs},\phi=\phi_{\rm gs}} = 0$$

- This is Hohenberg-Kohn DFT extended to pairing!
- We need a method to carry out the inversion
  - For Kohn-Sham DFT, apply inversion methods
  - We need to renormalize!

Kohn-Sham Inversion Method Revisited

- Order-by-order matching in EFT expansion parameter λ

$$\begin{aligned} W[J,j,\lambda] &= W_0[J,j] + \lambda W_1[J,j] + \lambda^2 W_2[J,j] + \cdots \\ J[\rho,\phi,\lambda] &= J_0[\rho,\phi] + \lambda J_1[\rho,\phi] + \lambda^2 J_2[\rho,\phi] + \cdots \\ j[\rho,\phi,\lambda] &= j_0[\rho,\phi] + \lambda j_1[\rho,\phi] + \lambda^2 j_2[\rho,\phi] + \cdots \\ \Gamma[\rho,\phi,\lambda] &= \Gamma_0[\rho,\phi] + \lambda \Gamma_1[\rho,\phi] + \lambda^2 \Gamma_2[\rho,\phi] + \cdots \end{aligned}$$

- 0^{th} order is Kohn-Sham system with potentials $J_0(\mathbf{x})$ and $j_0(\mathbf{x})$ $\Longrightarrow$ yields the exact densities $\rho(\mathbf{x})$ and $\phi(\mathbf{x})$
  - introduce single-particle orbitals and solve (cf. HFB)

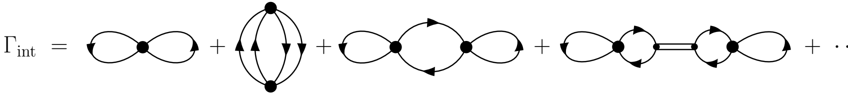
$$\begin{pmatrix} h_0(\mathbf{x}) - \mu_0 & j_0(\mathbf{x}) \\ j_0(\mathbf{x}) & -h_0(\mathbf{x}) + \mu_0 \end{pmatrix} \begin{pmatrix} u_i(\mathbf{x}) \\ v_i(\mathbf{x}) \end{pmatrix} = E_i \begin{pmatrix} u_i(\mathbf{x}) \\ v_i(\mathbf{x}) \end{pmatrix}$$

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

with conventional orthonormality relations for u_i, v_i

Diagrammatic Expansion of W_i

- Same diagrams, but with Nambu-Gor'kov Green's functions



$$iG = \begin{pmatrix} \langle T\psi_\uparrow(x)\psi_\uparrow^\dagger(x')\rangle_0 & \langle T\psi_\uparrow(x)\psi_\downarrow(x')\rangle_0 \\ \langle T\psi_\downarrow^\dagger(x)\psi_\uparrow^\dagger(x')\rangle_0 & \langle T\psi_\downarrow^\dagger(x)\psi_\downarrow(x')\rangle_0 \end{pmatrix} \equiv \begin{pmatrix} iG_{\rm ks}^0 & iF_{\rm ks}^0 \\ iF_{\rm ks}^{0\,\dagger} & -iG_{\rm ks}^0 \end{pmatrix}$$

- In frequency space, the Green's functions are

$$iG_{\rm ks}^0(\mathbf{x},\mathbf{x}';\omega) = \sum_i \left[\frac{u_i(\mathbf{x})\,u_i^*(\mathbf{x}')}{\omega - E_i + i\eta} + \frac{v_i(\mathbf{x}')\,v_i^*(\mathbf{x})}{\omega + E_i - i\eta}\right]$$

$$iF_{\rm ks}^0(\mathbf{x},\mathbf{x}';\omega) = -\sum_i \left[\frac{u_i(\mathbf{x})\,v_i^*(\mathbf{x}')}{\omega - E_i + i\eta} - \frac{u_i(\mathbf{x}')\,v_i^*(\mathbf{x})}{\omega + E_i - i\eta}\right]$$

Kohn-Sham Self-Consistency Procedure

- Same iteration procedure as in Skyrme or RMF with pairing
- In terms of the orbitals, the fermion density is

$$\rho(\mathbf{x}) = 2\sum_i |v_i(\mathbf{x})|^2$$

and the pair density is (warning: divergent!)

$$\phi(\mathbf{x}) = \sum_i [u_i^*(\mathbf{x})v_i(\mathbf{x}) + u_i(\mathbf{x})v_i^*(\mathbf{x})]$$

- The chemical potential μ_0 is fixed by $\int \rho(\mathbf{x}) = A$
- Diagrams for $\widetilde{\Gamma}[\rho, \phi] = -E[\rho, \phi]$ (with LDA+) yields KS potentials

$$J_0(\mathbf{x})\Big|_{\rho=\rho_{\rm gs}} = \frac{\delta\widetilde{\Gamma}_{\rm int}[\rho,\phi]}{\delta\rho(\mathbf{x})}\bigg|_{\rho=\rho_{\rm gs}} \quad \text{and} \quad j_0(\mathbf{x})\Big|_{\phi=\phi_{\rm gs}} = \frac{\delta\widetilde{\Gamma}_{\rm int}[\rho,\phi]}{\delta\phi(\mathbf{x})}\bigg|_{\phi=\phi_{\rm gs}}$$

Outline

Overview: Microscopic DFT

Effective Actions and DFT

Issues and Ideas and Open Problems

Summary

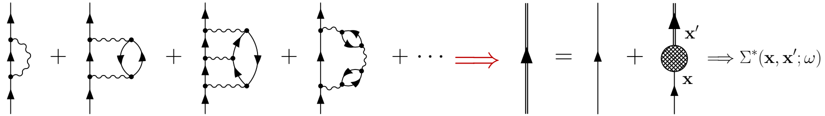
Questions about DFT and Nuclear Structure

- How do we connect to the free NN$\cdots$N interaction?
  - Chiral EFT $\xrightarrow{RG}$ low-momentum interactions: Power counting?
- What can you calculate in a DFT approach?
  - What about single-particle properties? Excited states?
- How is Kohn-Sham DFT more than “mean field”?
  - Where are the approximations? How do we truncate?
  - How do we include long-range effects (correlations)?
- What about broken symmetries? (translation, rotation, . . .)
- What about the “Dirac sea” in covariant DFT?
- What about UV divergences in DFT pairing?
  - Can we (should we) decouple *pp* and *ph*?
  - Are higher-order contributions important?

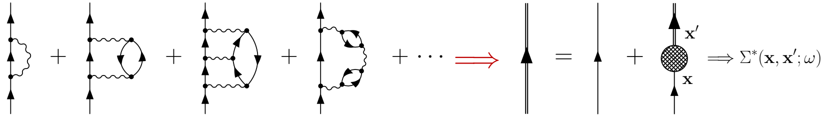
Questions about DFT and Nuclear Structure

- How do we connect to the free $NN\cdots N$ interaction?
  - Chiral EFT $\xrightarrow{RG}$ low-momentum interactions: Power counting?
- What can you calculate in a DFT approach?
  - What about single-particle properties? Excited states?
- How is Kohn-Sham DFT more than “mean field”?
  - Where are the approximations? How do we truncate?
  - How do we include long-range effects (correlations)?
- What about broken symmetries? (translation, rotation, . . .)
- What about the “Dirac sea” in covariant DFT?
- What about UV divergences in DFT pairing?
  - Can we (should we) decouple *pp* and *ph*?
  - Are higher-order contributions important?

How is the Full G Related to G_{ks}? [nucl-th/0410105]



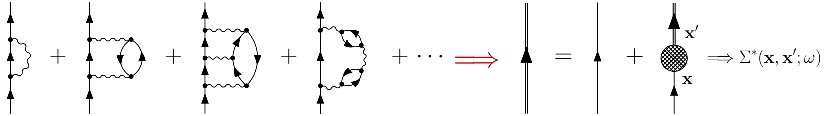
How is the Full G Related to $G_{\rm ks}$? [nucl-th/0410105]



- Add a non-local source $\xi(x', x)$ coupled to $\psi(x)\psi^\dagger(x')$:

$$Z[J,\xi] = e^{iW[J,\xi]} = \int D\psi D\psi^\dagger \; e^{i\int d^4x\;[\mathcal{L} + J(x)\psi^\dagger(x)\psi(x) + \int d^4x'\;\psi(x)\xi(x,x')\psi^\dagger(x')]}$$

How is the Full G Related to $G_{\rm ks}$? [nucl-th/0410105]

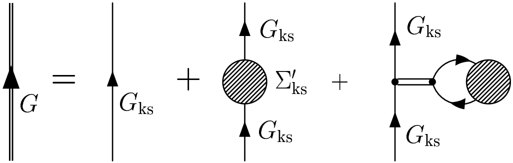


- Add a non-local source $\xi(x',x)$ coupled to $\psi(x)\psi^\dagger(x')$:

$$Z[J,\xi] = e^{iW[J,\xi]} = \int D\psi D\psi^\dagger \, e^{i\int d^4x\, [\mathcal{L} + J(x)\psi^\dagger(x)\psi(x) + \int d^4x'\, \psi(x)\xi(x,x')\psi^\dagger(x')]}$$

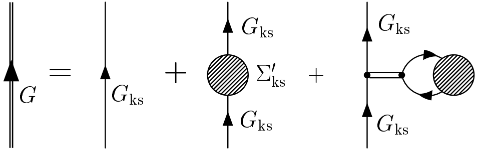
- With $\Gamma[\rho,\xi] = \Gamma_0[\rho,\xi] + \Gamma_{\rm int}[\rho,\xi]$,

$$G(x,x') = \left.\frac{\delta W}{\delta \xi}\right|_J = \left.\frac{\delta \Gamma}{\delta \xi}\right|_\rho = G_{\rm ks}(x,x') + G_{\rm ks}\left[\frac{1}{i}\frac{\delta \Gamma_{\rm int}}{\delta G_{\rm ks}} + \frac{\delta \Gamma_{\rm int}}{\delta \rho}\right] G_{\rm ks}$$



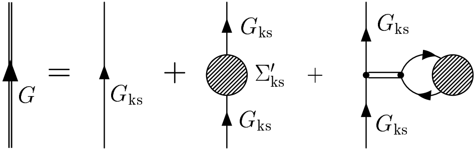
G and $G_{\rm ks}$ Yield the Same Density by *Construction*

- Claim: $\rho_{\rm ks}(\mathbf{x}) = -i\nu G^0_{\rm KS}(x, x^+)$ equals $\rho(\mathbf{x}) = -i\nu G(x, x^+)$
- Start with

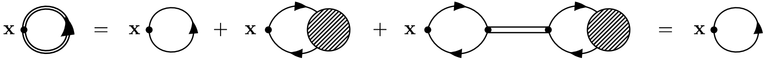


G and $G_{\rm ks}$ Yield the Same Density by *Construction*

- Claim: $\rho_{\rm ks}(\mathbf{x}) = -i\nu G^0_{\rm KS}(x,x^+)$ equals $\rho(\mathbf{x}) = -i\nu G(x,x^+)$
- Start with



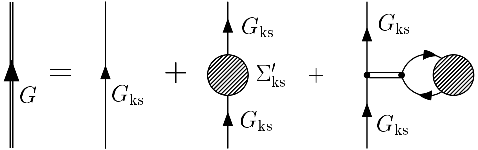
- Simple diagrammatic demonstration:



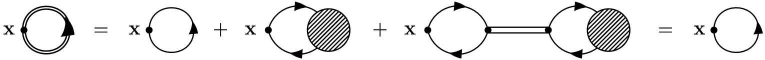
- Densities agree by construction!

G and $G_{\rm ks}$ Yield the Same Density by *Construction*

- Claim: $\rho_{\rm ks}(\mathbf{x}) = -i\nu G^0_{\rm KS}(x, x^+)$ equals $\rho(\mathbf{x}) = -i\nu G(x, x^+)$
- Start with



- Simple diagrammatic demonstration:



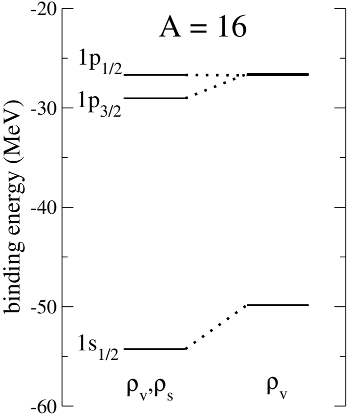
- Densities agree by construction!
- Is the Kohn-Sham basis a useful one for G?

How Close is $G_{\rm KS}$ to G?

- It depends on what sources are used!

$$G(x,x') = \frac{\delta W}{\delta \xi}\bigg|_J = \frac{\delta \Gamma}{\delta \xi}\bigg|_\rho = G_{\rm ks}(x,x') + G_{\rm ks}\left[\frac{1}{i}\frac{\delta \Gamma_{\rm int}}{\delta G_{\rm ks}} + \frac{\delta \Gamma_{\rm int}}{\delta \rho}\right] G_{\rm ks}$$

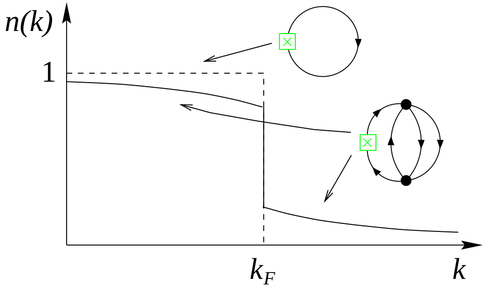
- Nonrel. M^* in $\Gamma[\rho]$ vs. $\Gamma[\rho,\tau]$ vs. $\cdots$ (see Anirban's talk)
- Covariant case at LO:
  $\Gamma[\rho_V]$ vs. $\Gamma[\rho_V, \rho_S]$
- Higher orders?



Questions about DFT and Nuclear Structure

- How do we connect to the free $\mathrm{NN}\cdots\mathrm{N}$ interaction?
  - Chiral EFT $\xrightarrow{RG}$ low-momentum interactions: Power counting?
- What can you calculate in a DFT approach?
  - What about single-particle properties? Excited states?
- How is Kohn-Sham DFT more than "mean field"?
  - Where are the approximations? How do we truncate?
  - How do we include long-range effects (correlations)?
- What about broken symmetries? (translation, rotation, . . .)
- What about the "Dirac sea" in covariant DFT?
- What about UV divergences in DFT pairing?
  - Can we (should we) decouple *pp* and *ph*?
  - Are higher-order contributions important?

Kohn-Sham DFT and “Mean-Field” Models



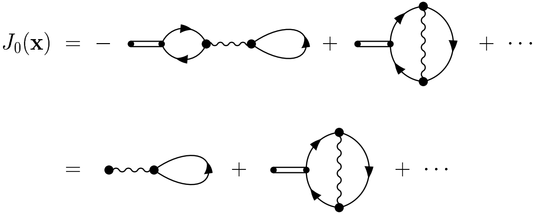
1. Kohn-Sham propagator *always* has “mean-field” structure
   $\Longrightarrow$ doesn’t mean that correlations aren’t included in $\Gamma[\rho]$!
2. $n(\mathbf{k}) = \langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}} \rangle$ is resolution dependent (not observable!)
   $\Longrightarrow$ operator related to experiment is more complicated
3. Is the Kohn-Sham basis a useful one for other observables?

Approximating and Fitting the Functional

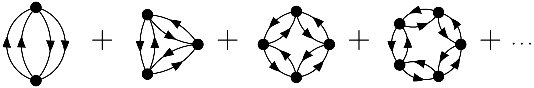
- Need a truncated expansion to carry out inversion method
  - Chiral EFT expansion is well-defined
  - Power counting for low-momentum interactions?
- Gradient expansions?
  - Density matrix expansion
  - Semiclassical expansions used in Coulomb DFT
  - Derivative expansion techniques developed for (one-loop) effective actions?
- How should we “fine tune” a DFT functional?
  - What does EFT say about what knobs to adjust?
  - EFT tells about theoretical errors $\Longrightarrow$ use in fits (e.g., Bayesian)

Long-range Effects

- Long-range forces (e.g., pion exchange) $\Longrightarrow$ limits of DME++



- Non-localities from near-on-shell particle-hole excitations



Questions about DFT and Nuclear Structure

- How do we connect to the free NN$\cdots$N interaction?
  - Chiral EFT $\xrightarrow{RG}$ low-momentum interactions: Power counting?
- What can you calculate in a DFT approach?
  - What about single-particle properties? Excited states?
- How is Kohn-Sham DFT more than “mean field”?
  - Where are the approximations? How do we truncate?
  - How do we include long-range effects (correlations)?
- What about broken symmetries? (translation, rotation, . . .)
- What about the “Dirac sea” in covariant DFT?
- What about UV divergences in DFT pairing?
  - Can we (should we) decouple *pp* and *ph*?
  - Are higher-order contributions important?

Symmetry Breaking and Zero Modes

- What about breaking of translational, rotational invariance, particle number?
- No guidance from Coulomb DFT (?)
- Effective action $\Longrightarrow$ zero modes
  - cf. soliton zero modes and projection methods
  - Fadeev-Popov games?
- Energy functional for the intrinsic density? $\Longrightarrow$ J. Engel: one-dimensional laboratory

Questions about DFT and Nuclear Structure

- How do we connect to the free NN$\cdots$N interaction?
  - Chiral EFT $\xrightarrow{RG}$ low-momentum interactions: Power counting?
- What can you calculate in a DFT approach?
  - What about single-particle properties? Excited states?
- How is Kohn-Sham DFT more than "mean field"?
  - Where are the approximations? How do we truncate?
  - How do we include long-range effects (correlations)?
- What about broken symmetries? (translation, rotation, . . .)
- What about the "Dirac sea" in covariant DFT?
- What about UV divergences in DFT pairing?
  - Can we (should we) decouple *pp* and *ph*?
  - Are higher-order contributions important?

UV Divergences in Nonrelativistic and Relativistic Effective Actions

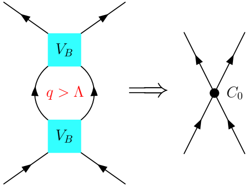
- *All* low-energy effective theories have incorrect UV behavior
- Sensitivity to short-distance physics signalled by divergences
  but finiteness (e.g., with cutoff) doesn't mean not sensitive!
  $\Longrightarrow$ must absorb (and correct) sensitivity by renormalization
- Instances of UV divergences

nonrelativistic	covariant
scattering	scattering
pairing	pairing
	anti-nucleons

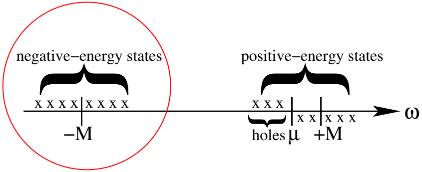
Power Counting Lost / Power Counting Regained

- Gasser, Sainio, Svarc $\Longrightarrow$ ChPT for πN with relativistic N's
  - loop and momentum expansions don't agree
    $\Longrightarrow$ systematic power counting lost
  - heavy-baryon EFT restores power counting by $1/M$ expansion
- Hua-Bin Tang (1996) [and with Paul Ellis]:

  ". . . EFT's permit useful low-energy expansions only if we absorb all of the hard-momentum effects into the parameters of the Lagrangian."



and



- Becher/Leutwyler IR $\Longrightarrow$ Schindler-Gegelia-Scherer version

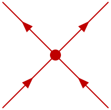
Moving Dirac Sea Physics into Coefficients

- Absorb the "hard" part of a diagram into parameters,
  $\Longrightarrow$ the remaining "soft" part satisfies chiral power counting
  - original πN prescription by H.B. Tang (expand, integrate term-by-term, and resum propagators)
  - systematized for πN by Becher and Leutwyler: "infrared regularization" or IR
  - not unique; e.g., Fuchs et al. additional finite subtractions in DR
- Extension of IR to multiple heavy particles [Lehmann/Prézeau]
  - convenient reformulation by Schindler, Gegelia, Scherer
  - tadpoles, $N\overline{N}$ loops in free space vanish!
  - particle-particle loop reduces to nonrelativistic DR/MS result

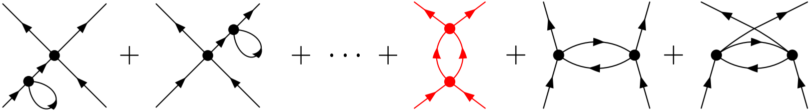
Consequences for Free-Space Natural Fermions

- Tadpoles, $N\overline{N}$ loops in free space vanish!
- Leading order (LO) has scalar, vector, etc. vertices

$$\mathcal{L}_{\rm eft} = \cdots - \frac{C_s}{2}(\overline{\psi}\psi)(\overline{\psi}\psi) - \frac{C_v}{2}(\overline{\psi}\gamma^\mu\psi)(\overline{\psi}\gamma_\mu\psi) + \cdots \Longrightarrow$$



- At NLO, only particle-particle loop survives IR



- Only forward-going nucleons contribute
  $\Longrightarrow$ same scattering amplitude as nonrel. DR/MS for small k

Comments on Vacuum Physics

- Unlike QED DFT, “no sea” for nuclear structure is a misnomer
  - include “vacuum physics” in coefficients via renormalization
- Renormalization versus Renormalizability
  - Renormalization is required to account for short-distance behavior but can be implicit
  - Renormalizability at the hadronic level corresponds to making a model for the short-distance behavior
    - not a good model phenomenologically
    - Please don’t send me any more RHA papers to referee!
  - Fixing short-distance behavior is not the same thing as throwing away negative-energy states
- For a long time, we looked for *unique* “relativistic effects”; these were largely misguided efforts

Questions about DFT and Nuclear Structure

- How do we connect to the free NN$\cdots$N interaction?
  - Chiral EFT $\xrightarrow{RG}$ low-momentum interactions: Power counting?
- What can you calculate in a DFT approach?
  - What about single-particle properties? Excited states?
- How is Kohn-Sham DFT more than “mean field”?
  - Where are the approximations? How do we truncate?
  - How do we include long-range effects (correlations)?
- What about broken symmetries? (translation, rotation, . . .)
- What about the “Dirac sea” in covariant DFT?
- What about UV divergences in DFT pairing?
  - Can we (should we) decouple *pp* and *ph*?
  - Are higher-order contributions important?

UV Divergences in Nonrelativistic and Relativistic Effective Actions

- *All* low-energy effective theories have incorrect UV behavior
- Sensitivity to short-distance physics signalled by divergences
  but finiteness (e.g., with cutoff) doesn't mean not sensitive!
  $\Longrightarrow$ must absorb (and correct) sensitivity by renormalization
- Instances of UV divergences

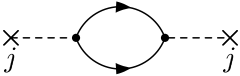
nonrelativistic	covariant
scattering	scattering
pairing	pairing
	anti-nucleons

Divergences: Dilute Fermi System

- Generating functional with constant sources μ and j:

$$e^{-W} = \int D(\psi^\dagger\psi)\, e^{-\int d^4x\, [\psi_\alpha^\dagger(\frac{\partial}{\partial\tau} - \frac{\nabla^2}{2M} - \mu)\psi_\alpha + \frac{C_0}{2}\psi_\uparrow^\dagger\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow + j(\psi_\uparrow\psi_\downarrow + \psi_\downarrow^\dagger\psi_\uparrow^\dagger)]}$$

  - cf. adding integration over auxiliary field $\int D(\Delta^*,\Delta)\, e^{-\frac{1}{|C_0|}\int|\Delta|^2}$
    $\Longrightarrow$ shift variables to eliminate $\psi_\uparrow^\dagger\psi_\downarrow^\dagger\psi_\downarrow\psi_\uparrow$ for $\Delta^*\psi_\uparrow\psi_\downarrow$
- New divergences because of $j \Longrightarrow$ e.g., expand to $\mathcal{O}(j^2)$

$W[\mu,j] = \cdots +$  $+ \cdots$

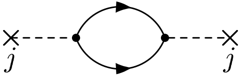
  - Same linear divergence as in 2-to-2 scattering

Divergences: Dilute Fermi System

- Generating functional with constant sources μ and j:

$$e^{-W} = \int D(\psi^\dagger\psi)\, e^{-\int d^4x\, [\psi^\dagger_\alpha(\frac{\partial}{\partial\tau} - \frac{\nabla^2}{2M} - \mu)\psi_\alpha + \frac{C_0}{2}\psi^\dagger_\uparrow\psi^\dagger_\downarrow\psi_\downarrow\psi_\uparrow + j(\psi_\uparrow\psi_\downarrow + \psi^\dagger_\downarrow\psi^\dagger_\uparrow) + \frac{1}{2}\zeta j^2]}$$

  - cf. adding integration over auxiliary field $\int D(\Delta^*, \Delta)\, e^{-\frac{1}{|C_0|}\int|\Delta|^2}$
    $\Longrightarrow$ shift variables to eliminate $\psi^\dagger_\uparrow\psi^\dagger_\downarrow\psi_\downarrow\psi_\uparrow$ for $\Delta^*\psi_\uparrow\psi_\downarrow$
- New divergences because of j $\Longrightarrow$ e.g., expand to $\mathcal{O}(j^2)$

$W[\mu, j] = \cdots +$  $+ \cdots$

  - Same linear divergence as in 2-to-2 scattering
- Strategy: Add counterterm $\frac{1}{2}\zeta j^2$ to $\mathcal{L}$
  - additive to W (cf. $|\Delta|^2$) $\Longrightarrow$ no effect on scattering
  - Energy interpretation? Finite part?

Renormalized Uniform System Observables

- To find the energy density, evaluate Γ at the stationary point:

$$\frac{E}{V} = (\Gamma_0 + \Gamma_1)|_{j_0=-\frac{1}{2}|C_0|\phi} = \int \frac{d^3k}{(2\pi)^3}\left[\xi_k - E_k + \frac{1}{2}\frac{j_0^2}{E_k}\right] + \left[\mu_0 - \frac{1}{4}|C_0|\rho\right]\rho$$

with

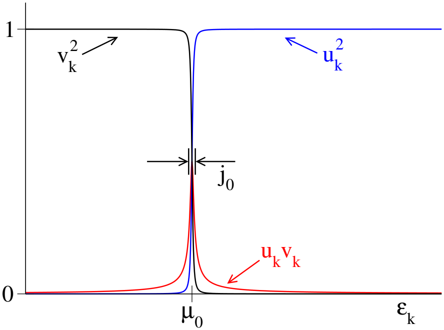
$$\rho = \int \frac{d^3k}{(2\pi)^3}\left(1 - \frac{\xi_k}{E_k}\right) \quad \text{and} \quad \phi = -\int \frac{d^3k}{(2\pi)^3}\frac{j_0}{E_k} + \zeta^{(0)} j_0$$

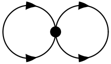
- Explicitly finite and dependence on $\zeta^{(0)}$ cancels out
- Finite system $\Longrightarrow$ optimize renormalization (see Bulgac et al.)

Higher Order: Induced Interaction

- As $j_0 \to 0$, $u_k v_k$ peaks at μ_0
- Leading order $T = 0$:

$$\Delta_{LO}/\mu_0 = \frac{8}{e^2}\, e^{-1/N(0)|C_0|} = \frac{8}{e^2}\, e^{-\pi/2k_{\rm F}|a_s|}$$



$\Gamma_1 =$  $+\, CTC + \cdots \Longrightarrow j_1 = \dfrac{\delta\Gamma_1}{\delta\phi} = \dfrac{1}{2}|C_0|\phi$

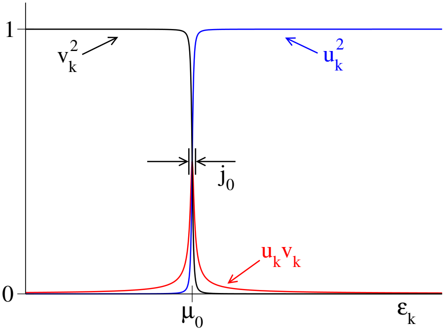
- Same renormalization works (Furnstahl/Hammer)
  $\Longrightarrow$ energy interpretation? finite system?

Higher Order: Induced Interaction

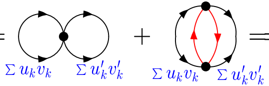
- As $j_0 \to 0$, $u_k v_k$ peaks at μ_0
- Leading order $T = 0$:

$$\Delta_{LO}/\mu_0 = \frac{8}{e^2} e^{-1/N(0)|C_0|} = \frac{8}{e^2} e^{-\pi/2k_F|a_s|}$$

- NLO modifies exponent
  $\Longrightarrow$ changes prefactor
- $\Delta_{NLO} \approx \Delta_{LO}/(4e)^{1/3}$



$$\Gamma_1 + \Gamma_2 = $$



$$\Longrightarrow j_1 + j_2 = \frac{1}{2}|C_0|\left[1 - |C_0|\langle\Pi_0\rangle_{|\mathbf{k}|=|\mathbf{k}'|=k_F}\right]\phi$$

- Same renormalization works (Furnstahl/Hammer)
  $\Longrightarrow$ energy interpretation? finite system?

Outline

Overview: Microscopic DFT

Effective Actions and DFT

Issues and Ideas and Open Problems

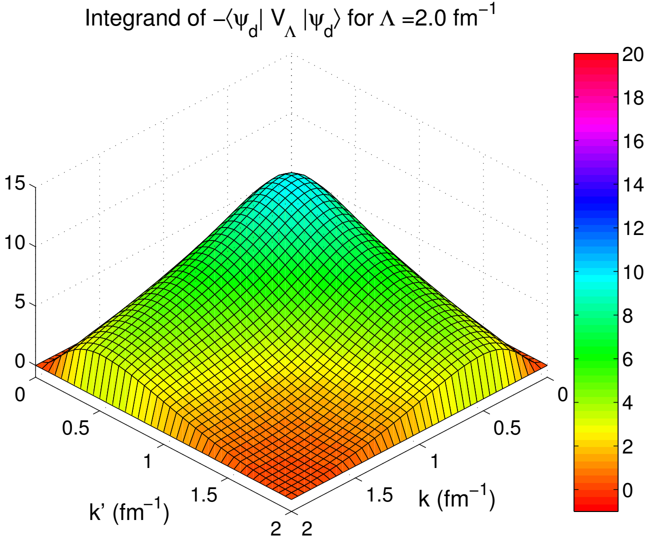
Summary

Summary

- Plan: Chiral EFT $\longrightarrow$ low momentum $V_{NN}, V_{NNN}, \ldots$
  $\longrightarrow$ DFT for nuclei
- Effective action formalism provides framework
- Many issues to resolve (my list for today)
  - gradient expansions (DME++, ...), long-range effects
  - isospin dependence, many-body contributions, low-density limit
  - symmetry breaking and restoration
  - higher-order pairing
  - how to fine-tune?
  - systematic covariant DFT
  - $\vdots$

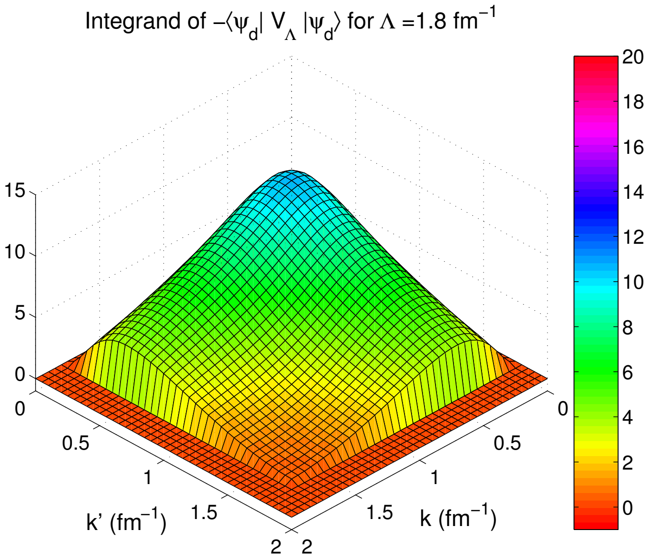
The Deuteron at Different Resolutions

back



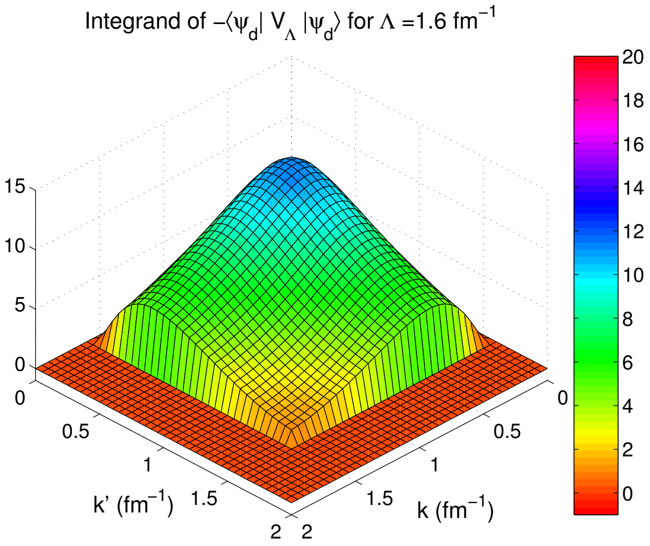
The Deuteron at Different Resolutions

back



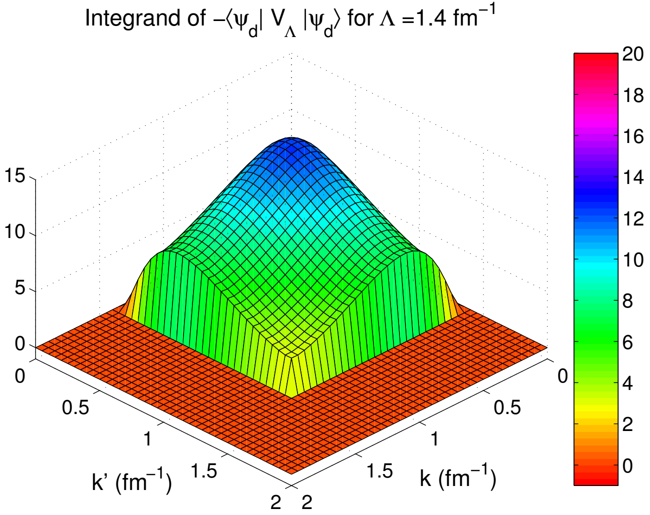
The Deuteron at Different Resolutions

back



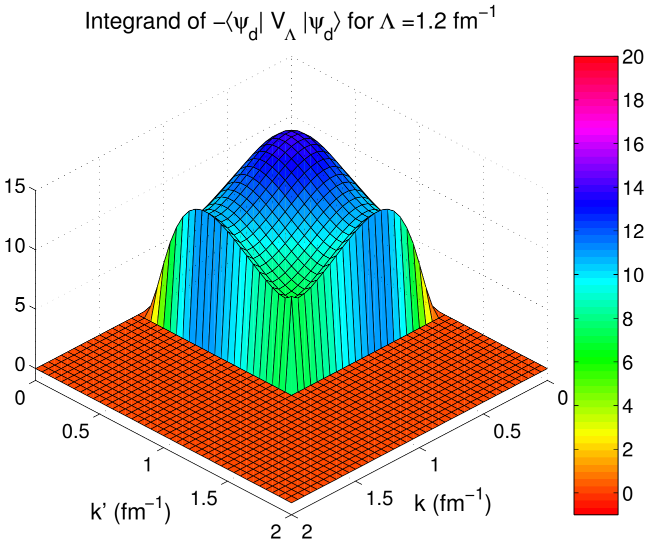
The Deuteron at Different Resolutions

back



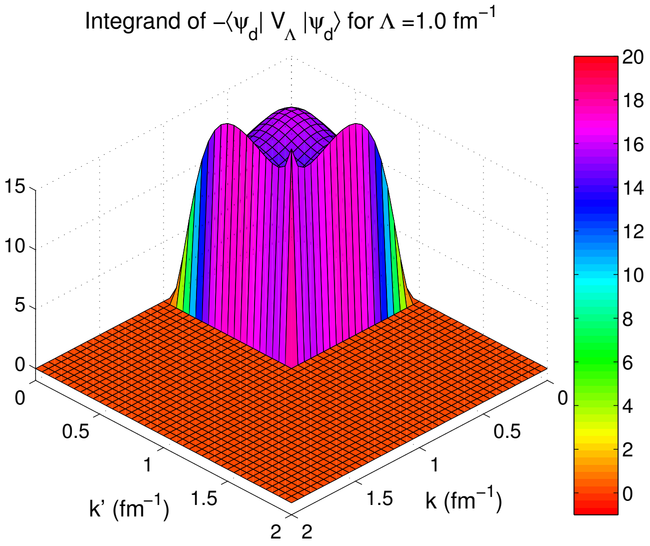
The Deuteron at Different Resolutions

back



The Deuteron at Different Resolutions

back



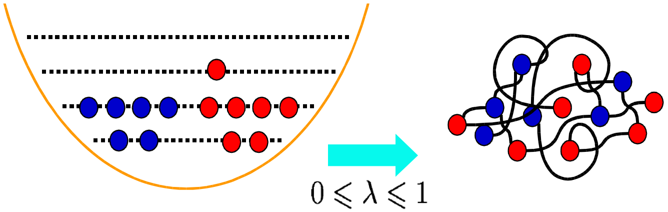
Effective Action as Energy Functional: Minkowski

back

- See, e.g., Weinberg, Vol. II

Polonyi-Schwenk RG Approach to DFT

back



Non-interacting fermions in background mean-field potential V at $\lambda = 0$

Gradually switch off background potential and turn on the microscopic interaction U as $\lambda \to 1$

$$S_{\lambda,1}[\psi^\dagger,\psi] = \int dx\, \psi^\dagger_\alpha(x) \left(\frac{\partial}{\partial t} - \frac{\nabla^2_{\mathbf{x}}}{2M} + (1-\lambda) V_{\lambda;\alpha}(\mathbf{x}) \right) \psi_\alpha(x)$$

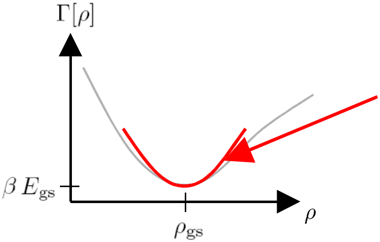
$$S_{\lambda,2}[\psi^\dagger,\psi] = \frac{\lambda}{2} \int\!\!\int (\psi^\dagger \psi) \cdot U \cdot (\psi^\dagger \psi)$$

Density Functional = Effective Action for Density

back

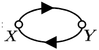
- Effective action $\Gamma[\rho] = -W[J] + J \cdot \rho$ is minimal at the physical (zero source) ground state density:

$$\left.\frac{\delta\Gamma[\rho]}{\delta\rho}\right|_{\rho_{\rm gs}} = 0 \quad\Longrightarrow\quad E_{\rm gs} = E[\rho_{\rm gs}] = \lim_{\beta\to\infty}\frac{1}{\beta}\Gamma[\rho_{\rm gs}]$$



Curvature will include correlations

$$\left(\left.\frac{\delta^2\Gamma[\rho]}{\delta\rho\,\delta\rho}\right|_{\rho_{\rm gs}}\right)^{-1} = \left.\frac{\delta^2 W[J]}{\delta J\,\delta J}\right|_{J=0}$$

$=$  $+$ interactions

Evolution of Effective Action with Parameter λ

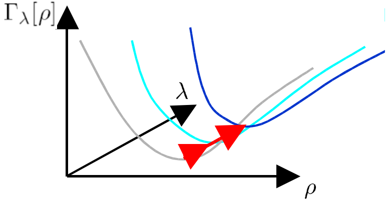
back

Δ background Hartree exchange-correlations

$$\partial_\lambda \Gamma_\lambda[\rho] = \partial_\lambda[(1-\lambda)V_\lambda]\cdot\rho + \frac{1}{2}\rho\cdot U\cdot\rho + \frac{1}{2}\mathrm{Tr}\left[U\cdot\left(\frac{\delta^2\Gamma_\lambda[\rho]}{\delta\rho\,\delta\rho}\right)^{-1}\right]$$

Expand density functional about evolving ground-state density

$$\Gamma_\lambda[\rho] = \Gamma[\rho_{\mathrm{gs},\lambda}]^{(0)} + \sum_{n\geq 2}\int\cdots\int \frac{1}{n!}\Gamma[\rho_{\mathrm{gs},\lambda}]^{(n)}\cdot(\rho-\rho_{\mathrm{gs},\lambda})_1\cdots(\rho-\rho_{\mathrm{gs},\lambda})_n$$

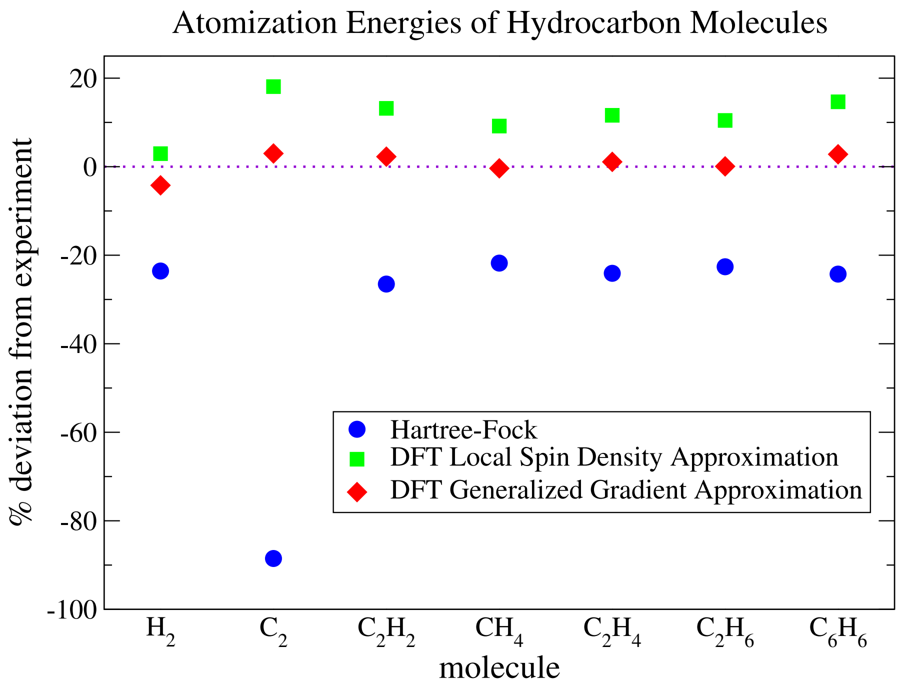


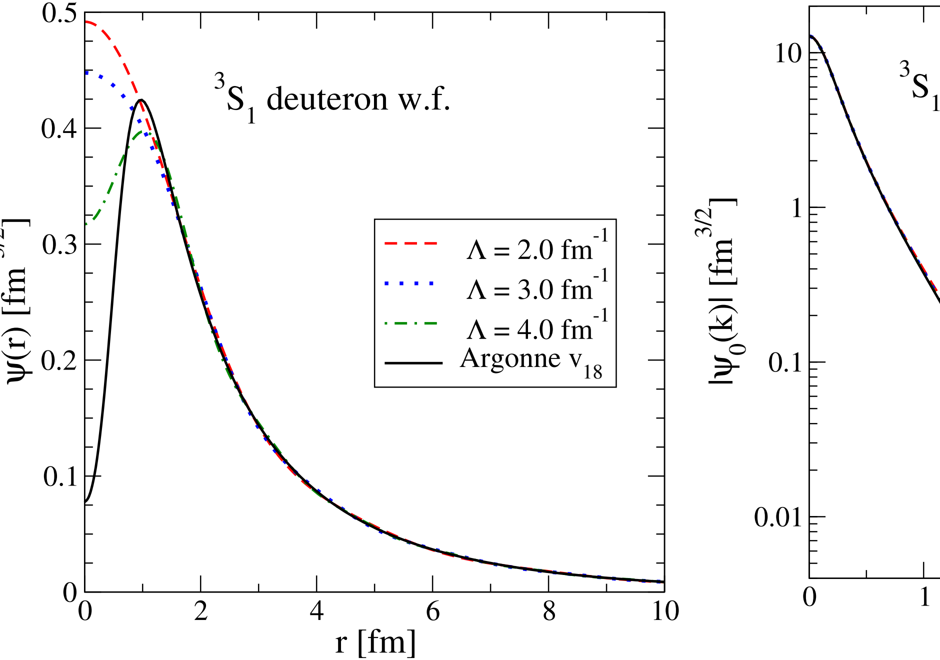
Evolution equations for expansion coefficients build up correlations through dressed ph propagator

Auxiliary Fields [Faussurier]

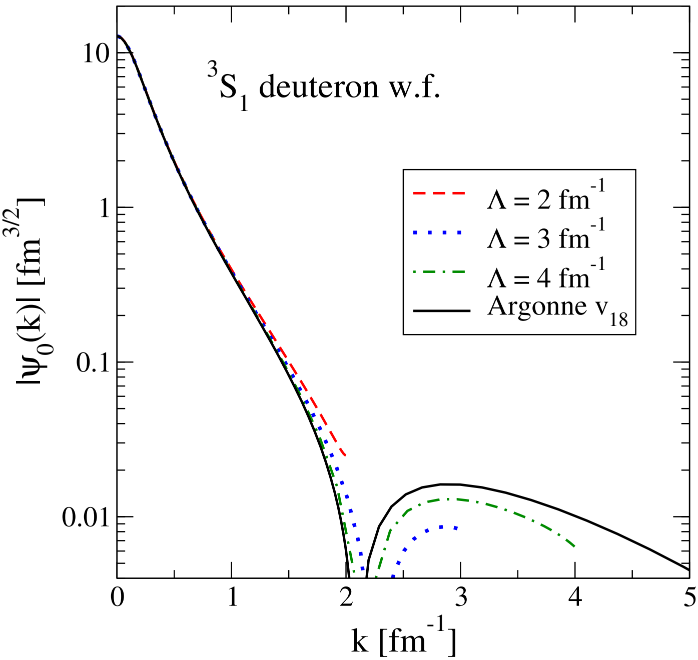
back

- Introduce scalar field φ coupled to $\psi^\dagger\psi$
- Construct $\widetilde{S}[\psi^\dagger,\psi,\varphi]$ such that $\psi,\psi^\dagger$ is only in $\psi^\dagger[G^{-1}(\varphi)]\psi$ and
$$\int \mathcal{D}\varphi\, e^{i\widetilde{S}[\psi^\dagger,\psi,\varphi]} \Longrightarrow e^{iS[\psi^\dagger,\psi]}$$
- Integrate out $\psi^\dagger\psi \Longrightarrow$ determinant $\Longrightarrow \mathrm{Tr}\ln[G^{-1}(\varphi)] + \cdots$
- Keep only leading saddle point $\phi_0(\mathbf{x}) \Longrightarrow$ Hartree
  - fluctuation corrections generate loop expansion
  - freedom to choose mean field [Kerman et al. (1983)]
    cf., $H = (T+U) + (V-U)$ for arbitrary U
- Kohn-Sham: choose special saddle-point evaluation
  - reference local potential ϕ_{xc} such that $-\mathrm{Tr}\, G_{\mathrm{xc}}(x,x^+) = n(\mathbf{x})$
  - expand $\mathrm{Tr}\ln[G_{\mathrm{xc}}^{-1} + \delta\phi]$ in $\delta\phi = \phi - \phi_{\mathrm{xc}}$
    $\Longrightarrow \Gamma_{\mathrm{xc}}[n]$ with $\phi_{\mathrm{xc}}(\mathbf{x}) = \delta\Gamma_{\mathrm{xc}}[n]/\delta n(\mathbf{x})$
  - introduce orbitals $\{\psi_\alpha, \epsilon_\alpha\}$ to diagonalize $\mathrm{Tr}\ln[G_{\mathrm{xc}}^{-1}]$


Atomization Energies of Hydrocarbon Molecules
% deviation from experiment
20
0
-20
-40
-60
-80
-100
H2
C2
C2H2
CH4
C2H4
C2H6
C6H6
molecule
Hartree-Fock
DFT Local Spin Density Approximation
DFT Generalized Gradient Approximation

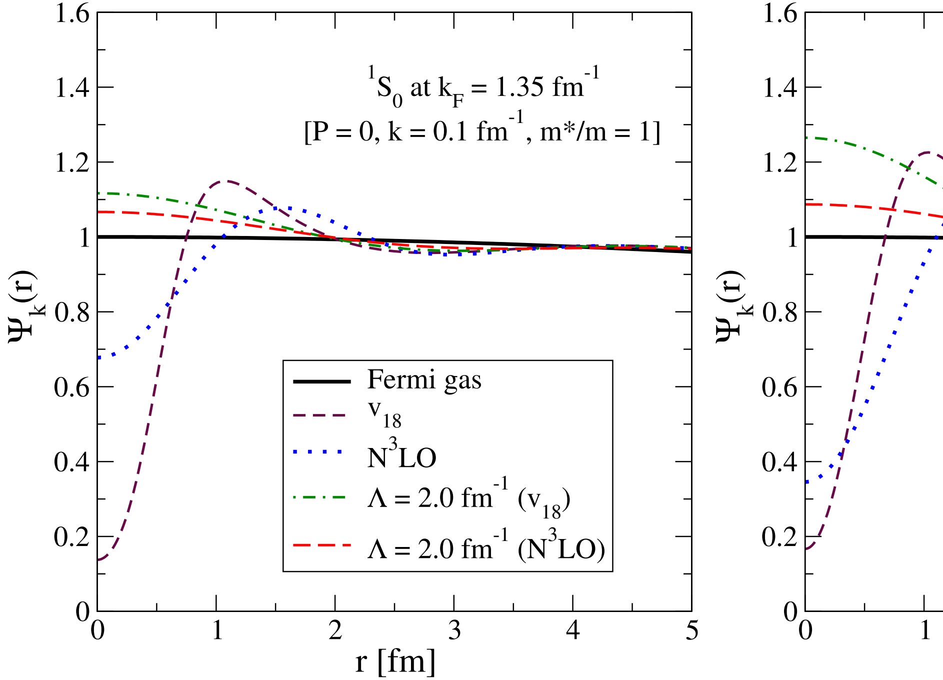


$^3S_1$ deuteron w.f.
Λ = 2.0 fm^{-1}
Λ = 3.0 fm^{-1}
Λ = 4.0 fm^{-1}
Argonne v_{18}
$\psi(r)$ [fm$^{-3/2}$]
r [fm]
$|\psi_0(k)|$ [fm$^{3/2}$]
$^3S_1$

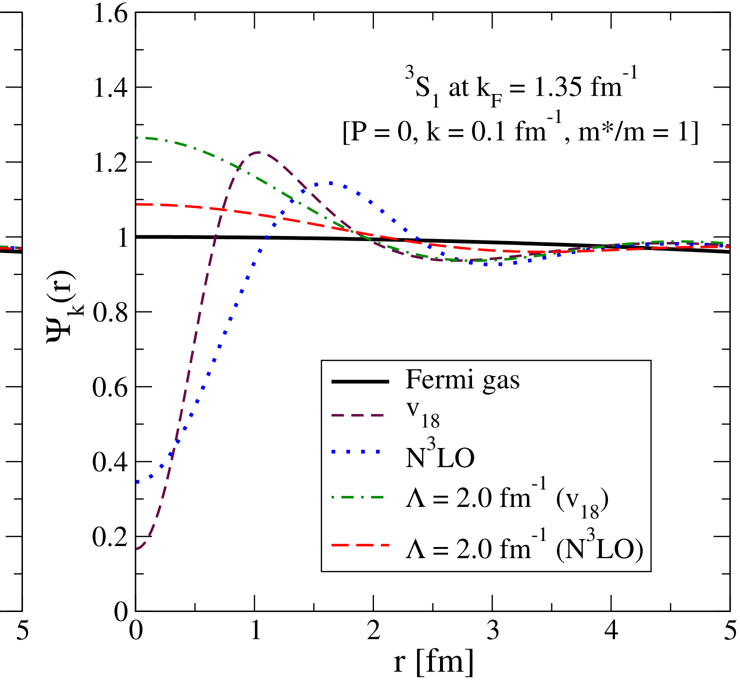


$^3S_1$ deuteron w.f.
Λ = 2 fm^{-1}
Λ = 3 fm^{-1}
Λ = 4 fm^{-1}
Argonne v_{18}
$|\psi_0(k)|$ [fm$^{3/2}$]
k [fm^{-1}]
10
1
0.1
0.01
0
1
2
3
4
5

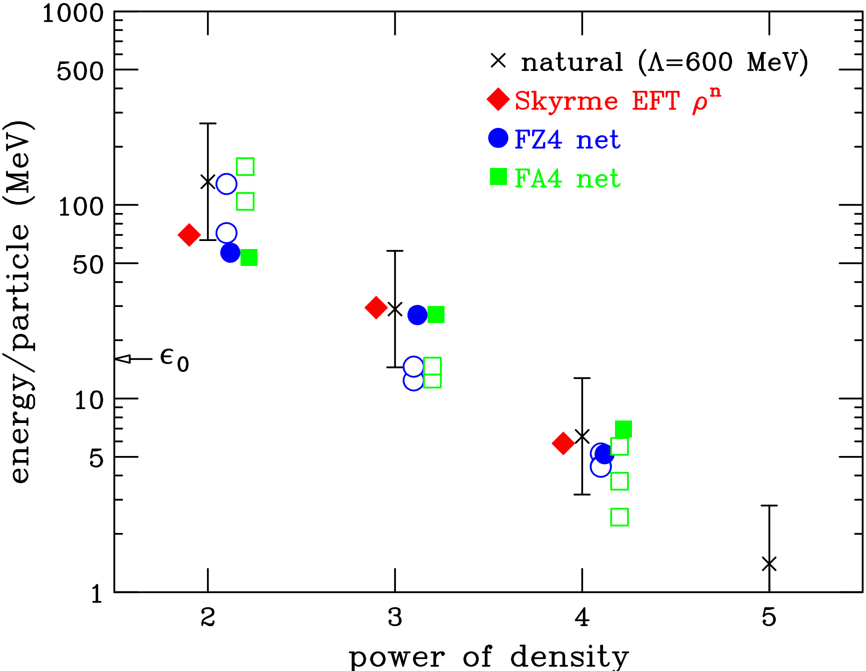
0



$^1S_0$ at k_F = 1.35 fm^{-1}
[P = 0, k = 0.1 fm^{-1}, m*/m = 1]
$\Psi_k(r)$
r [fm]
Fermi gas
v_{18}
N^3LO
Λ = 2.0 fm^{-1} (v_{18})
Λ = 2.0 fm^{-1} (N^3LO)



$^3S_1$ at k_F = 1.35 fm^{-1}
[P = 0, k = 0.1 fm^{-1}, m*/m = 1]
$\Psi_k(r)$
r [fm]
Fermi gas
v_{18}
N^3LO
Λ = 2.0 fm^{-1} (v_{18})
Λ = 2.0 fm^{-1} (N^3LO)



natural (Λ=600 MeV)
Skyrme EFT ρ^n
FZ4 net
FA4 net
ϵ_0
energy/particle (MeV)
power of density
1000
500
100
50
10
5
1
2
3
4
5