Effective Field Theory for Density Functional Theory III

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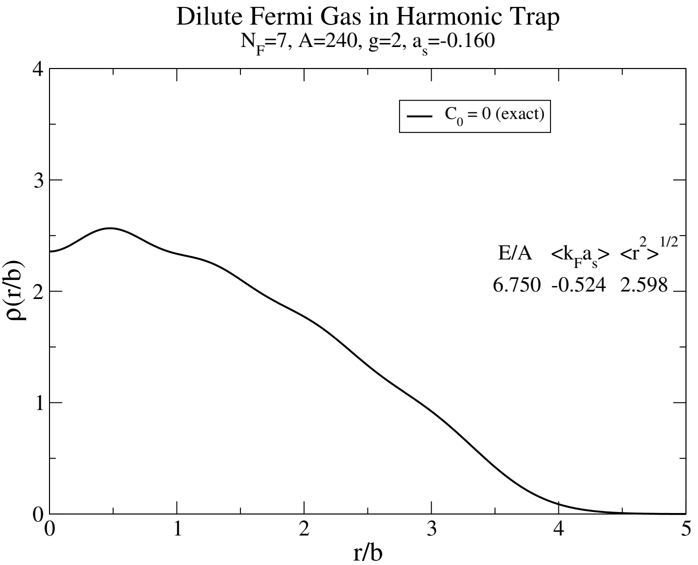
I. Overview of EFT, RG, DFT for fermion many-body systems

II. EFT/DFT for dilute Fermi systems

III. Refinements: Toward EFT/DFT for nuclei

IV. Loose ends and challenges, Cold atoms, RG/DFT

Recall Our Example [nucl-th/0212071]



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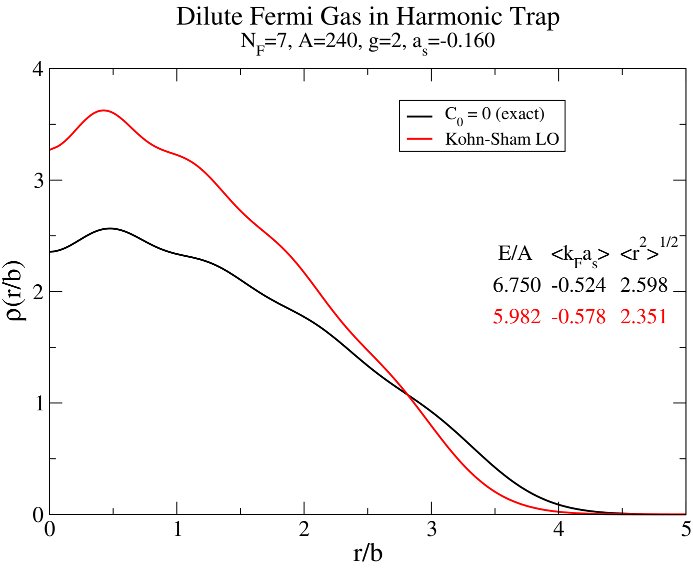

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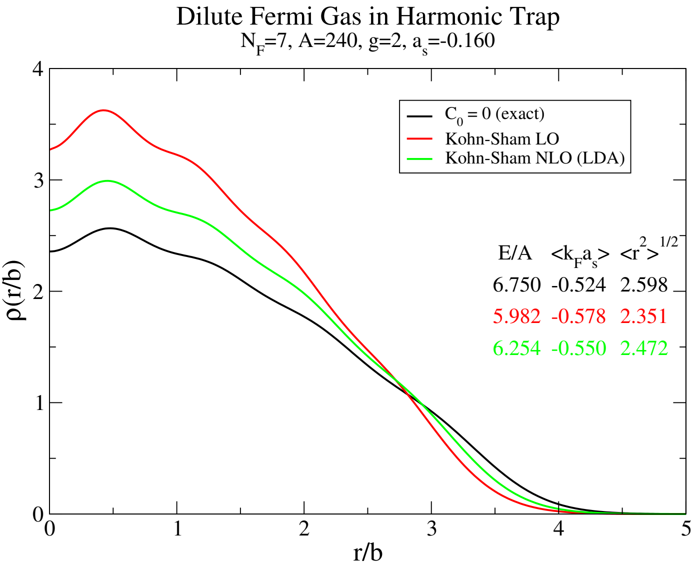

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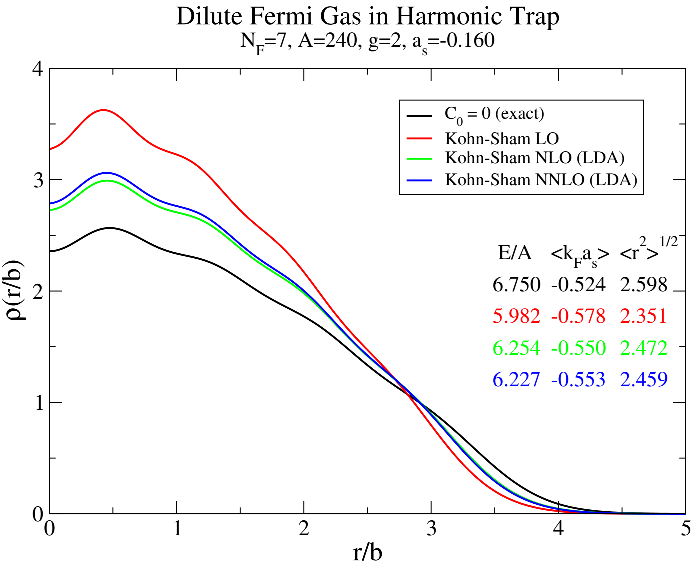
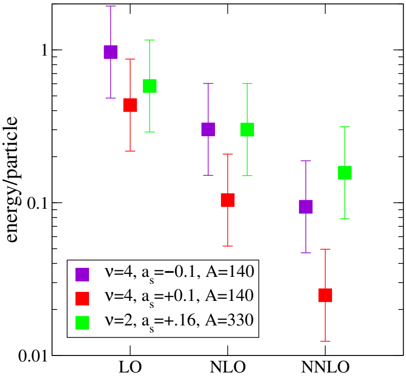


Power Counting Terms in Energy Functionals

- Scale contributions according to average density or $\langle k_{\rm F} \rangle$



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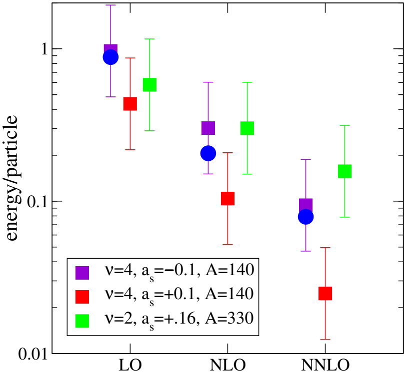

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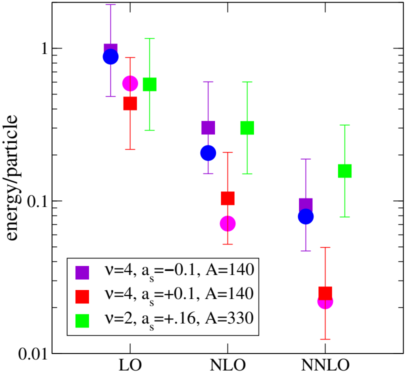

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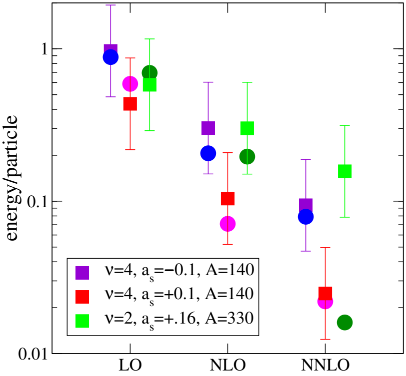

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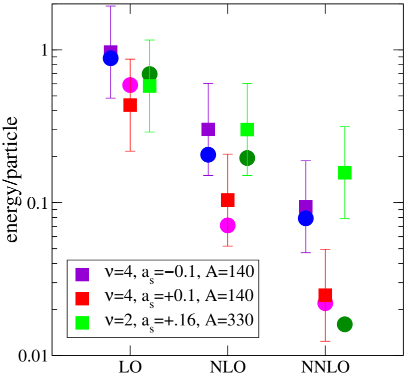

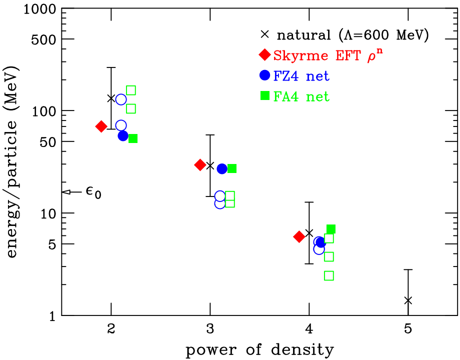

- Reasonable estimates $\Longrightarrow$ truncation errors understood

Questions about DFT and Nuclear Structure

- 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 can you calculate in a DFT approach?
  - What about single-particle properties? Excited states?
- How does pairing work in DFT?
  - Can we (should we) decouple *pp* and *ph*?
  - Are higher-order contributions important?
- What about broken symmetries? (translation, rotation, . . .)
- How do we connect to the free NN$\cdots$N interaction?
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Outline

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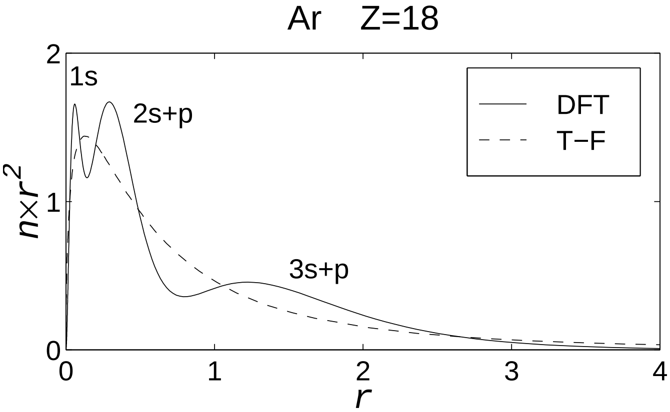
Extensions to DFT/EFT

Pairing in Kohn-Sham DFT

Summary III

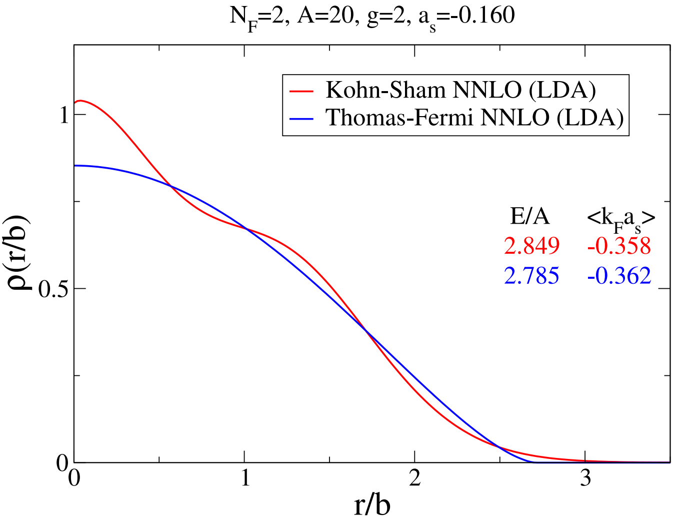
LDA I: Kohn-Sham vs. Thomas-Fermi

- Entire energy functional is treated in LDA in Thomas-Fermi
- In Kohn-Sham DFT, treat kinetic energy non-locally
  $\Longrightarrow$ shell structure in atoms:



LDA I: Kohn-Sham vs. Thomas-Fermi

- and in cold atoms in a trap:



Beyond Kohn-Sham LDA: Kinetic Energy Density

- Skyrme E is functional of ρ *and* $\tau \equiv \langle \nabla\psi^\dagger \cdot \nabla\psi \rangle$

$$E[\rho, \tau, \mathbf{J}] = \int d^3x \left\{ \frac{1}{2M}\tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau \right.$$
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- To do this in DFT/EFT, add to Lagrangian $+\eta(\mathbf{x})\,\nabla\psi^\dagger\nabla\psi$

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

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- Two Kohn-Sham potentials:

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

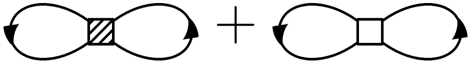
- Kohn-Sham equation $\Longrightarrow$ defines $\frac{1}{2M^*(\mathbf{x})} \equiv \frac{1}{2M} - \eta_0(\mathbf{x})$:

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

First Step: HF Diagrams With ∇'s [nucl-th/0408014]

- Consider bowtie diagrams from vertices with derivatives:

$$\mathcal{L}_{\text{eft}} = \ldots + \frac{C_2}{16}\left[(\psi\psi)^\dagger(\psi\overleftrightarrow{\nabla}^2\psi) + \text{h.c.}\right] + \frac{C_2'}{8}(\psi\overleftrightarrow{\nabla}\psi)^\dagger\cdot(\psi\overleftrightarrow{\nabla}\psi) + \ldots$$



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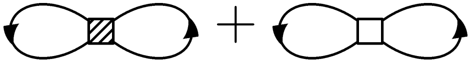

- Energy density in Kohn-Sham LDA ($\nu = 2$):

$$\mathcal{E}_{\rm int}[\rho] = \ldots + \frac{C_2}{8}\left[\frac{3}{5}\left(\frac{6\pi^2}{\nu}\right)^{2/3}\rho^{8/3}\right] + \frac{3C_2'}{8}\left[\frac{3}{5}\left(\frac{6\pi^2}{\nu}\right)^{2/3}\rho^{8/3}\right] + \ldots$$

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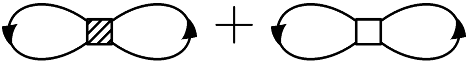

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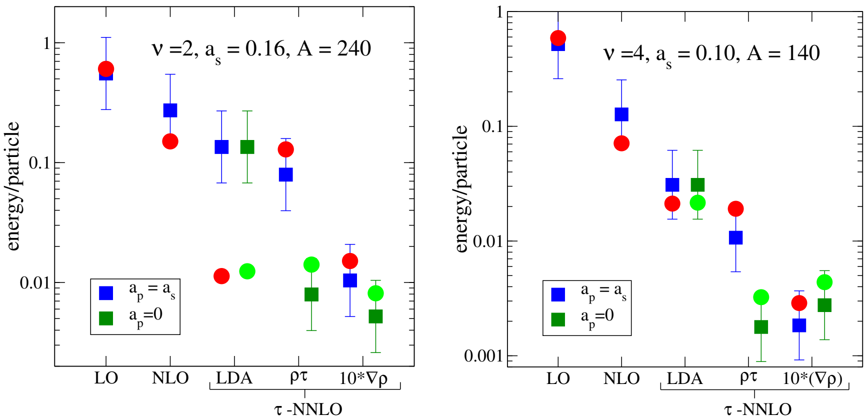
- Energy density in Kohn-Sham with τ ($\nu = 2$):

$$\mathcal{E}_{\rm int}[\rho,\tau] = \ldots + \frac{C_2}{8}\left[\rho\tau + \frac{3}{4}(\boldsymbol{\nabla}\rho)^2\right] + \frac{3C_2'}{8}\left[\rho\tau - \frac{1}{4}(\boldsymbol{\nabla}\rho)^2\right] + \ldots$$

Power Counting Estimates Work for Gradients!



Comparing Skyrme and Dilute Functionals

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

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

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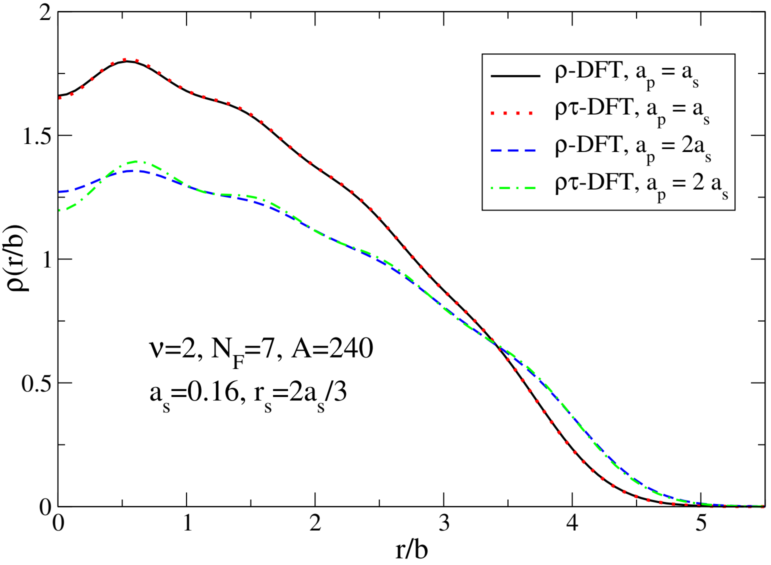
- Same functional as dilute Fermi gas with $t_i \leftrightarrow C_i$
  - equivalent $a_0 \approx -2$–3 fm but $|k_{\rm F}a_p|, |k_{\rm F}r_0| < 1$ (with $a_p < 0$)
  - missing non-analytic terms, NNN, . . .

Kohn-Sham LDA ρ vs. $\rho\tau$ [Anirban Bhattacharyya]



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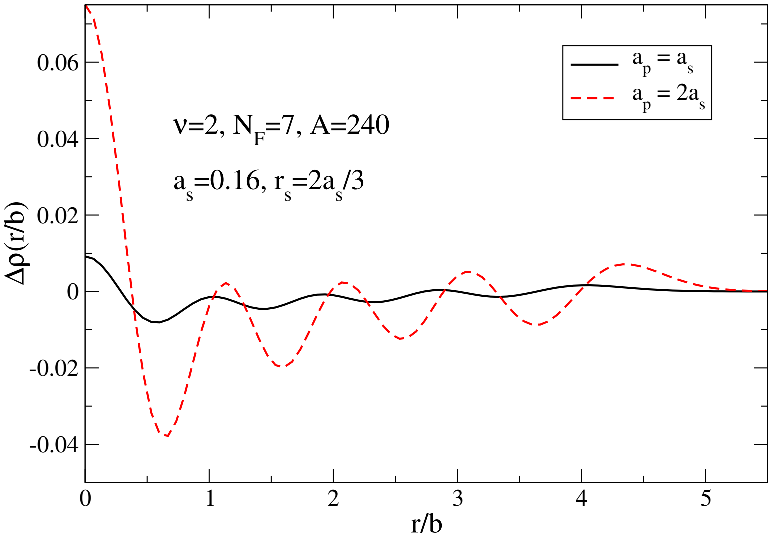
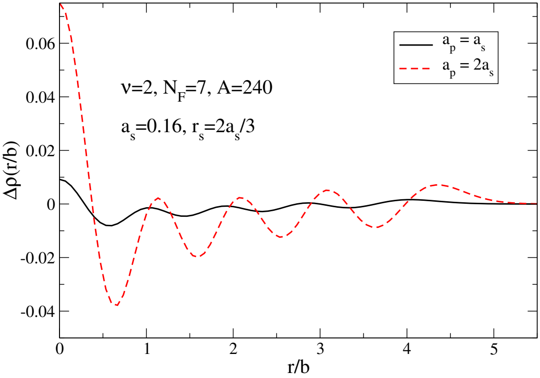


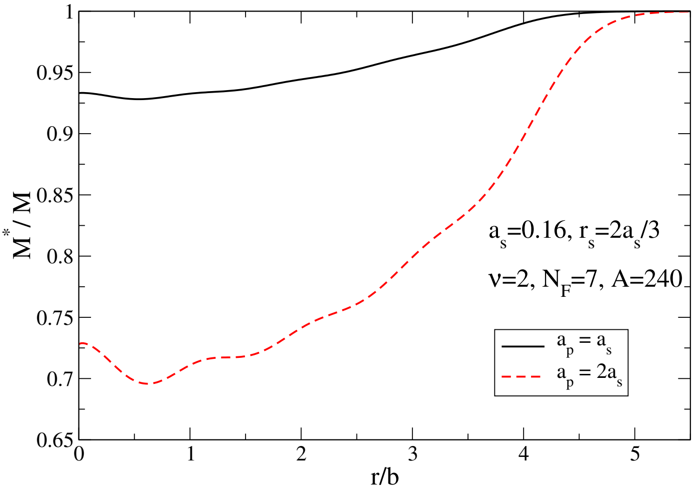
Kohn-Sham LDA ρ vs. $\rho\tau$: Differences

$a_p = a_s$	E/A	$\sqrt{\langle r^2 \rangle}$
ρ	7.66	2.87
$\rho\tau$	7.65	2.87

$a_p = 2a_s$	E/A	$\sqrt{\langle r^2 \rangle}$
ρ	8.33	3.10
$\rho\tau$	8.30	3.09

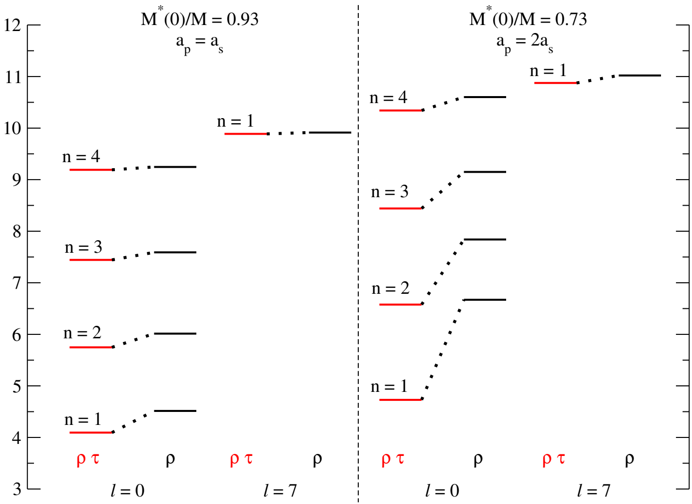


Effective Mass and the Single-Particle Spectrum



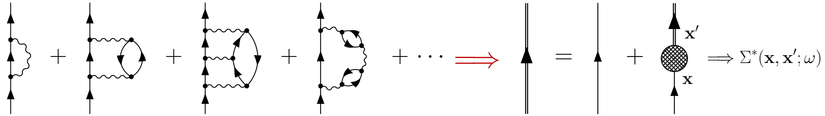
- Effective mass M^* related to single-particle levels

Effective Mass and the Single-Particle Spectrum



- Uniform system: $\varepsilon^{\rho}_{\mathbf{k}} - \varepsilon^{\rho\tau}_{\mathbf{k}} = \frac{\pi}{\nu}[(\nu-1)a_s^2 r_s + 2(\nu+1)a_p^3]\,\frac{k_F^2 - \mathbf{k}^2}{2M}\,\rho$

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



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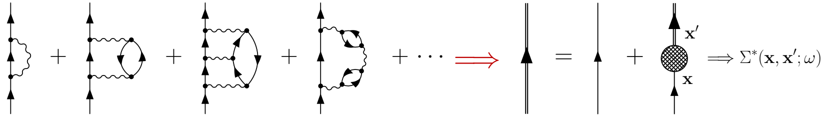

- Add a non-local source $\xi(x',x)$ coupled to $\psi(x)\psi^\dagger(x')$:

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

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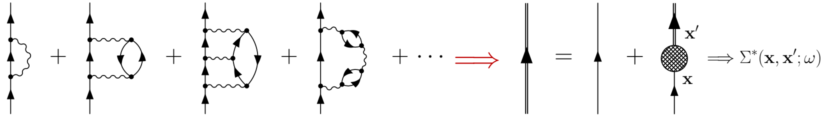

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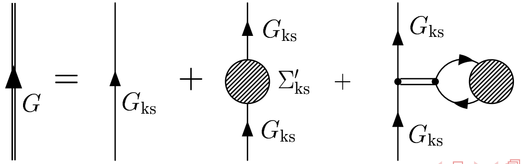
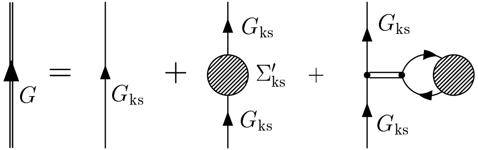
- With $\Gamma[\rho,\xi] = \Gamma_0[\rho,\xi] + \Gamma_{\rm int}[\rho,\xi]$,

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



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



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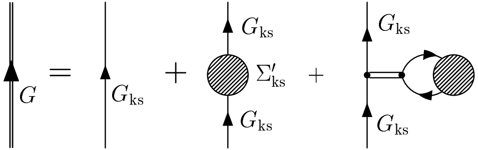
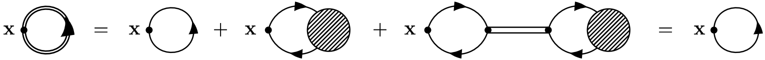


- Simple diagrammatic demonstration:



- Densities agree by construction!

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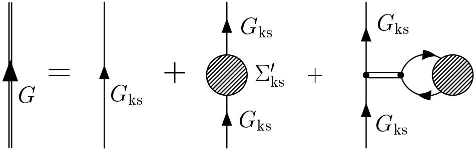

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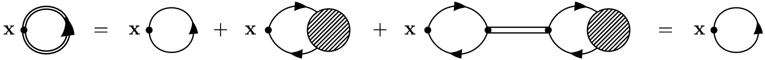


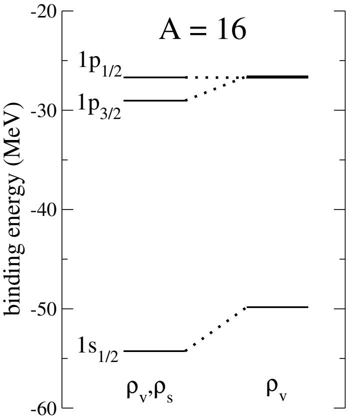
- Densities agree by construction!
- Is the Kohn-Sham basis a useful one for G?

How Close is G_{KS} to G?

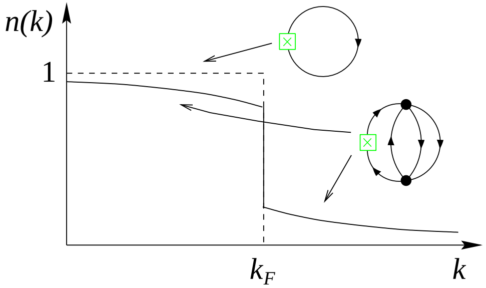
- It depends on what sources are used!

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

- Nonrel. M^* in $\Gamma[\rho]$ vs. $\Gamma[\rho,\tau]$ vs. $\ldots$
- Covariant case at LO: $\Gamma[\rho_v]$ vs. $\Gamma[\rho_v, \rho_s]$
- Higher orders?



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)

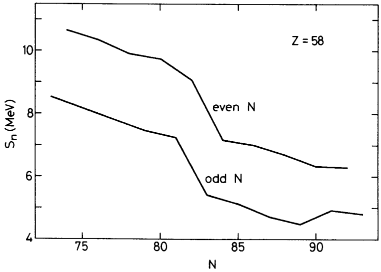
Outline

Extensions to DFT/EFT

Pairing in Kohn-Sham DFT

Summary III

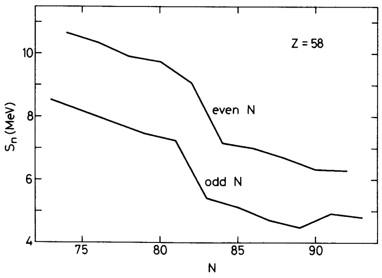
Experimental Evidence for Pairing in Nuclei



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

- Odd-even staggering of binding energies

Experimental Evidence for Pairing in Nuclei



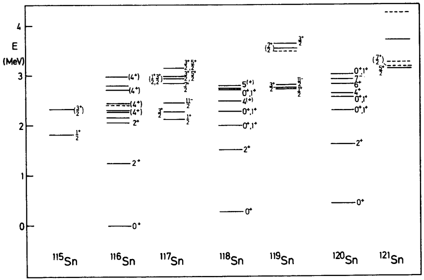
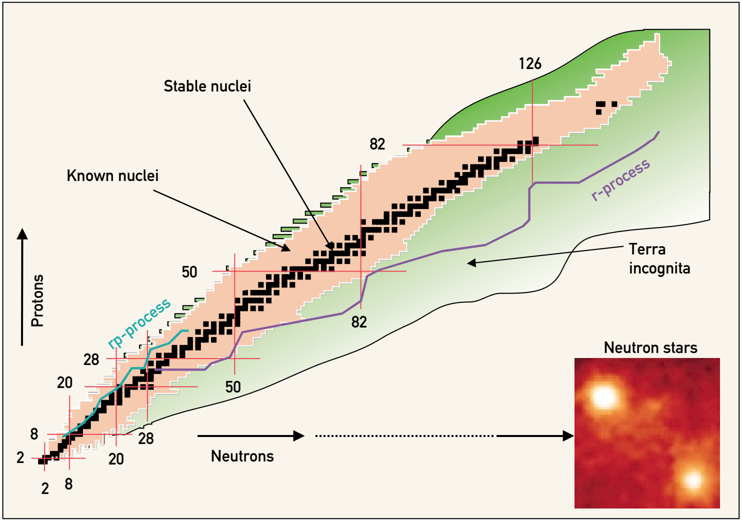


Figure 6.1. Excitation spectra of the $_{50}$Sn isotopes.

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

Table of the Nuclides



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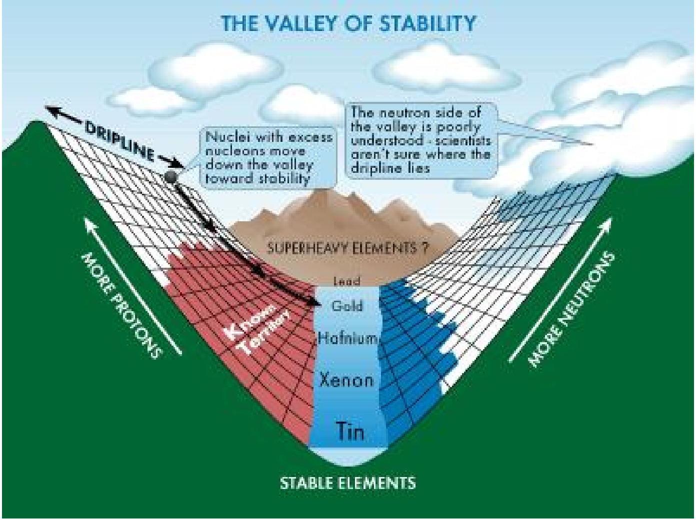
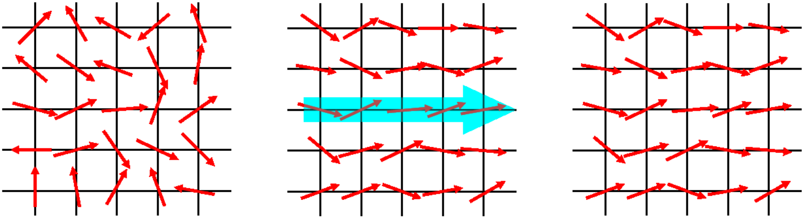


Effective Actions and Broken Symmetries

- 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 $F(H)$:

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

  - since $H = \partial\Gamma/\partial M \longrightarrow 0$, minimize Γ to find ground state



Pairing from Effective Actions

- For pairing, the broken symmetry is a $U(1)$ [phase] symmetry
- Textbook effective action treatment in condensed matter
  - introduce contact interaction: $g\,\psi^\dagger\psi^\dagger\psi\psi$
  - Hubbard-Stratonovich with auxiliary pairing field $\hat{\Delta}(x)$ coupled to $\psi^\dagger\psi^\dagger \Longrightarrow$ eliminate contact interaction
  - construct 1PI $\Gamma[\Delta]$ with $\Delta = \langle\hat{\Delta}\rangle$, look for $\frac{\delta\Gamma}{\delta\Delta} = 0$
  - to leading order in the loop expansion (mean field) $\Longrightarrow$ BCS weak-coupling gap equation with gap Δ

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- Alternative: Combine an expansion (e.g., EFT) and the *inversion* method for effective actions (Fukuda et al.)
  - external current $j(x)$ coupled to pair density breaks symmetry
  - natural generalization of Kohn-Sham DFT (Bulgac et al.)
  - cf. DFT with nonlocal source (Oliveira et al.; Kurth et al.)

Local Composite Effective Action with Pairing

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

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

- Densities found by functional derivatives wrt J, j:

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

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

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

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

Claims (Hopes?) About Effective Action

- $\Gamma[\rho, \phi] \propto$ (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:

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

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- This is Hohenberg-Kohn DFT extended to pairing!
- We need a method to carry out the Legendre transforms
  - To get Kohn-Sham DFT, apply inversion methods
- Can we renormalize consistently?

Kohn-Sham Inversion Method (General)

- Order-by-order matching in counting parameter λ

diagrams	$\Longrightarrow$	$W[J,j,\lambda] = W_0[J,j] + \lambda W_1[J,j] + \lambda^2 W_2[J,j] + \cdots$
assume	$\Longrightarrow$	$J[\rho,\phi,\lambda] = J_0[\rho,\phi] + \lambda J_1[\rho,\phi] + \lambda^2 J_2[\rho,\phi] + \cdots$
assume	$\Longrightarrow$	$j[\rho,\phi,\lambda] = j_0[\rho,\phi] + \lambda j_1[\rho,\phi] + \lambda^2 j_2[\rho,\phi] + \cdots$
derive	$\Longrightarrow$	$\Gamma[\rho,\phi,\lambda] = \Gamma_0[\rho,\phi] + \lambda \Gamma_1[\rho,\phi] + \lambda^2 \Gamma_2[\rho,\phi] + \cdots$

- Start with exact expressions for Γ and ρ

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

$\Longrightarrow$ plug in expansions with ρ, ϕ treated as order unity

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\end{aligned}$$

- 0^{th} order is Kohn-Sham system with potentials $J_0(\mathbf{x})$ and $j_0(\mathbf{x})$
  $\implies$ exact densities $\rho(\mathbf{x})$ and $\phi(\mathbf{x})$ by construction

$$\Gamma_0[\rho,\phi] = W_0[J_0,j_0] - \int J_0\,\rho - \int j_0\,\phi \implies \rho(x) = \frac{\delta W_0[\,]}{\delta J_0(x)}\,, \quad \phi(x) = \frac{\delta W_0[\,]}{\delta j_0(x)}$$

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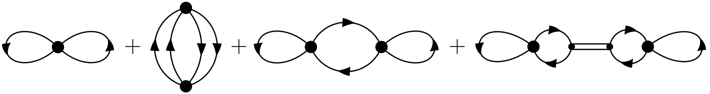
- Introduce single-particle orbitals and solve (cf. HFB)

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

where $h_0(\mathbf{x}) \equiv -\dfrac{\boldsymbol{\nabla}^2}{2M} + V_{\rm trap}(\mathbf{x}) - J_0(\mathbf{x})$

Diagrammatic Expansion of W_i

- Lines in diagrams are KS Nambu-Gor'kov Green's functions

$\Gamma_{\rm int} =$  $+ \cdots$

$$
\mathbf{G} = \begin{pmatrix} \langle T_\tau \psi_\uparrow(x)\psi_\uparrow^\dagger(x')\rangle_0 & \langle T_\tau \psi_\uparrow(x)\psi_\downarrow(x')\rangle_0 \\ \langle T_\tau \psi_\downarrow^\dagger(x)\psi_\uparrow^\dagger(x')\rangle_0 & \langle T_\tau \psi_\downarrow^\dagger(x)\psi_\downarrow(x')\rangle_0 \end{pmatrix} \equiv \begin{pmatrix} G_{\rm ks}^0 & F_{\rm ks}^0 \\ F_{\rm ks}^{0\,\dagger} & -\widetilde{G}_{\rm ks}^0 \end{pmatrix}
$$

  - Extra diagrams enforce inversion (here removes anomalous)

- In frequency space, the Kohn-Sham Green's functions are

$$
G_{\rm ks}^0(\mathbf{x},\mathbf{x}';\omega) = \sum_j \left[\frac{u_j(\mathbf{x})\,u_j^*(\mathbf{x}')}{i\omega - E_j} + \frac{v_j(\mathbf{x}')\,v_j^*(\mathbf{x})}{i\omega + E_j} \right]
$$

$$
F_{\rm ks}^0(\mathbf{x},\mathbf{x}';\omega) = -\sum_j \left[\frac{u_j(\mathbf{x})\,v_j^*(\mathbf{x}')}{i\omega - E_j} - \frac{u_j(\mathbf{x}')\,v_j^*(\mathbf{x})}{i\omega + E_j} \right]
$$

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

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

- The chemical potential μ_0 is fixed by $\int \rho(\mathbf{x}) = A$
- Diagrams for $\Gamma[\rho,\phi] \propto E_0[\rho,\phi] + E_{\rm int}[\rho,\phi]$ yields KS potentials

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

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Divergences: Uniform Dilute Fermi System

- Generating functional with constant sources μ and j:

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

- 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 $\Delta^*\psi_\uparrow\psi_\downarrow$

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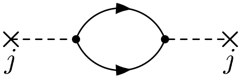
$W[\mu, j] = \cdots +$  $+ \cdots$

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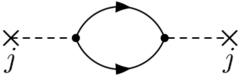
$W[\mu,j] = \cdots +$  $+ \cdots$

  - Same linear divergence as in 2-to-2 scattering
- Renormalization: Add counterterm $\frac{1}{2}\zeta|j|^2$ to $\mathcal{L}$ (cf. Zinn-Justin)
  - Additive to W (cf. $|\Delta|^2$) $\Longrightarrow$ no effect on scattering
  - How to determine ζ? Energy interpretation of Γ?

Use Dimensional Regularization (DR)

- Generalize Papenbrock & Bertsch DR/MS calculation
- DR/PDS $\Longrightarrow$ generate explicit Λ to "check" renormalization
  - Basic free-space integral in D spatial dimensions

$$\left(\frac{\Lambda}{2}\right)^{3-D}\int\frac{d^Dk}{(2\pi)^D}\,\frac{1}{p^2-k^2+i\epsilon}\xrightarrow{\text{PDS}}-\frac{1}{4\pi}(\Lambda+ip)\qquad\left[\text{note: }\int\frac{1}{\epsilon_k^0}\longrightarrow\frac{M\Lambda}{2\pi}\right]$$

  - Renormalizing free-space scattering yields:

$$C_0(\Lambda)=\frac{4\pi a_s}{M}+\frac{4\pi a_s^2}{M}\Lambda+\mathcal{O}(\Lambda^2)=C_0^{(1)}+C_0^{(2)}+\cdots\longrightarrow\frac{4\pi a_s}{M}\,\frac{1}{1-a_s\Lambda}$$

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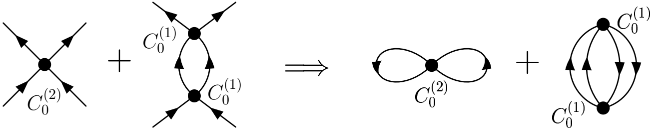
  - Recover DR/MS with $\Lambda=0$
- E.g., verify NLO renormalization $\Longrightarrow$ independent of Λ



Kohn-Sham Non-Interacting System

- Bare density ρ:

$$\rho = -\frac{1}{\beta V}\frac{\partial W_0[]}{\partial \mu_0} = \frac{2}{V}\sum_{\mathbf{k}} v_k^2$$

$$= \int \frac{d^3k}{(2\pi)^3}\left(1 - \frac{\epsilon_k^0 - \mu_0}{E_k}\right)$$

- Bare pair density ϕ_B:

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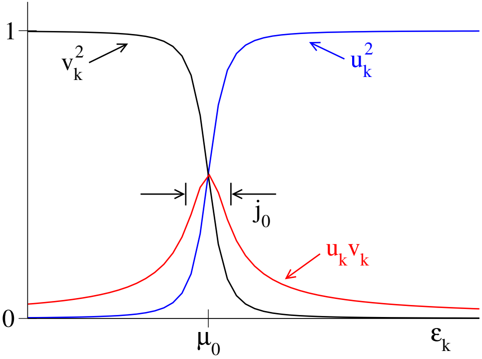

- j_0 plays role of constant gap

$$E_k = \sqrt{(\epsilon_k^0 - \mu_0)^2 + j_0^2}\,, \quad \epsilon_k^0 = \frac{k^2}{2M}$$

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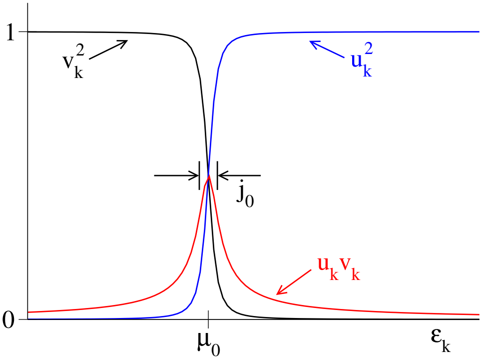

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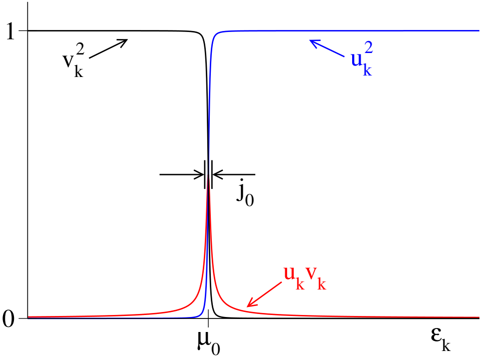

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$$\rho = -\frac{1}{\beta V}\frac{\partial W_0[]}{\partial \mu_0} = \frac{2}{V}\sum_{\mathbf{k}} v_k^2$$

$$= \int \frac{d^3k}{(2\pi)^3}\left(1 - \frac{\epsilon_k^0 - \mu_0}{E_k}\right)$$

- Bare pair density ϕ_B:

$$\phi_B = \frac{1}{\beta V}\frac{\partial W_0[]}{\partial j_0} = \frac{2}{V}\sum_{\mathbf{k}} u_k v_k$$

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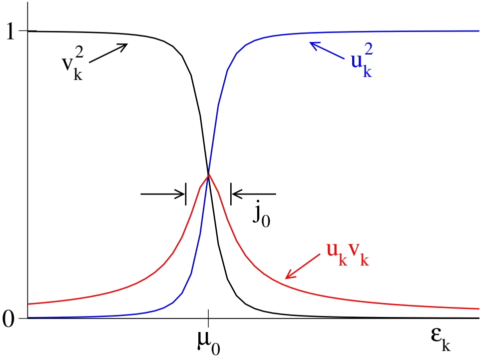

- j_0 plays role of constant gap

$$E_k = \sqrt{(\epsilon_k^0 - \mu_0)^2 + j_0^2}\,, \quad \epsilon_k^0 = \frac{k^2}{2M}$$

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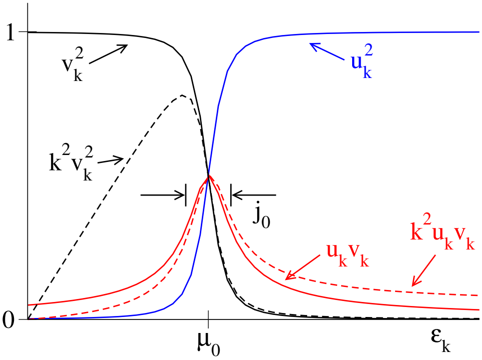

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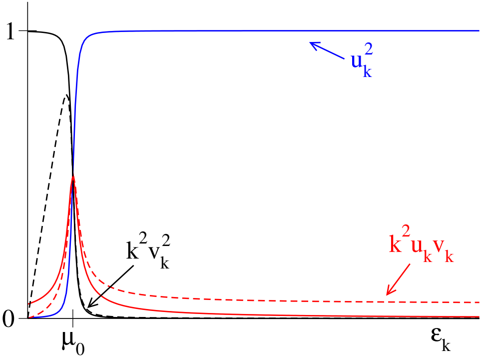

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- The basic DR/PDS integral in D dimensions, with $x \equiv j_0/\mu_0$, is

$$I(\beta) \equiv \left(\frac{\Lambda}{2}\right)^{3-D} \int \frac{d^D k}{(2\pi)^D} \frac{(\epsilon_k^0)^\beta}{\sqrt{(\epsilon_k^0 - \mu_0)^2 + j_0^2}} = \frac{M\Lambda}{2\pi} \mu_0^\beta \left(1 - \delta_{\beta,2} \frac{x^2}{2}\right)$$

$$+ (-)^{\beta+1} \frac{M^{3/2}}{\sqrt{2\pi}} [\mu_0^2(1+x^2)]^{(\beta+1/2)/2} P^0_{\beta+1/2}\left(\frac{-1}{\sqrt{1+x^2}}\right)$$

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- Check the KS density equation $\Longrightarrow$ Λ dependence cancels:

$$\rho = -\frac{1}{\beta V}\frac{\partial W_0[\,]}{\partial \mu_0} = \int \frac{d^3k}{(2\pi)^3}\left(1 - \frac{\epsilon_k^0}{E_k} + \frac{\mu_0}{E_k}\right) \longrightarrow 0 - I(1) + \mu_0 I(0)$$

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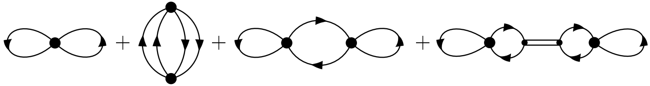
- The KS equation for the pair density ϕ fixes $\zeta^{(0)}$:

$$\phi = \frac{1}{\beta V}\frac{\partial W_0[\,]}{\partial j_0} = -\int \frac{d^3k}{(2\pi)^3}\frac{j_0}{E_k} + \zeta^{(0)} j_0 \longrightarrow -j_0 I(0) + \zeta^{(0)} j_0 \Longrightarrow \zeta^{(0)} = \frac{M\Lambda}{2\pi}$$

Calculating to n^{th} Order

- Find $\Gamma_{1\le i\le n}[\rho,\phi]$ from $W_{1\le i\le n}[\mu_0(\rho,\phi), j_0(\rho,\phi)]$
  - including additional Feynman rules

$\Gamma_{\mathrm{int}} =$  $+\cdots$

- Calculate μ_i, j_i from Γ_i, then use $\sum_{i=0}^{n} j_i = j \to 0$ to find j_0
- Renormalization conditions:
  - No freedom in choosing $C_0(\Lambda) \implies \Lambda$'s must cancel!
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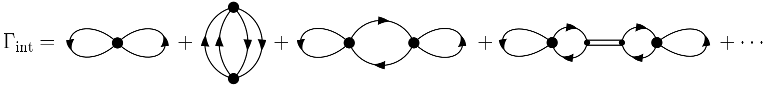

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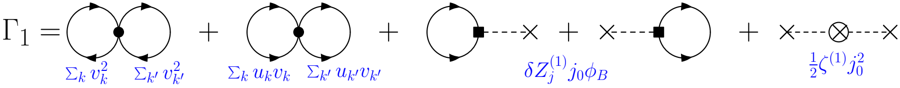
  - Choose $\delta Z_j^{(n)}$ and $\zeta^{(n)}$ to convert ϕ_B to renormalized ϕ
- Leading order: Diagrams for $\Gamma_1[\rho,\phi] = W_1[\mu_0(\rho,\phi), j_0(\rho,\phi)]$



$$\Longrightarrow \quad \frac{1}{\beta V}\Gamma_1[\rho,\phi] = \frac{1}{4}C_0^{(1)}\rho^2 + \frac{1}{4}C_0^{(1)}\phi^2 \quad \text{with } C_0^{(1)} = \frac{4\pi a_s}{M}$$

The “Gap” Equation at Leading Order (LO)

- Γ_1 dependence on ρ and ϕ explicit $\Longrightarrow$ easy to find μ_1 and j_1:

$$\mu_1 = \frac{1}{\beta V}\frac{\partial \Gamma_1}{\partial \rho} = \frac{1}{2}C_0^{(1)}\rho \qquad \text{and} \qquad j_1 = -\frac{1}{\beta V}\frac{\partial \Gamma_1}{\partial \phi} = -\frac{1}{2}C_0^{(1)}\phi$$

- “Gap” equation from $j = j_0 + j_1 = 0$

$$j_0 = -j_1 = -\frac{1}{2}|C_0^{(1)}|\phi = \frac{1}{2}|C_0^{(1)}|j_0\left(\int \frac{d^3k}{(2\pi)^3}\frac{1}{\sqrt{(\epsilon_k^0 - \mu_0)^2 + j_0^2}} - \zeta^{(0)}\right)$$

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- DR/PDS reproduces Papenbrock/Bertsch (with $x \equiv |j_0/\mu_0|$)

$$1 = \sqrt{2M\mu_0}a_s(1+x^2)^{1/4}P^0_{1/2}\left(\frac{-1}{\sqrt{1+x^2}}\right) \xrightarrow{x\to 0} k_{\mathrm{F}}a_s\left[\frac{4-6\log 2}{\pi}+\frac{2}{\pi}\log x\right]$$

$$\Longrightarrow \text{ if } k_{\mathrm{F}}a_s < 1,\ \frac{j_0}{\mu_0} = \frac{8}{e^2}e^{-\pi/2k_{\mathrm{F}}|a_s|} \text{ holds}$$

Renormalized Energy Density at LO

- Renormalized effective action $\Gamma = \Gamma_0 + \Gamma_1$:

$$\frac{1}{\beta V}\Gamma = \int(\epsilon_k^0 - \mu_0 - E_k) + \frac{1}{2}\zeta^{(0)} j_0^2 + \mu_0\rho - j_0\phi + \frac{1}{4}C_0^{(1)}\rho^2 + \frac{1}{4}C_0^{(1)}\phi^2$$

- Check for Λ's:

$$\frac{1}{\beta V}\Gamma = 0 - I(2) + 2\mu_0 I(1) - (\mu_0^2 + j_0^2)I(0) + \frac{1}{2}\frac{M\Lambda}{2\pi}j_0^2 + \cdots$$

$$\longrightarrow \frac{M\Lambda}{2\pi}\Big(-\mu_0^2(1 - j_0^2/2\mu_0^2) + 2\mu_0^2 - \mu_0^2 - j_0^2 + \frac{1}{2}j_0^2\Big) = 0$$

- To find the energy density, evaluate Γ at the stationary point $j_0 = -\frac{1}{2}|C_0^{(1)}|\phi$ with μ_0 fixed by the equation for ρ
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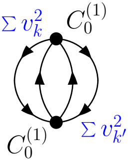
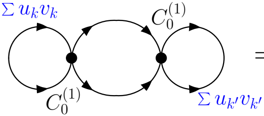
  $\Longrightarrow$ same results as Papenbrock/Bertsch (plus HF term)
- Life gets more complicated at NLO
  - dependence of Γ_2 on ρ, ϕ is no longer explicit
  - analytic formulas for DR integrals not available

Γ_2 at Next-to-Leading Order (NLO)



$$\Longrightarrow \quad -(C_0^{(1)})^2 \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3q}{(2\pi)^3} \frac{1}{E_p + E_k + E_{p-q} + E_{k+q}} \times \Big[u_p^2\, u_k^2\, v_{p-q}^2\, v_{k+q}^2 - 2u_p^2\, v_k^2\, (uv)_{p-q}\, (uv)_{k+q} + (uv)_p\, (uv)_k\, (uv)_{p-q}\, (uv)_{k+q} \Big]$$



$$\Longrightarrow \quad -(C_0^{(1)})^2 \int \frac{d^3k}{(2\pi)^3} \frac{1}{2E_k} \left[\rho (u_k v_k)^2 + \frac{1}{2}\phi_B (u_k^2 - v_k^2)\right]^2$$

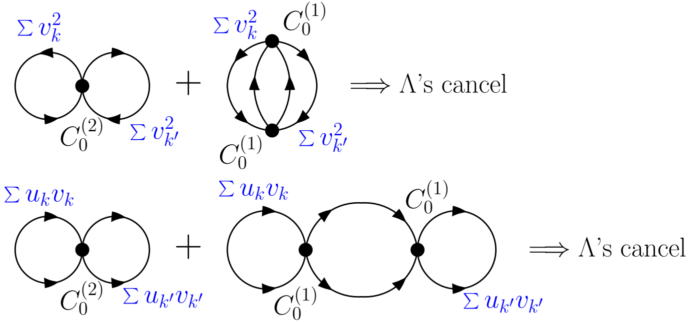
- UV divergences identified from

$$v_k^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right) \xrightarrow{k\to\infty} \frac{j_0^2 M^2}{k^4} \qquad u_k^2 = \frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right) \xrightarrow{k\to\infty} 1 - \frac{j_0^2 M^2}{k^4}$$

$$u_k v_k = -\frac{j_0}{2E_k} \xrightarrow{k\to\infty} -\frac{j_0 M}{k^2} \qquad \frac{1}{E_k} \xrightarrow{k\to\infty} \frac{2M}{k^2}$$

Next-To-Leading-Order (NLO) Renormalization

- Bowtie with $C_0^{(2)} = \dfrac{4\pi a_s^2}{M}\Lambda$ vertex must precisely cancel Λ's from beachballs with $C_0^{(1)} = \dfrac{4\pi a_s}{M}$ vertices:



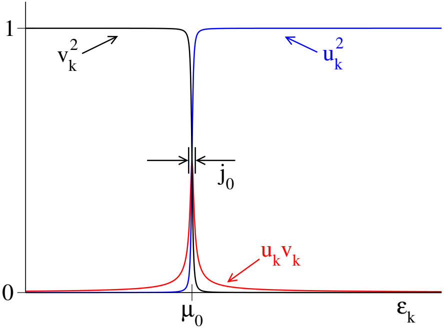
(Note that $\delta Z_j^{(1)}$ vertex takes $\phi_B \to \phi$)

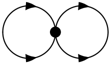
- How do we see cancellation of Λ's and evaluate renormalized results without analytic formulas? [but first . . .]

Standard Induced Interaction Result Recovered

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

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





$$\Gamma_1 = \bigcirc\!\!\bullet\!\!\bigcirc + CTC + \cdots \Longrightarrow j_1 = \frac{\delta\Gamma_1}{\delta\phi} = \frac{1}{2}|C_0|\phi$$

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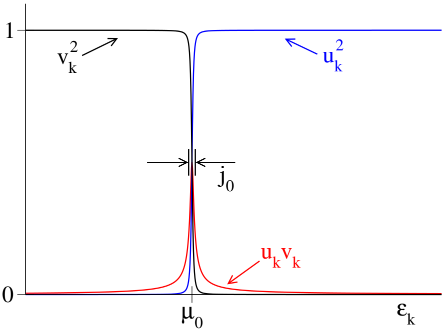
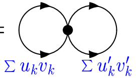
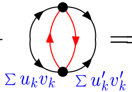
- NLO modifies exponent $\Longrightarrow$ changes prefactor
- $\Delta_{NLO} \approx \Delta_{LO}/(4e)^{1/3}$



$\Gamma_1+\Gamma_2 =$  $+$  $\Longrightarrow j_1+j_2 = \frac{1}{2}|C_0|\left[1 - |C_0|\langle\Pi_0\rangle_{|\mathbf{k}|=|\mathbf{k}'|=k_\mathrm{F}}\right]\phi$

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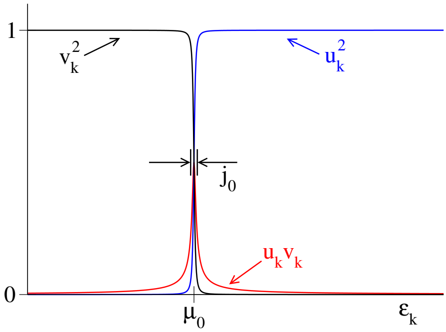
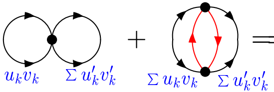


$\Gamma_1 + \Gamma_2 =$  $\Longrightarrow j_1 + j_2 = \frac{1}{2}|C_0| \left[1 - |C_0| \langle \Pi_0 \rangle_{|\mathbf{k}|=|\mathbf{k}'|=k_{\rm F}}\right] \phi$

- How does the Kohn-Sham gap compare to “real” gap?

Renormalizing with Subtractions

- NLO integrals over $E_k = \sqrt{(\epsilon_k - \mu_0)^2 + j_0^2}$ are intractable, but

$$\int \frac{1}{E_1 + E_2 + E_3 + E_4} = \int \left[\frac{1}{E_1 + E_2 + E_3 + E_4} - \frac{\mathcal{P}}{\epsilon_1^0 + \epsilon_2^0 - \epsilon_3^0 - \epsilon_4^0} \right]$$

plus a DR/PDS integral that is proportional to Λ

$\Longrightarrow$ just make the substitution in [ ]'s for renormalized result

- When applied at LO,

$$\int \frac{1}{E_k} = \int \left[\frac{1}{E_k} - \frac{\mathcal{P}}{\epsilon_k^0} \right] + \frac{M\Lambda}{2\pi}$$

- Cf. subtraction to eliminate C_0 in gap equation

$$\frac{M}{4\pi a_s} + \frac{1}{|C_0|} = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\epsilon_k^0} \Longrightarrow \frac{M}{4\pi a_s} = -\frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \left[\frac{1}{E_k} - \frac{1}{\epsilon_k^0} \right]$$

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- Any equivalent subtraction works, e.g.,

$$\int \frac{d^3k}{(2\pi)^3} \frac{\mathcal{P}}{\epsilon_k^0 - \mu_0} = \int \frac{d^3k}{(2\pi)^3} \frac{1}{\epsilon_k^0}$$

Anomalous Density in Finite Systems

- How do we renormalize the pair density in a finite system?

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

  - cf. scalar density $\rho_s = \sum_i \overline{\psi}(\mathbf{x})\psi(\mathbf{x})$ for relativistic mft

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- Plan: Use subtracted expression for ϕ in uniform system

$$\phi = \int^{k_c} \frac{d^3k}{(2\pi)^3} j_0 \left(\frac{1}{\sqrt{(\epsilon_k^0 - \mu_0)^2 + j_0^2}} - \frac{1}{\epsilon_k^0} \right) \overset{k_c\to\infty}{\longrightarrow} \text{finite}$$

- Apply this in a local density approximation (Thomas-Fermi)

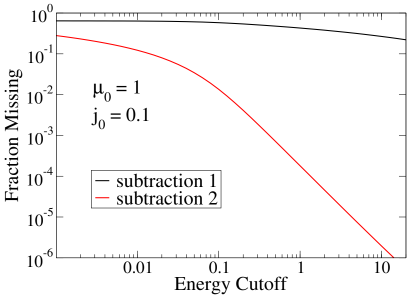
$$\phi(\mathbf{x}) = 2\sum_i^{E_c} u_i(\mathbf{x})v_i(\mathbf{x}) - j_0(\mathbf{x})\frac{M\,k_c(\mathbf{x})}{2\pi^2} \quad \text{with} \quad E_c = \frac{k_c^2(\mathbf{x})}{2M} + J(\mathbf{x}) - \mu_0$$

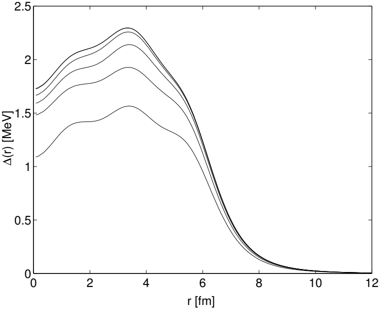
Bulgac Renormalization [Bulgac/Yu PRL 88 (2002) 042504]

- Convergence is very slow as the energy cutoff is increased
  $\Longrightarrow$ Bulgac/Yu: make a different subtraction

$$\phi = \int^{k_c} \frac{d^3k}{(2\pi)^3} j_0 \left(\frac{1}{\sqrt{(\epsilon_k^0 - \mu_0)^2 + j_0^2}} - \frac{\mathcal{P}}{\epsilon_k^0 - \mu_0} \right) \overset{k_c \to \infty}{\longrightarrow} \text{finite}$$

- Compare convergence in uniform system, in nuclei with LDA





- How do we generalize this?

Energy Interpretation

- Effective actions of local composite operators 30 years ago
  - “Sentenced to death” by Banks and Raby
  - Underlying problems from new UV divergences
- Connection between effective action and variational energy
  - Euclidean space (see Zinn-Justin)

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

  - Minkowski space constrained minimization (see Weinberg)
    - source terms serve as Lagrange multipliers
  - Are these properties invalidated by nonlinear source terms?

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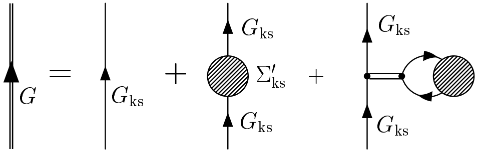
    - source terms serve as Lagrange multipliers
  - Are these properties invalidated by nonlinear source terms?
- Potential ambiguities in the renormalization
  - Arbitrary finite part of added counterterms $\Longrightarrow$ shift minima
  - Verschelde et al. claim not arbitrary
- Are the stationary points valid in any case?

Kohn-Sham Questions

- How are Kohn-Sham “gap” and conventional gap related?
  - Kohn-Sham Green’s function vs. full Green’s function

$$G(x,x') = G_{\rm ks}(x,x') + G_{\rm ks}\left[\frac{1}{i}\frac{\delta\Gamma_{\rm int}}{\delta G_{\rm ks}} + \frac{\delta\Gamma_{\rm int}}{\delta\rho}\right]G_{\rm ks}$$



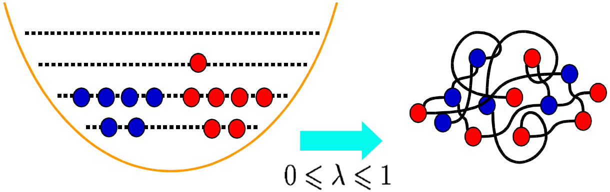
  - When do we need the “real” gap?
- What about broken symmetries?
  - E.g., number projection for pairing
  - How to accomodate within effective action framework?

Better Alternatives to Local Kohn-Sham?

- Couple source to non-local pair field (Oliveira et al.):

$$\widehat{H} \longrightarrow \widehat{H} - \int dx\, dx' \, [D^*(x,x')\psi_\uparrow(x)\psi_\downarrow(x') + \text{H.c.}]$$

  - CJT 2PI effective action $\Gamma[\rho, \Delta]$ with $\Delta(x,x') = \langle \psi_\uparrow(x)\psi_\downarrow(x')\rangle$
- Auxiliary fields: Introduce $\widehat{\Delta}^*(x)\psi(x)\psi(x) + \text{H.c.}$ via H.S.
  - 1PI effective action in $\Delta(x) = \langle \widehat{\Delta}(x)\rangle$
  - Special saddle point evaluation $\Longrightarrow$ Kohn-Sham DFT
- DFT from Renormalization Group (Polonyi-Schwenk)



Outline

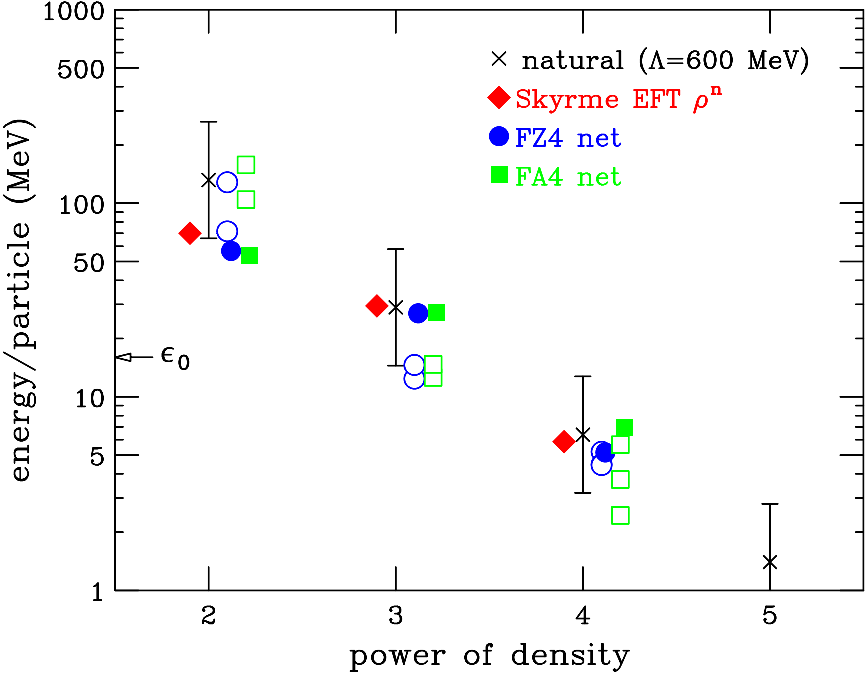
Extensions to DFT/EFT

Pairing in Kohn-Sham DFT

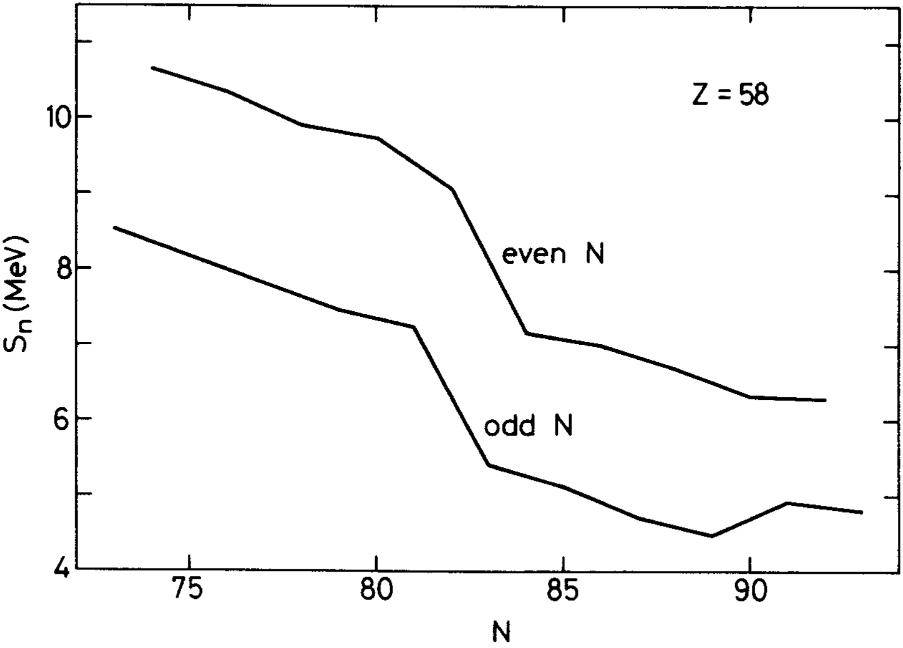
Summary III

Summary III

- Extensions to DFT by adding external fields
  - With kinetic energy and spin-orbit densities
    $\Longrightarrow$ looks like Skyrme functional!
- Effective action formalism generates Kohn-Sham DFT
  with local pairing fields $\Longrightarrow$ systematic expansion
- Some of the open issues:
  - Energy interpretation and ambiguities
  - Number projection
  - Renormalization in finite systems
  - Efficient numerical implementation
  - Implementing low-momentum potential $\Longrightarrow$ Power counting
  - Better alternatives?



× natural (Λ=600 MeV)
Skyrme EFT ρ^n
FZ4 net
FA4 net
energy/particle (MeV)
power of density
ε0
1000
500
100
50
10
5
1
2
3
4
5



Z = 58
even N
odd N
S_n (MeV)
10
8
6
4
75
80
85
90
N

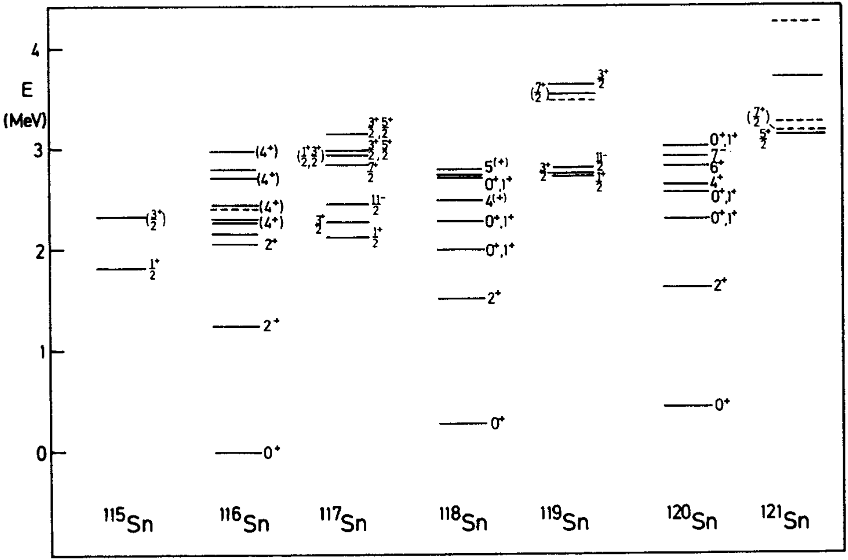
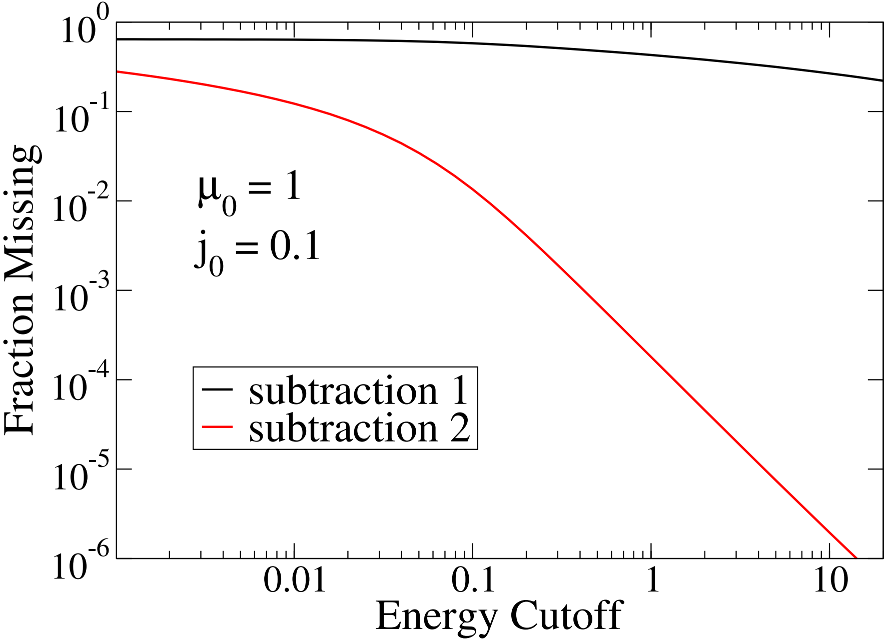


Figure 6.1. Excitation spectra of the $_{50}$Sn isotopes.



Fraction Missing
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
$\mu_0 = 1$
$j_0 = 0.1$
subtraction 1
subtraction 2
0.01
0.1
1
10
Energy Cutoff