

# Pairing from Effective Field Theory and Density Functional Theory

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## References:

- “Effective field theory for dilute fermions with pairing,” rjf, H.-W. Hammer, S. Puglia, Ann. Phys. (NY) **322**, 2703 (2007)
- “Toward ab initio density functional theory for nuclei,” J. Drut, rjf, L. Platter, Prog. Part. Nucl. Phys. **64**, 120 (2009)

# Outline

**Overview: Pairing in EFT/DFT**

**Kohn-Sham DFT with pairing from effective action**

**Renormalization issues**

**Going forward: ideas, questions, tools**

# Outline

## Overview: Pairing in EFT/DFT

Kohn-Sham DFT with pairing from effective action

Renormalization issues

Going forward: ideas, questions, tools

# Effective Field Theory ingredients

Simplest case: short-distance, *natural* interactions

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

- $$\mathcal{L}_{\text{eft}} = \psi^\dagger \left[ i \frac{\partial}{\partial t} + \frac{\nabla^2}{2M} \right] \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 - \frac{D_0}{6} (\psi^\dagger \psi)^3 + \dots$$

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**3** Well-defined power counting  $\implies$  small expansion parameter

- use separation of scales  $\implies \frac{k}{\Lambda}$  with  $\Lambda \sim 1/R \implies ka_s \ll 1$ , etc.
- Recovers scattering expansion order-by-order with diagrams

$$f_0(k) \propto \frac{1}{k \cot \delta_0(k) - ik} \longrightarrow a_s [1 - ia_s k - (a_s^2 - a_s r_0/2) k^2 + \mathcal{O}(k^3 a_s^3)]$$

$$\longrightarrow R [1 - ikR - 2k^2 R^2/3 + \mathcal{O}(k^3 R^3)] \quad [\text{e.g., hard spheres}]$$

- with DR/MS, one power of  $k$  per diagram, *natural* coefficients
- estimate truncation error from dimensional analysis
- valid for *any* natural short-range interaction!

# Effective Field Theory ingredients

Apply at finite density (no pairing) [Hammer, rjf, nucl-th/0004043]

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- 2 Declaration of regularization and renormalization scheme

- natural  $a_s \implies$  dimensional regularization and min. subtraction

- 3 Well-defined power counting  $\implies$  small expansion parameters

- use separation of scales  $\implies \frac{k_F}{\Lambda}$  with  $\Lambda \sim 1/R \implies k_F a_s \ll \pi$ , etc.

$$\mathcal{O}(k_F^6) : \text{blue bubble diagram} \quad \mathcal{O}(k_F^7) : \text{green bubble diagram} + \text{black bubble diagram with red X}$$

$$\mathcal{E} = \rho \frac{k_F^2}{2M} \left[ \frac{3}{5} + \frac{2}{3} (k_F a_s / \pi) + \frac{4}{35} (11 - 2 \ln 2) (k_F a_s / \pi)^2 + \dots \right]$$

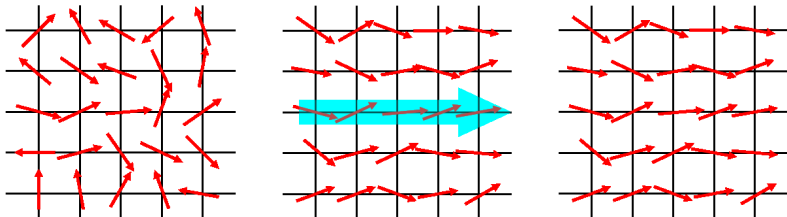
- cleanly recovers perturbative free-space ERE and in-medium energy density (including 3-body logs), plus error estimates

# Laundry list of EFT/DFT pairing issues

- Questions:
  - To what extent is an EDF unique? Kohn-Sham gap? (and so on)
  - Can we motivate/constrain ASLDA near the unitary limit?
  - For nuclei, do we want/need to include the pion explicitly?
- Ideas from other contexts:
  - Alternative (Kohn-Sham) DFT — e.g., auxiliary fields, non-local
  - Beyond quasi-local: orbital-based methods for long-range correlations (cf., RPA with OEP in Coulomb systems)
- Tools/methods:
  - Renormalized sums in finite systems (from RHA/soliton studies)
  - Operator Product Expansion (e.g., cancellation of divergences)
  - Collective coordinate methods (e.g., BRST invariance)

## Effective actions and broken symmetries

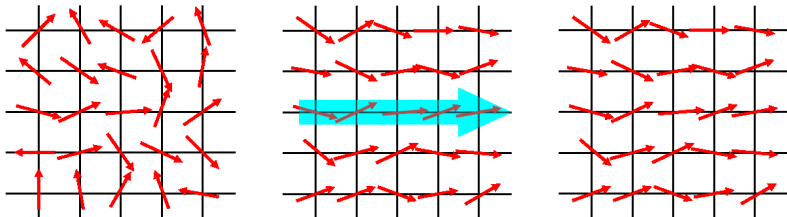
- Natural framework for spontaneous symmetry breaking
  - e.g., test for zero-field magnetization  $M$  in a spin system
  - introduce an external field  $H$  to break rotational symmetry



- if  $F[H]$  calculated perturbatively,  $M[H = 0] = 0$  to all orders

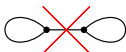

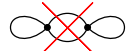
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- if  $F[H]$  calculated perturbatively,  $M[H = 0] = 0$  to all orders
- Legendre transform Helmholtz free energy  $F(H)$ :
 
$$\text{invert } M = -\partial F(H)/\partial H \xrightarrow{H(M)} \Gamma[M] = F[H(M)] + MH(M)$$
  - since  $H = \partial\Gamma/\partial M \rightarrow 0$ , stationary points of  $\Gamma \Rightarrow$  ground state
- Can couple source “ $H$ ” many ways (and multiple sources)

# A bestiary of effective actions

- Couple source to local Lagrangian field, e.g.,  $J(x)\phi(x)$ 
  - $\Gamma[\varphi]$  where  $\varphi(x) = \langle \phi(x) \rangle \implies$  1PI effective action 
  - Arises from fermion  $\mathcal{L}$ 's by introducing auxiliary fields
  - Can approximate with stationary phase  $\implies$  loop expansion
- Couple  $J$  to **non-local** composite op, e.g.,  $J(x, x')\phi(x)\phi(x')$ 
  - $\Gamma[G, \varphi] \implies$  2PI effective action [CJT] 
  - cf. Baym-Kadanoff conserving (“ $\Phi$ -derivable”) approximations
  - Often applied to hot, nonequilibrium QCD
- Source coupled to **local** composite operator, e.g.,  $J(x)\phi^2(x)$ 
  - 1.5PI effective action? Almost: 
  - Kohn-Sham DFT from **inversion method**
  - Careful: new divergences likely (e.g., pairing)

## Partition function in $\beta \rightarrow \infty$ limit [see Zinn-Justin]

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

$$\hat{H}(J) = \hat{H} + \int J \hat{\phi} \quad \text{or} \quad \hat{H}(J) = \hat{H} + \int J \psi^\dagger \psi$$

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

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

- As  $\beta \rightarrow \infty$ ,  $\mathcal{Z}[J] \implies$  ground state of  $\hat{H}(J)$  with energy  $E_0(J)$

$$\mathcal{Z}[J] = e^{-W[J]} \sim \text{Tr} e^{-\beta(\hat{H} + J\hat{\rho})} \implies E_0(J) = \lim_{\beta \rightarrow \infty} -\frac{1}{\beta} \log \mathcal{Z}[J] = \frac{1}{\beta} W[J]$$

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- $\Gamma[\rho]$ : expectation value of  $\hat{H}$  in ground state generated by  $J[\rho]$

$$\frac{1}{\beta} \Gamma[\rho] = E_0(J) - \int J \rho = \langle \hat{H} + J\hat{\rho} \rangle_J - \int J \rho = \langle \hat{H} \rangle_J \xrightarrow{J \rightarrow 0} E_0$$

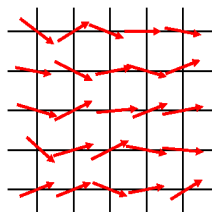
$$J(\mathbf{x}) = -\frac{\delta \Gamma[\rho]}{\delta \rho(\mathbf{x})} \xrightarrow{J \rightarrow 0} \left. \frac{\delta \Gamma[\rho]}{\delta \rho(\mathbf{x})} \right|_{\rho_{\text{gs}}(\mathbf{x})} = 0 \implies \text{variational } F_{\text{HK}}[\rho] \quad (?)$$

# DFT and effective actions (Fukuda et al., Polonyi, ...)

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

Legendre transform  $\implies \Gamma[M] = F[H] + HM$

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



source magnet

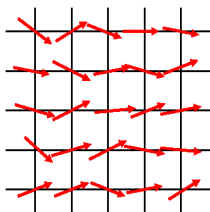
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source magnet

- Partition function with sources ( $J \rightarrow v$ ) that adjust (any) densities:

$$\mathcal{Z}[v] = e^{-W[v]} \sim \text{Tr} e^{-\beta(\hat{H} + v\hat{\rho})} \implies \text{e.g., path integral for } W[v]$$

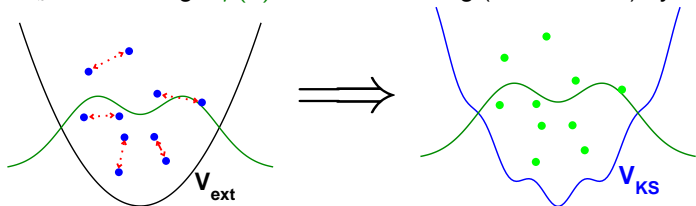
- Invert* to find  $v[\rho]$  and Legendre transform from  $v$  to  $\rho$ :

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

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

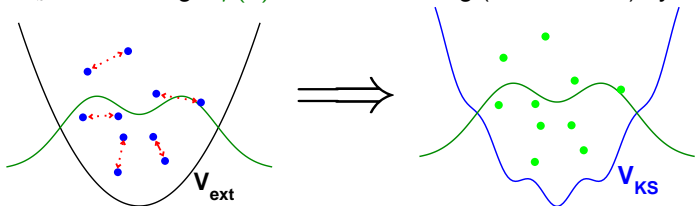
## Construct $W[v]$ and then $\Gamma[\rho]$ order-by-order

- Need a diagrammatic *expansion* (e.g., MBPT or EFT)
- **Inversion method**  $\implies$  Split source  $v(\mathbf{x}) = V_{\text{KS}} + v_1 + v_2 + \dots$ 
  - $V_{\text{KS}}$  *chosen* to get  $\rho(\mathbf{x})$  in noninteracting (Kohn-Sham) system:



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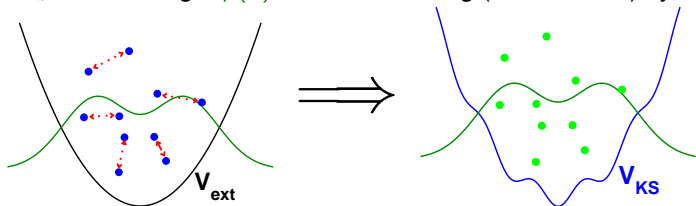
- Orbitals  $\{\psi_\alpha(\mathbf{x})\}$  in **local** potential  $V_{\text{KS}}([\rho], \mathbf{x})$

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

- Self-consistency from  $v(\mathbf{x}) \rightarrow v_{\text{ext}}(\mathbf{x}) \implies V_{\text{KS}}(\mathbf{x}) \propto \delta\Gamma_{\text{int}}[\rho]/\delta\rho(\mathbf{x})$

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- Alternative: Do MBPT with **single particle potential**  $U(\mathbf{x})$  and  $H = (T + U) + (V - U + v_{\text{ext}})$  **and choose**  $U = V_{\text{KS}}$  (no  $\Delta\rho(\mathbf{x})$ )

# 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  $\psi^\dagger \psi^\dagger \implies$  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)  
 $\implies$  BCS weak-coupling gap equation with gap  $\Delta$
  - Can we construct a Kohn-Sham DFT this way? ph channel?

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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 **local** Kohn-Sham DFT (Bulgac et al.)
  - cf. DFT with nonlocal source (Oliveira et al.; Kurth et al.)

# Outline

Overview: Pairing in EFT/DFT

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## Local composite effective action with pairing

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

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

- Densities found by functional derivatives wrt  $J, j$ :

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

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

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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 more

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

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

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

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

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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  $\lambda$

diagrams  $\implies W[J, j, \lambda] = W_0[J, j] + \lambda W_1[J, j] + \lambda^2 W_2[J, j] + \dots$

assume  $\implies J[\rho, \phi, \lambda] = J_0[\rho, \phi] + \lambda J_1[\rho, \phi] + \lambda^2 J_2[\rho, \phi] + \dots$

assume  $\implies j[\rho, \phi, \lambda] = j_0[\rho, \phi] + \lambda j_1[\rho, \phi] + \lambda^2 j_2[\rho, \phi] + \dots$

derive  $\implies \Gamma[\rho, \phi, \lambda] = \Gamma_0[\rho, \phi] + \lambda \Gamma_1[\rho, \phi] + \lambda^2 \Gamma_2[\rho, \phi] + \dots$

- Start with exact expressions for  $\Gamma$  and  $\rho$

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

$\implies$  plug in expansions with  $\rho, \phi$  treated as order unity

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- 0<sup>th</sup> 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**

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

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

- Diagonalize with single-particle orbitals (cf. HFB with gap  $j_0$ )

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

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

# Diagrammatic expansion of $W_i$

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

$$\Gamma_{\text{int}} = \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} + \dots$$

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

- Extra diagrams enforce inversion (here removes anomalous)
- In frequency space, the Kohn-Sham Green's functions are

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

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

# 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  $\mu_0$  is fixed by  $\int \rho(\mathbf{x}) = A$
- Diagrams for  $\Gamma[\rho, \phi] \propto E_0[\rho, \phi] + E_{\text{int}}[\rho, \phi]$  yields KS potentials

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

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# Outline

Overview: Pairing in EFT/DFT

Kohn-Sham DFT with pairing from effective action

**Renormalization issues**

Going forward: ideas, questions, tools

## 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!  
 $\implies$  must absorb (and correct) sensitivity by renormalization
- Instances of UV divergences

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- Can we consistently renormalize within inversion method?
- Strategy: Verify renormalization using scale parameter  $\Lambda$

# Divergences: uniform dilute Fermi system

- Generating functional with constant sources  $\mu$  and  $j$ :

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

- cf. adding integration over auxiliary field  $\int D(\Delta^*, \Delta) e^{-\frac{1}{|C_0|} \int |\Delta|^2}$   
 $\implies$  shift variables to eliminate  $\psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow$  for  $\Delta^* \psi_\uparrow \psi_\downarrow$

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- Renormalization: Add counterterm  $\frac{1}{2} \zeta |j|^2$  to  $\mathcal{L}$  (cf. Zinn-Justin)
  - Additive to  $W$  (cf.  $|\Delta|^2$ )  $\implies$  no effect on scattering
  - How to determine  $\zeta$ ? Energy interpretation of  $\Gamma$ ?

## Use dimensional regularization (DR)

- Generalize Papenbrock & Bertsch DR/MS calculation
- DR/PDS  $\implies$  generate explicit  $\Lambda$  to “check” renormalization
  - Basic free-space integral in  $D$  spatial dimensions

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

- Renormalizing free-space scattering yields:

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

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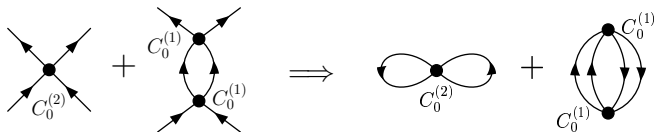
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- Recover DR/MS with  $\Lambda = 0$
- E.g., verify NLO renormalization  $\implies$  independent of  $\Lambda$



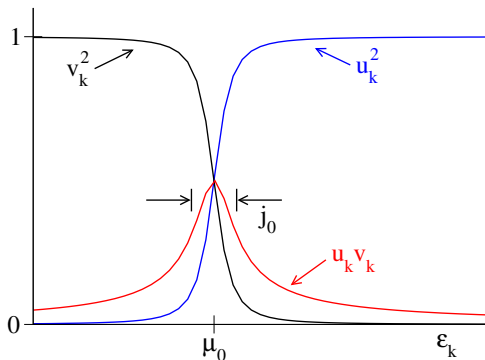
# Kohn-Sham non-interacting system

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$$\begin{aligned}\rho &= -\frac{1}{\beta V} \frac{\partial W_0[\rho]}{\partial \mu_0} = \frac{2}{V} \sum_{\mathbf{k}} v_k^2 \\ &= \int \frac{d^3 k}{(2\pi)^3} \left( 1 - \frac{\epsilon_k^0 - \mu_0}{E_k} \right)\end{aligned}$$

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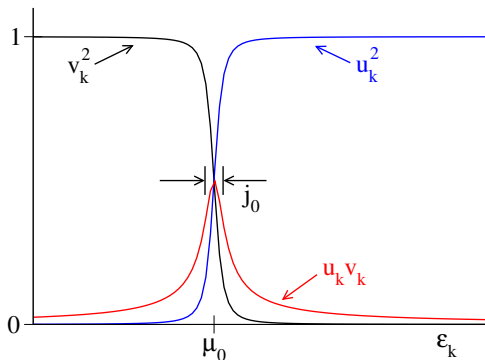
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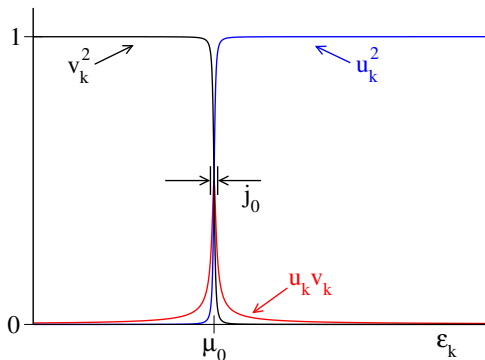
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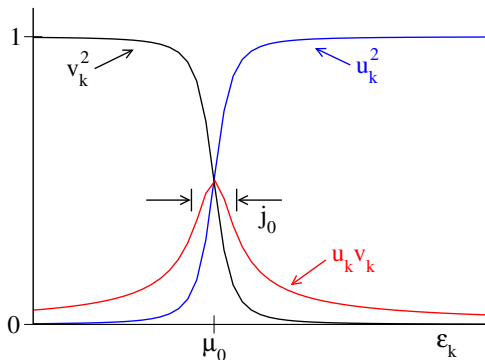
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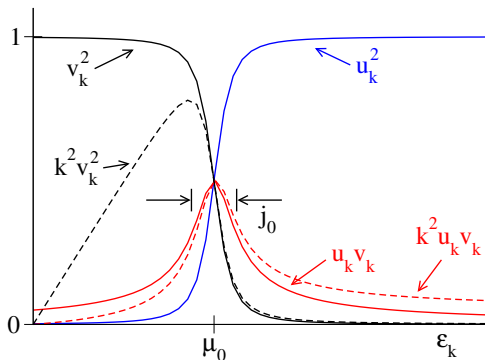
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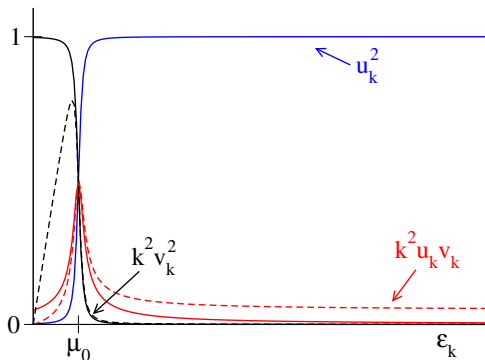
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- The basic DR/PDS integral in  $D$  dimensions, with  $x \equiv j_0/\mu_0$ , is

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

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

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## Calculating to $n^{\text{th}}$ Order

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

$$\Gamma_{\text{int}} = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \text{[diagram 4]} + \dots$$

- Calculate  $\mu_i, j_i$  from  $\Gamma_i$ , then use  $\sum_{i=0}^n j_i = j \rightarrow 0$  to find  $j_0$
- Renormalization conditions:**
  - No freedom in choosing  $C_0(\Lambda) \implies \Lambda$ 's must cancel!
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- Leading order: Diagrams for  $\Gamma_1[\rho, \phi] = W_1[\mu_0(\rho, \phi), j_0(\rho, \phi)]$

$$\Gamma_1 = \underbrace{\text{[diagram 1]}}_{\Sigma_k v_k^2 \quad \Sigma_{k'} v_{k'}^2} + \underbrace{\text{[diagram 2]}}_{\Sigma_k u_k v_k \quad \Sigma_{k'} u_{k'} v_{k'}} + \underbrace{\text{[diagram 3]}}_{\delta Z_j^{(1)} j_0 \phi_B} + \underbrace{\text{[diagram 4]}}_{\frac{1}{2} \zeta^{(1)} j_0^2} + \dots$$

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

# The “gap” equation at leading order (LO)

- $\Gamma_1$  dependence on  $\rho$  and  $\phi$  explicit  $\implies$  easy to find  $\mu_1$  and  $j_1$ :

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

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

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

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

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

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

$$1 = \sqrt{2M\mu_0} a_s (1+x^2)^{1/4} P_{1/2}^0 \left( \frac{-1}{\sqrt{1+x^2}} \right) \xrightarrow{x \rightarrow 0} k_F a_s \left[ \frac{4 - 6 \log 2}{\pi} + \frac{2}{\pi} \log x \right]$$

$$\implies \text{if } k_F a_s < 1, \frac{j_0}{\mu_0} = \frac{8}{e^2} e^{-\pi/2 k_F |a_s|} \text{ holds}$$

# 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  $\Lambda$  dependence:

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

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

- To find the energy density, evaluate  $\Gamma$  at the stationary point  $j_0 = -\frac{1}{2} |C_0^{(1)}| \phi$  with  $\mu_0$  fixed by the equation for  $\rho$   
 $\implies$  same results as Papenbrock/Bertsch (plus HF term)

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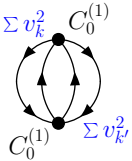
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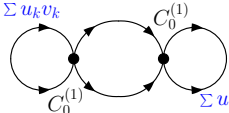
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- To find the energy density, evaluate  $\Gamma$  at the stationary point  $j_0 = -\frac{1}{2} |C_0^{(1)}| \phi$  with  $\mu_0$  fixed by the equation for  $\rho$   
 $\implies$  same results as Papenbrock/Bertsch (plus HF term)
- Life gets more complicated at NLO
  - dependence of  $\Gamma_2$  on  $\rho, \phi$  is no longer explicit
  - analytic formulas for DR integrals not available

## $\Gamma_2$ at next-to-leading order (NLO)



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



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

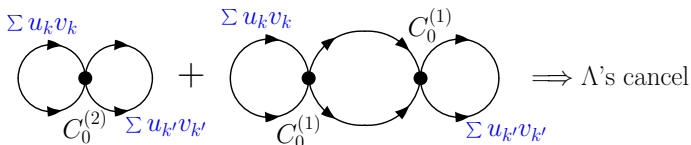
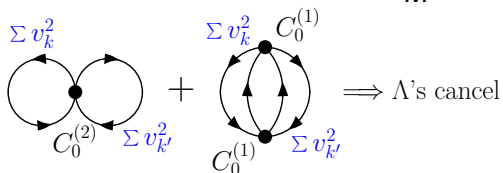
- UV divergences identified from

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

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

# Next-to-leading-order (NLO) renormalization

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



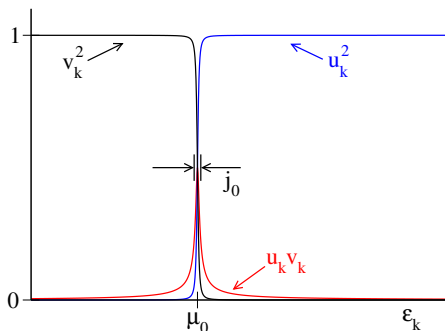
(Note that  $\delta Z_j^{(1)}$  vertex takes  $\phi_B \rightarrow \phi$ )

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

# Standard induced interaction result recovered

- Look at  $j_0 \Leftrightarrow \Delta$
- As  $j_0 \rightarrow 0$ ,  $u_k v_k$  peaks at  $\mu_0$
- Leading order  $T = 0$ :

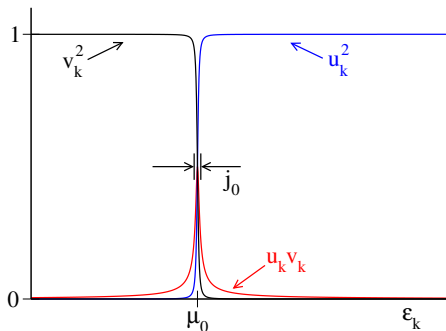
$$\begin{aligned} \Delta_{LO}/\mu_0 &= \frac{8}{e^2} e^{-1/N(0)|C_0|} \\ &= \frac{8}{e^2} e^{-\pi/2k_F|a_s|} \end{aligned}$$



$$\Gamma_1 = \underbrace{\text{Diagram}}_{\Sigma_k u_k v_k \quad \Sigma_{k'} u'_k v'_k} + CTC + \dots \implies j_1 = \frac{\delta \Gamma_1}{\delta \phi} = \frac{1}{2} |C_0| \phi$$

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



$$\Gamma_1 + \Gamma_2 = \begin{array}{c} \text{Diagram 1: Two circles sharing a central dot. Left circle has counter-clockwise arrow, right circle has clockwise arrow. Labels: } \Sigma u_k v_k \text{ (left), } \Sigma u'_k v'_k \text{ (right)} \\ + \text{Diagram 2: Two circles sharing a central dot. Left circle has counter-clockwise arrow, right circle has clockwise arrow. Red double-headed arrows connect the dots. Labels: } \Sigma u_k v_k \text{ (left), } \Sigma u'_k v'_k \text{ (right)} \end{array} \implies j_1 + j_2 = \frac{1}{2} |C_0| \left[ 1 - |C_0| \langle \Pi_0 \rangle_{|\mathbf{k}|=|\mathbf{k}'|=k_F} \right] \phi$$

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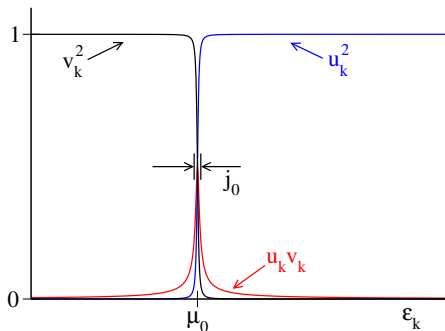
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$$\Gamma_1 + \Gamma_2 = \begin{array}{c} \text{Diagram 1: Two circles sharing a central dot, with arrows forming a loop.} \\ \Sigma u_k v_k \quad \Sigma u'_k v'_k \end{array} + \begin{array}{c} \text{Diagram 2: Two circles sharing a central dot, with arrows forming a loop.} \\ \Sigma u_k v_k \quad \Sigma u'_k v'_k \end{array} \Rightarrow j_1 + j_2 = \frac{1}{2} |C_0| \left[ 1 - |C_0| \langle \Pi_0 \rangle_{|\mathbf{k}|=|\mathbf{k}'|=k_F} \right] \phi$$

- 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  $\Lambda$

$\implies$  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

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

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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  $\rho_s = \sum_i \bar{\psi}(\mathbf{x})\psi(\mathbf{x})$  for relativistic mft

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- cf. scalar density  $\rho_s = \sum_i \bar{\psi}(\mathbf{x})\psi(\mathbf{x})$  for relativistic mft
- Usual plan: Subtracted expression for  $\phi$  in uniform system

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

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

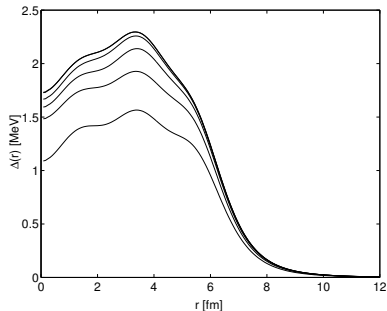
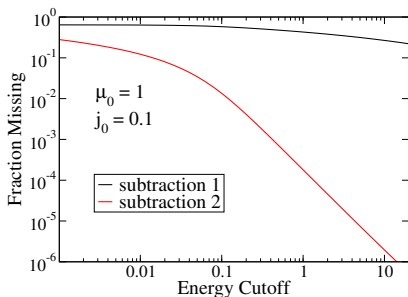
$$\phi(\mathbf{x}) = 2 \sum_i^{E_c} u_i(\mathbf{x})v_i(\mathbf{x}) - j_0(\mathbf{x}) \frac{M k_c(\mathbf{x})}{2\pi^2} \quad \text{with} \quad E_c = \frac{k_c^2(\mathbf{x})}{2M} + J(\mathbf{x}) - \mu_0$$

## Bulgac/Yu renormalization [PRL 88 (2002) 042504]

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

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

- Compare convergence in uniform system, in nuclei with LDA



- How do we generalize? Are RHA/soliton vacuum methods useful?

# Outline

Overview: Pairing in EFT/DFT

Kohn-Sham DFT with pairing from effective action

Renormalization issues

**Going forward: ideas, questions, tools**

# Laundry list of EFT/DFT pairing issues

- Questions:
  - To what extent is an EDF unique? Kohn-Sham gap? (and so on)
  - Can we motivate/constrain ASLDA near the unitary limit?
  - For nuclei, do we want/need to include the pion explicitly?
- Ideas from other contexts:
  - Alternative (Kohn-Sham) DFT — e.g., auxiliary fields, non-local
  - Beyond quasi-local: orbital-based methods for long-range correlations (cf., RPA with OEP in Coulomb systems)
- Tools/methods:
  - Renormalized sums in finite systems (from RHA/soliton studies)
  - Operator Product Expansion (e.g., cancellation of divergences)
  - Collective coordinate methods (e.g., BRST invariance)

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# Uniqueness of EDF's from EFT effective action

- What is the dependence of an energy density functional on the EFT representation or regularization or an RG  $\Lambda$ ?
- Appeal to authority: Zinn-Justin on observable quantities

$$e^{-W[J]} = \int [d\phi] e^{-S(\phi)+J\phi} = e^{-\Gamma[\varphi]+J\varphi}, \quad \varphi \equiv \langle \phi \rangle = \delta W / \delta J, \quad J = \delta \Gamma / \delta \varphi$$

$$e^{-\Gamma[\varphi]} = \int [d\phi] e^{-S(\phi) + \int dx (\phi(x) - \varphi(x)) \frac{\delta \Gamma}{\delta \varphi(x)}} \xrightarrow{\text{shift}} e^{-\Gamma[\varphi_c]} = \int [d\phi] e^{-S(\phi + \varphi_c)}$$

- Effective action evaluated at the **stationary point** is independent of the representation of the fields  $\phi'(x) = \sum_{k=1}^{\infty} C_k \phi^k(x)/k!$
- These are the “on shell” points; invariance is analogous to independence of the S-matrix to interpolating field
- Use field redefinitions to illustrate this point
- Consequences for DFT from EFT effective action
  - “Universal” does not mean unique!
  - What about LDA?

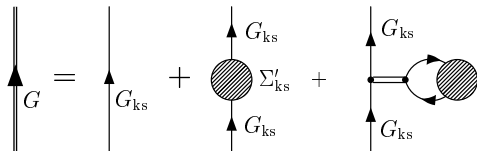
# Kohn-Sham pairing questions

- How are the Kohn-Sham “gap” and gap  $\Delta(\mathbf{q})$  related?
  - “Conventional” gap function from anomalous Green’s function:

$$\Delta(\mathbf{q}) = - \int \frac{d^4 k}{(2\pi)^4} V(\mathbf{q} - \mathbf{k}) \mathcal{F}_0(k_0, \mathbf{k}) e^{ik_0\eta}$$

- Kohn-Sham Green’s function vs. full Green’s function [more](#)

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



- When do we need the “real” gap from Green’s function?
- What about the gap from odd-even mass staggering?

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## Can EFT/DFT give insight into form of ASLDA?

- Simplified but phenomenologically successful ASLDA structure motivated by Bulgac and Forbes [arXiv:0808.1436]

$$E = \int d\mathbf{x} \left\{ \mathcal{E}[n_{a,b}(\mathbf{x}), \tau_{a,b}(\mathbf{x}), \nu(\mathbf{x})] + V_{\text{ext}}(\mathbf{x})[n_a(\mathbf{x}) + n_b(\mathbf{x}) + \text{sources} \dots] \right\}$$

$$\mathcal{E}[n_{a,b}, \tau_{a,b}, \nu] = \alpha_a(n_a, n_b) \frac{\tau_a}{2} + \alpha_b(n_a, n_b) \frac{\tau_b}{2} + D(n_a, n_b) + g_{\text{eff}}(n_a, n_b) \nu^* \nu$$

- Cancellation of divergences? ( $\alpha_a \tau_a / 2 + \alpha_b \tau_b / 2 - \Delta^* \nu$  is finite)
- Additional support for neglecting gradient terms?
- Power counting functionals of  $[(\alpha_a \tau_a + \alpha_b \tau_b) / 2 - \Delta^* \nu] / n^{5/3}$
- Decoupling of paired and normal states? (e.g., neglect of  $n$  dependence of pairing)
- Justification for semi-local form?

# Effective Field Theory ingredients for EFT( $\not{t}$ )

Low-energy QCD (nuclear physics) but no pions ...

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

- $\mathcal{L}_{\text{eft}} = \psi^\dagger \left[ i \frac{\partial}{\partial t} + \frac{\nabla^2}{2M} \right] \psi - \frac{C_0}{2} (\psi^\dagger P \psi)^2 - \frac{D_0}{6} (\psi^\dagger \psi)^3 + \dots$
- $P$  is a (schematic) spin/isospin projector

**2** Declaration of regularization and renormalization scheme

- dimensional (DR/PDS) and cutoff regularization both work
- unnatural  $a_0 \gg R \implies$  If it is to be a low-energy scale  $\implies$  nonperturbative renormalization

**3** Well-defined power counting  $\implies$  small expansion parameter

- use separation of scales  $\implies \frac{k}{\Lambda_b} \ll 1$  with  $\Lambda_b \sim m_\pi$
- $k|a_0| > 1 \implies$  leading order: sum **all** diagrams with just  $C_0$ 's
- Is there an additional counting for finite density? ( $1/N, \epsilon, \dots$ )

Same setup for an EFT for cold atoms!

## EFT/DFT in unitarity limit

- Only one paper? Rupak/Schäfer, Nucl. Phys. **816** (2009)
  - Not Kohn-Sham and has normal density  $\rho$  only  
 $\implies$  no pairing or kinetic energy density
- Work to NLO in gradient expansion
- Match to  $\epsilon$  expansion about  $d = 4 - \epsilon$  spatial dimensions:

$$\mathcal{E}(x) = n(x)v_{\text{ext}}(x) + 1.364 \frac{n(x)^{5/3}}{m} + 0.022 \frac{[\nabla n(x)]^2}{m n(x)} + \mathcal{O}(\nabla^4 n)$$

- Comparison to “extended Thomas-Fermi” for free nucleons:

$$\mathcal{E}_{\text{ETF}}(x) = n(x)v_{\text{ext}}(x) + 2.871 \frac{n(x)^{5/3}}{m} + 0.014 \frac{[\nabla n(x)]^2}{m n(x)} + \mathcal{O}(\nabla^4 n)$$

- Extension to motivate/justify form of ASLDA?
  - Use  $\epsilon$  or  $1/N$  expansion but with sources coupled to  $\rho$ ,  $\tau$ ,  
*and* pairing density
  - Apply inversion method

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# Effective Field Theory Ingredients

See, e.g., Epelbaum et al., Rev. Mod. Phys. **81**, 1773 (2009)

- 1** Use the most general  $\mathcal{L}$  with low-energy dof's consistent with the global and local symmetries of the underlying theory
- 2** Declaration of regularization and renormalization scheme
- 3** Well-defined power counting  $\implies$  expansion parameters

# Effective Field Theory Ingredients: Chiral NN

See, e.g., Epelbaum et al., Rev. Mod. Phys. **81**, 1773 (2009)

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

- $\mathcal{L}_{\text{eft}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN}$
- chiral symmetry  $\implies$  systematic long-distance pion physics

**2** Declaration of regularization and renormalization scheme

- momentum cutoff and “Weinberg counting” (still open!)  
 $\implies$  define irreducible potential and sum with LS eqn
- use cutoff sensitivity as measure of uncertainties

**3** Well-defined power counting  $\implies$  expansion parameters

- use the separation of scales  $\implies \frac{\{\mathbf{p}, m_\pi\}}{\Lambda_\chi}$  with  $\Lambda_\chi \sim 1 \text{ GeV}$
- chiral symmetry  $\implies V_{NN} = \sum_{\nu=\nu_{\min}}^{\infty} c_\nu Q^\nu$  with  $\nu \geq 0$
- naturalness: LEC's are  $\mathcal{O}(1)$  in appropriate units

# Long-range chiral EFT

$\implies$  **enhanced Skyrme**

- Add long-range ( $\pi$ -exchange) contributions in the density matrix expansion (DME)
  - NN/NNN through  $N^2\text{LO}$  [Gebremariam et al.]
- Refit Skyrme parameters for short-range parts
- Test for sensitivities and improved observables (e.g., isotope chains) [ORNL]
- Spin-orbit couplings from  $2\pi$  3NF particularly interesting
- Can we “see” the pion in medium to heavy nuclei?

		NN	3N	4N
LO	$\mathcal{O}\left(\frac{Q^0}{\Lambda^0}\right)$			
NLO	$\mathcal{O}\left(\frac{Q^2}{\Lambda^2}\right)$			
N <sup>2</sup> LO	$\mathcal{O}\left(\frac{Q^3}{\Lambda^3}\right)$			
N <sup>3</sup> LO	$\mathcal{O}\left(\frac{Q^4}{\Lambda^4}\right)$			
		+ ...	+ ...	+ ...

# Laundry list of EFT/DFT pairing issues

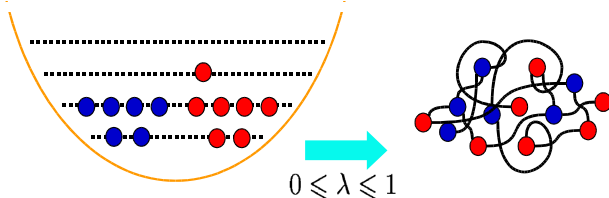
- Questions:
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## Better alternatives to local Kohn-Sham?

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

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

- CJT 2PI effective action  $\Gamma[\rho, \Delta]$  with  $\Delta(x, x') = \langle \psi_{\uparrow}(x)\psi_{\downarrow}(x') \rangle$ ?
- DFT from Renormalization Group (J. Braun, Polonyi-Schwenk)



- Auxiliary fields: Introduce  $\hat{\Delta}^*(x)\psi(x)\psi(x) + \text{H.c.}$  via H.S.
  - 1PI effective action in  $\Delta(x) = \langle \hat{\Delta}(x) \rangle$
  - Special saddle point evaluation  $\implies$  Kohn-Sham DFT

# HS decoupling in the Coulomb problem

From Atland and Simons “Condensed Matter Field Theory”:

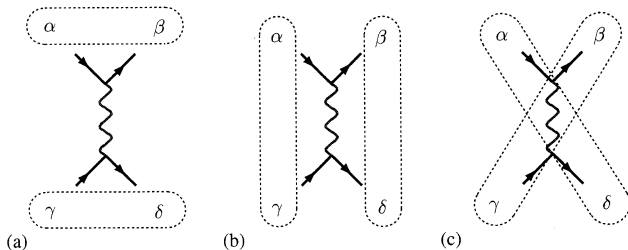


Figure 6.1 On the different channels of decoupling an interaction by Hubbard–Stratonovich transformation. (a) Decoupling in the “density” channel; (b) decoupling in the “pairing” or “Cooper” channel; and (c) decoupling in the “exchange” channel.

- May want to decouple in all three channels with  $q \ll |p_i|$ :

$$S_{\text{int}}[\bar{\psi}, \psi] \approx \frac{1}{2} \sum_{p, p', q} \left( \bar{\psi}_{\sigma p} \psi_{\sigma p+q} V(\mathbf{q}) \bar{\psi}_{\sigma' p'} \psi_{\sigma' p'-q} - \bar{\psi}_{\sigma p} \psi_{\sigma' p+q} V(\mathbf{p}' - \mathbf{p}) \bar{\psi}_{\sigma' p'+q} \psi_{\sigma' p'} \right. \\ \left. - \bar{\psi}_{\sigma p} \bar{\psi}_{\sigma' -p+q} V(\mathbf{p}' - \mathbf{p}) \psi_{\sigma' p'} \psi_{\sigma' -p'+q} \right)$$

## Auxiliary Fields [Faussurier]

- Introduce scalar field  $\varphi$  coupled to  $\psi^\dagger\psi$
- Construct  $\tilde{S}[\psi^\dagger, \psi, \varphi]$  such that  $\psi, \psi^\dagger$  is only in  $\psi^\dagger[G^{-1}(\varphi)]\psi$  and

$$\int \mathcal{D}\varphi e^{i\tilde{S}[\psi^\dagger, \psi, \varphi]} \implies e^{iS[\psi^\dagger, \psi]}$$

- Integrate out  $\psi^\dagger\psi \implies$  determinant  $\implies \text{Tr} \ln[G^{-1}(\varphi)] + \dots$
- Keep only leading saddle point  $\phi_0(\mathbf{x}) \implies$  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  $\phi_{xc}$  such that  $-\text{Tr} G_{xc}(x, x^+) = n(\mathbf{x})$
  - expand  $\text{Tr} \ln[G_{xc}^{-1} + \delta\phi]$  in  $\delta\phi = \phi - \phi_{xc}$   
 $\implies \Gamma_{xc}[n]$  with  $\phi_{xc}(\mathbf{x}) = \delta\Gamma_{xc}[n]/\delta n(\mathbf{x})$
  - introduce orbitals  $\{\psi_\alpha, \epsilon_\alpha\}$  to diagonalize  $\text{Tr} \ln[G_{xc}^{-1}]$

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## Orbital Dependent DFT (OEP, OPM, ...) [J. Drut, L. Platter, rjf]

- Expansion for  $E_{\text{int}}[\rho, \tau, \mathbf{J}, \dots]$ ; densities are sums over orbitals solving from Kohn-Sham S-eqn with  $V_{\text{KS}}(\mathbf{r}), \dots$
- Self-consistency  $\implies V_{\text{KS}}(\mathbf{r}) = \delta E_{\text{int}}[\rho, \dots] / \delta \rho(\mathbf{r}), \dots$ 
  - i.e., Kohn-Sham potential is functional derivative of interacting energy functional (or  $E_{\text{xc}}$ ) wrt (all) densities
  - How do we calculate this functional derivative?
- Approximations with **explicit**  $\rho(\mathbf{r})$  dependence: LDA, **DME**, ...

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- Approximations with **explicit**  $\rho(\mathbf{r})$  dependence: LDA, DME, ...
- Orbital-dependent DFT  $\implies$  full derivative via chain rule:

$$V_{\text{KS}}(\mathbf{r}) = \frac{\delta E_{\text{int}}[\phi_{\alpha}, \varepsilon_{\alpha}]}{\delta \rho(\mathbf{r})} = \int d\mathbf{r}' \frac{\delta V_{\text{KS}}(\mathbf{r}')}{\delta \rho(\mathbf{r})} \sum_{\alpha} \left\{ \int d\mathbf{r}'' \left[ \frac{\delta \phi_{\alpha}^{\dagger}(\mathbf{r}'')}{\delta V_{\text{KS}}(\mathbf{r}')} \frac{\delta E_{\text{int}}}{\delta \phi_{\alpha}^{\dagger}(\mathbf{r}'')} + \text{c.c.} \right] + \frac{\delta \varepsilon_{\alpha}}{\delta V_{\text{KS}}(\mathbf{r}')} \frac{\partial E_{\text{int}}}{\partial \varepsilon_{\alpha}} \right\}$$

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

$$\int d^3 r' \chi_s(\mathbf{r}, \mathbf{r}') V_{\text{KS}}(\mathbf{r}') = \Lambda_{\text{xc}}(\mathbf{r})$$

- $\Lambda_{\text{xc}}(\mathbf{r})$  is functional of the orbitals  $\phi_{\alpha}$ , eigenvalues  $\varepsilon_{\alpha}$ , and  $G_{\text{KS}}^0$

# Correlations beyond LDA: Coulomb RPA with OEP

- See Kummel and Kornik RMP article for examples/references
- RPA functional (simplified with KS dynamic response  $\chi_{\text{KS}}$ )

$$E_{\text{xc}} = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \int_0^1 d\lambda \left( -\frac{1}{\pi} \int_0^\infty d\omega \text{Im} \chi_{\text{KS}}(\mathbf{r}, \mathbf{r}', \omega) - n(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') \right)$$

$$\chi_{\text{KS}}(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\sigma=\uparrow, \downarrow} \sum_{j,k} (f_{k,\sigma} - f_{j,\sigma}) \frac{\phi_{j,\sigma}(\mathbf{r})\phi_{k,\sigma}^*(\mathbf{r})\phi_{j,\sigma}^*(\mathbf{r}')\phi_{k,\sigma}(\mathbf{r}')}{\omega - (\epsilon_{j,\sigma} - \epsilon_{k,\sigma}) + i\eta}$$

- Separate interaction into long- and short-range parts

$$\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} = \frac{\text{erf}(\mu|\mathbf{r}_i - \mathbf{r}_j|)}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1 - \text{erf}(\mu|\mathbf{r}_i - \mathbf{r}_j|)}{|\mathbf{r}_i - \mathbf{r}_j|}$$

- Treat short-range with semi-local density functional (DF) and long-range by non-local DF (or with CI)

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## Are RHA or soliton vacuum methods useful?

- Casimir energy sums in finite system analogous to pairing energy sum and  $\sum_{\alpha} \bar{\psi}(\mathbf{x})\psi(\mathbf{x})$  similar to  $\sum_{\alpha} u_{\alpha}^{*}(\mathbf{x})v_{\alpha}(\mathbf{x})$

$$E_{\text{vac}} \sim \sum_{\epsilon_i^0 < \Lambda} (\epsilon_i - \epsilon_i^0) + E_{\text{counterterms}}(\Lambda)$$

- Sum of energy differences with and without background field
- Many approaches to go beyond Thomas-Fermi approximation
- E.g., Wasson and Koonin, Phys. Rev. D **43**, 3400 (1991)
- Strategies:
  - Derivative expansion with functional methods (e.g., R. Perry)
  - WKB approximations for contribution of modes with energies above cutoff  $\implies$  accelerated convergence
  - and others in the literature . . .

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## Aside: Operator Product Expansion (OPE) more

- Energy for unitary gas with separately finite terms (Tan)

$$E = \sum_{\sigma} \int \frac{d^3k}{(2\pi)^3} \frac{k^2}{2m} \left( \rho_{\sigma}(\mathbf{k}) - \frac{C}{k^4} \right) + \frac{C}{4\pi m a_s} + \langle V \rangle$$

- “Contact”  $C$  appears in many relations
- OPE used by Braaten, Kang, Platter to extend Tan relations
  - In general:  $\mathcal{O}_A(\mathbf{R} - \frac{1}{2}\mathbf{r})\mathcal{O}_A(\mathbf{R} + \frac{1}{2}\mathbf{r}) = \sum_C C_{A,B}^C(\mathbf{r})\mathcal{O}_C(\mathbf{R})$
- Momentum distribution can be written

$$\rho_{\sigma}(\mathbf{k}) = \int d^3R \int d^3r e^{i\mathbf{k}\cdot\mathbf{r}} \langle X | \psi_{\sigma}^{\dagger}(\mathbf{R} - \frac{1}{2}\mathbf{r}) \psi_{\sigma}(\mathbf{R} + \frac{1}{2}\mathbf{r}) | X \rangle$$

- Apply OPE standard diagrammatic techniques to get:

$$\psi_{\sigma}^{\dagger}(\mathbf{R} - \frac{1}{2}\mathbf{r}) \psi_{\sigma}(\mathbf{R} + \frac{1}{2}\mathbf{r}) = \psi_{\sigma}^{\dagger} \psi_{\sigma}(\mathbf{R}) + \frac{1}{2} \mathbf{r} \cdot [\psi_{\sigma}^{\dagger} \nabla \psi_{\sigma}(\mathbf{R}) - \nabla \psi_{\sigma}^{\dagger} \psi_{\sigma}(\mathbf{R})] - \frac{r}{8\pi} g^2 \psi_1^{\dagger} \psi_2^{\dagger} \psi_2 \psi_1(\mathbf{R}) + \dots$$

- Power law in  $1/k$  from function of  $|\mathbf{r}|$
- Contact is finite:  $C = \int d^3R \langle X | g(\Lambda)^2 \psi_1^{\dagger} \psi_2^{\dagger} \psi_2 \psi_1(\mathbf{R}) | X \rangle$
- Use  $g(\Lambda) = -\frac{\Lambda}{2\pi^2} g^2 + \frac{1}{4\pi a_s} g^2$  to split into two terms

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# Collective coordinates and functional integrals

- What about dealing broken symmetries?
  - E.g., number projection for pairing
  - How to accommodate within effective action DFT framework?  
 $\implies$  consequences are zero-frequency modes (divergent perturbation expansion)
  - Transformation to collective variables  $\implies$  work with overcomplete dof's  $\implies$  system with constraints
  - "A theory with constraints is a gauge theory in the sense that it possesses a gauge symmetry which is generated by the constraints" [Müller-Kirsten/Zhang, PRD 50]
- Possible approach: use BRST invariance
  - E.g., Bes and Kurchan, "The treatment of collective coordinates in many-body systems: An application of the BRST invariance"
  - Add *more* fermionic variables (ghosts) so more overcomplete
  - Apparent complication is actually a simplification because in gauge systems there is a supersymmetry
  - Can procedure be adapted to DFT?

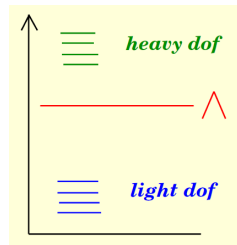
# Summary

- EFT + effective action formalism generates Kohn-Sham DFT with local pairing fields  $\implies$  systematic expansion
  - Consistent treatment of renormalization through NLO
  - Energy interpretation and ambiguities?
- Some of the more general open issues for EFT-based DFT
  - Auxiliary fields or other alternatives?
  - Quasi-local functionals vs. orbital-based functionals
  - Number projection (collective coordinates)
  - Renormalization in finite systems (convergence, induced interaction)
  - Implementing low-momentum potentials  $\implies$  Power counting

# Effective Field Theory Ingredients

Now QCD is the underlying theory ...

- 1** Use the most general  $\mathcal{L}$  with low-energy dof's consistent with global and local symmetries of underlying theory
    - What are the low-energy dof's for QCD?
    - What are the relevant symmetries?
  - 2** Declaration of regularization and renormalization scheme
    - What choices are there?
    - Will we be able to use dimensional regularization again?
  - 3** Well-defined power counting  $\implies$  small expansion parameter
    - Usually  $Q/\Lambda$ . What are the QCD scales?
- General procedures:
    - QFT: trees + loops  $\rightarrow$  renormalization
    - Include long-range physics explicitly
    - Short-distance physics captured in a few LEC's (calculated from underlying or fit to data). Check naturalness.



# Unraveling the magic of DFT [Kutzelnigg (2008)]

- Wavefunction-based: for anti-symmetric  $A$ -body  $|\Psi\rangle$ , find  $E_{gs} = \min_{\Psi} \langle \Psi | \hat{H} | \Psi \rangle$  (CI, CC use a single-particle basis for  $|\Psi\rangle$ )
- DFT: fermion densities as basic variables
  - Common but misleading statements:
    - “All information about a quantum mechanical ground state is contained in its electron density  $\rho$ .”
    - “The energy is completely expressible in terms of the density alone.”
  - At odds with kinetic and interaction energies needing  $(1, 2, \dots)$ -particle density matrices!

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  - At odds with kinetic and interaction energies needing  $(1, 2, \dots)$ -particle density matrices!
- Key: WF formulation deals with *single, fixed Hamiltonian*,  $E$  stationary to density matrix (or  $\Psi$ ) variations, not just  $\rho(\mathbf{x})$
- DFT: Consider a *family* of Hamiltonians  $\hat{H}[v] \rightarrow E[v]$ , then
 
$$F_{\text{HK}}[\rho] = \min_v \left\{ E[v] - \int d\mathbf{x} v(\mathbf{x}) \rho(\mathbf{x}) \right\} \text{ and}$$

$$E[v] = \min_{\rho} \left\{ F[\rho] + \int d\mathbf{x} v(\mathbf{x}) \rho(\mathbf{x}) \right\} \equiv \min_{\rho} \{ E_v[\rho] \}$$

## DFT as Legendre transform

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

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

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

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

⇒ This is our energy function!

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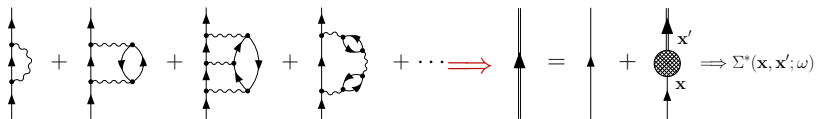
$\implies$  This is our energy function!

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

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

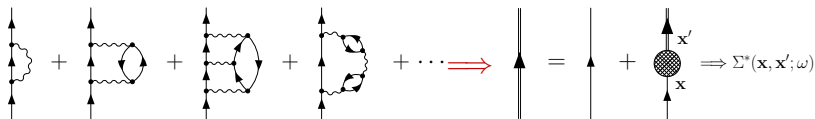
- LT from  $\ln Z[v(\mathbf{x})]$  to  $\Gamma[\rho(\mathbf{x})]$ , where  $\rho = \langle \psi^\dagger \psi \rangle_v \implies$  DFT!

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

[back](#)


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

back

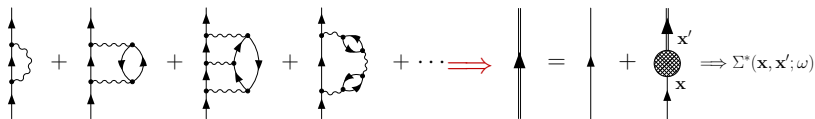


- Add a non-local source  $\xi(x', x)$  coupled to  $\psi(x)\psi^\dagger(x')$ :

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

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

back

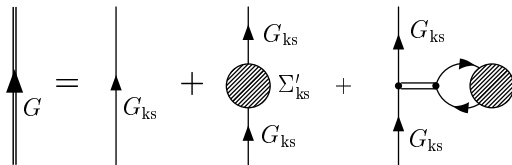


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- With  $\Gamma[\rho, \xi] = \Gamma_0[\rho, \xi] + \Gamma_{\text{int}}[\rho, \xi]$ ,

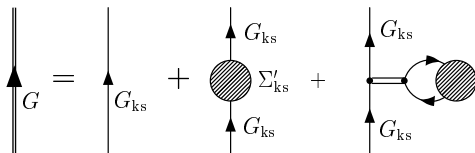
$$G(x, x') = \left. \frac{\delta W}{\delta \xi} \right|_J = \left. \frac{\delta \Gamma}{\delta \xi} \right|_\rho = G_{\text{ks}}(x, x') + G_{\text{ks}} \left[ \frac{1}{i} \frac{\delta \Gamma_{\text{int}}}{\delta G_{\text{ks}}} + \frac{\delta \Gamma_{\text{int}}}{\delta \rho} \right] G_{\text{ks}}$$



# $G$ and $G_{\text{KS}}$ Yield the Same Density by *Construction*

- Claim:  $\rho_{\text{KS}}(\mathbf{x}) = -i\nu G_{\text{KS}}^0(x, x^+)$  equals  $\rho(\mathbf{x}) = -i\nu G(x, x^+)$

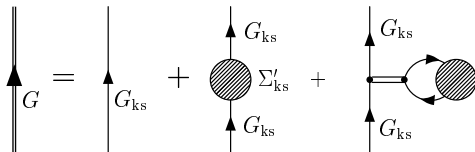
- Start with



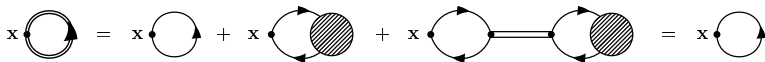
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- Simple diagrammatic demonstration:

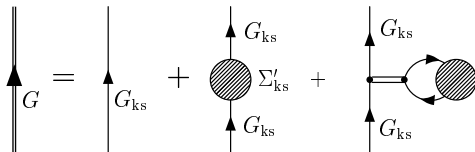


- Densities agree by construction!

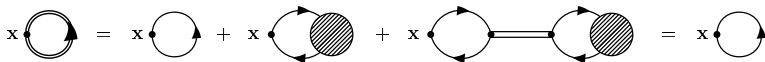
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- Start with



- Simple diagrammatic demonstration:



- Densities agree by construction!
- Is the Kohn-Sham basis a useful one for  $G$ ?
- Better single-particle energies with more sources

## Add Sources [Bhattacharyya, rjf, nucl-th/0408014]

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

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

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

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

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

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

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

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

## Beyond Kohn-Sham LDA: Kinetic energy density

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

$$E[\rho, \tau, \mathbf{J}] = \int d^3x \left\{ \frac{1}{2M} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho \tau \right. \\ \left. + \frac{1}{64} (9t_1 - 5t_2) (\nabla \rho)^2 - \frac{3}{4} W_0 \rho \nabla \cdot \mathbf{J} + \frac{1}{32} (t_1 - t_2) \mathbf{J}^2 \right\}$$

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- Two Kohn-Sham potentials:

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

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# First step: HF diagrams with $\nabla$ 's [nucl-th/0408014]

- Consider bowtie diagrams from vertices with derivatives:

$$\mathcal{L}_{\text{eft}} = \dots + \frac{C_2}{16} [(\psi\psi)^\dagger (\psi \overleftrightarrow{\nabla}^2 \psi) + \text{h.c.}] + \frac{C'_2}{8} (\psi \overleftrightarrow{\nabla} \psi)^\dagger \cdot (\psi \overleftrightarrow{\nabla} \psi) + \dots$$



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

$$\mathcal{E}_{\text{int}}[\rho] = \dots + \frac{C_2}{8} \left[ \frac{3}{5} \left( \frac{6\pi^2}{\nu} \right)^{2/3} \rho^{8/3} \right] + \frac{3C'_2}{8} \left[ \frac{3}{5} \left( \frac{6\pi^2}{\nu} \right)^{2/3} \rho^{8/3} \right] + \dots$$

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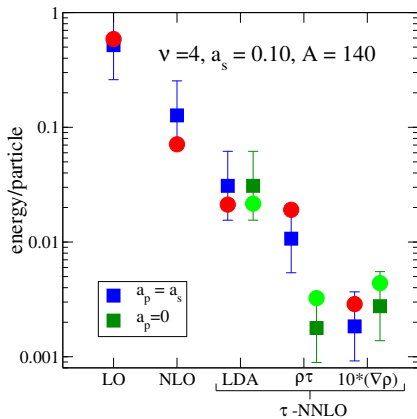
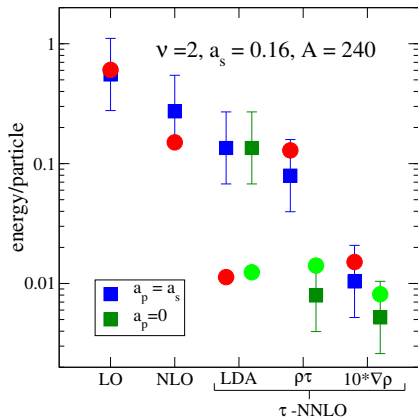
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- Energy density in Kohn-Sham with  $\tau$  ( $\nu = 2$ ):

$$\mathcal{E}_{\text{int}}[\rho, \tau] = \dots + \frac{C_2}{8} [\rho\tau + \frac{3}{4}(\nabla\rho)^2] + \frac{3C'_2}{8} [\rho\tau - \frac{1}{4}(\nabla\rho)^2] + \dots$$

# Power counting estimates work for gradients!



## Comparing Skyrme and dilute functionals

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

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

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

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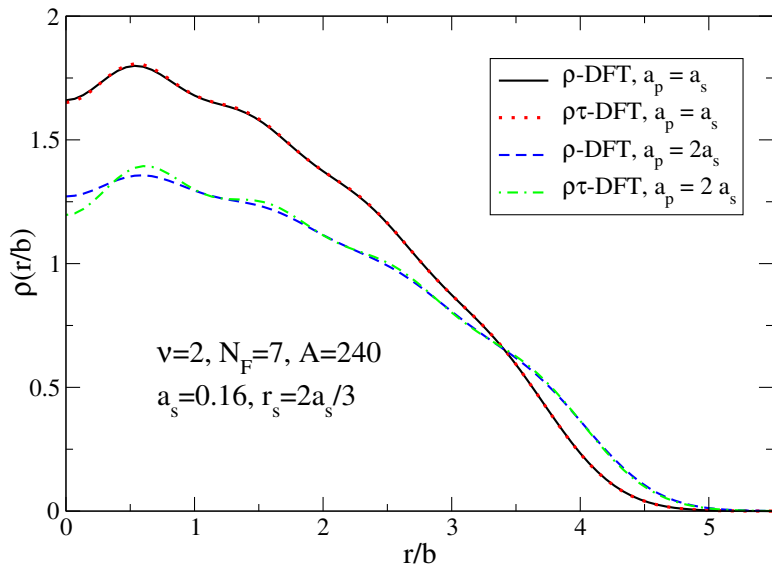
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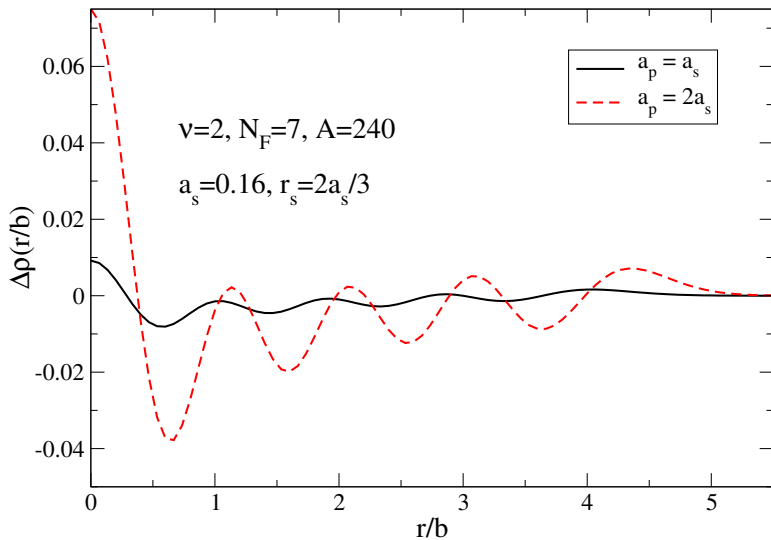
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- Same functional as dilute Fermi gas with  $t_i \leftrightarrow C_i$ 
  - equivalent  $a_s \approx -2-3$  fm but  $|k_F a_p|, |k_F r_0| < 1$  (with  $a_p < 0$ )
  - missing non-analytic terms, NNN, ...

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



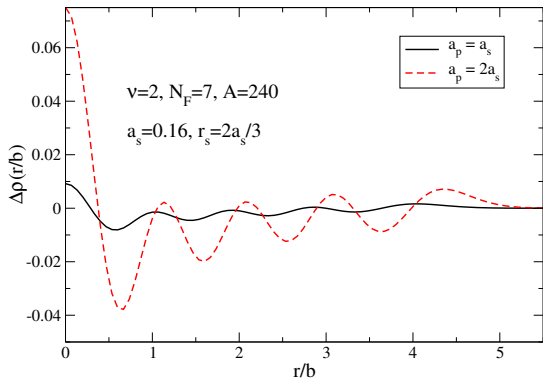
# Kohn-Sham LDA $\rho$ vs. $\rho_T$ [Anirban Bhattacharyya]



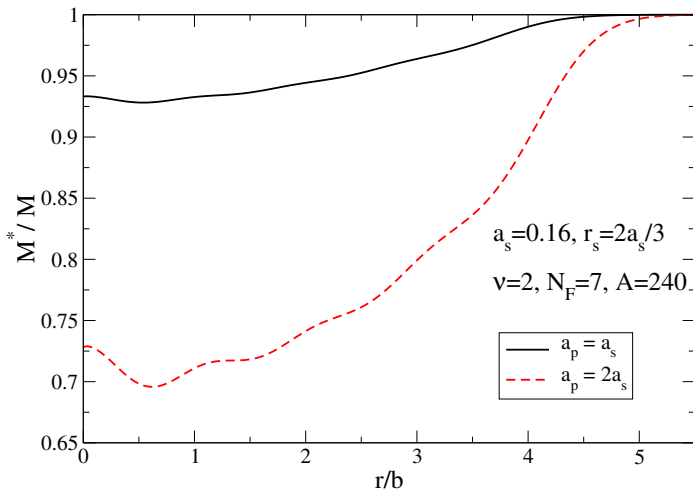
# Kohn-Sham LDA $\rho$ vs. $\rho\tau$ : Differences

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

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

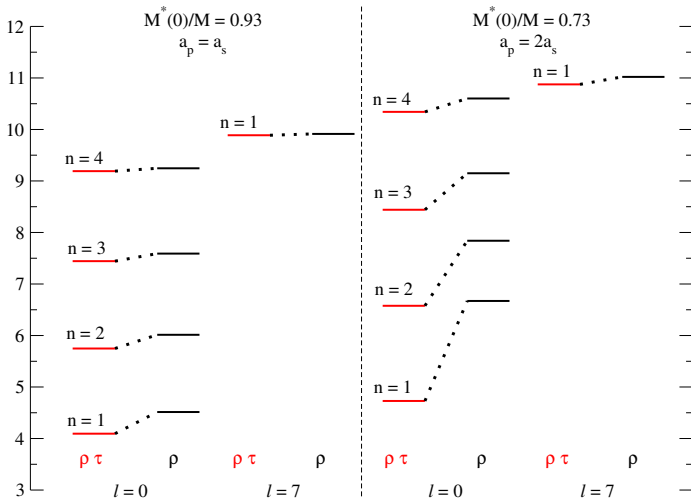


# Effective mass and the single-particle spectrum



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

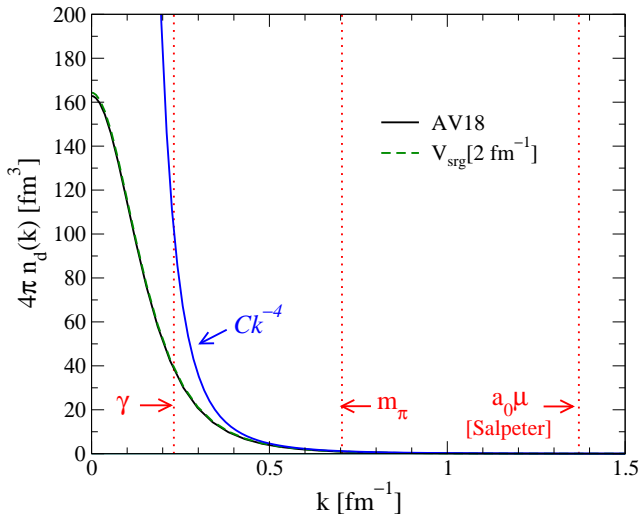
# Effective mass and the single-particle spectrum



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

# $1/k^4$ in deuteron momentum distribution?

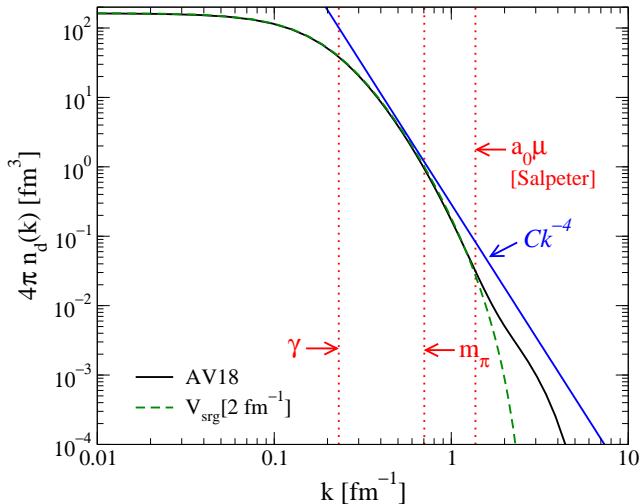
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Salpeter wave function:  $\phi(\mathbf{k}) \propto \frac{1}{(k^2 + \gamma^2)(k^2 + (a_0\mu)^2)}$

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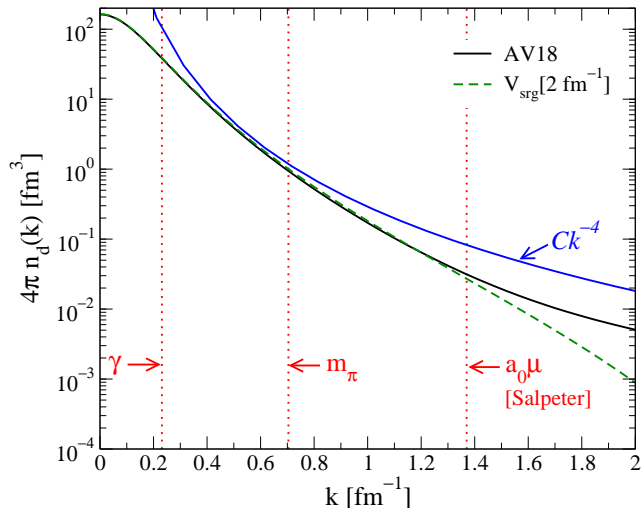
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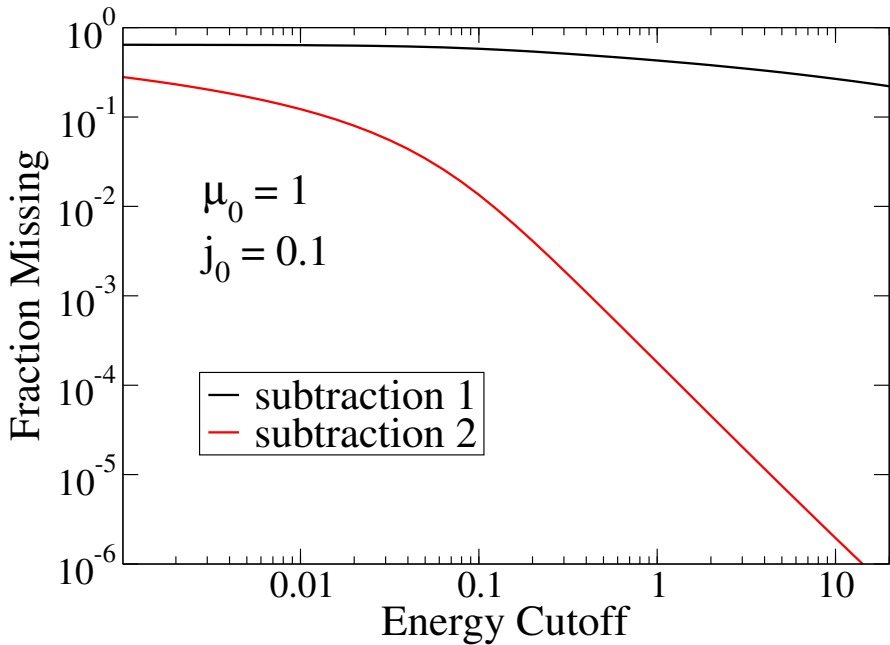
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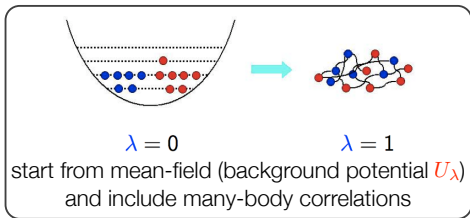


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# Density Functional RG for Nuclei

Density Functional:  $\Gamma_\lambda[\rho] = \ln \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S_\lambda[\psi^\dagger, \psi] + f \frac{\delta \Gamma_\lambda}{\delta \rho} \cdot (\psi^\dagger \psi)}$



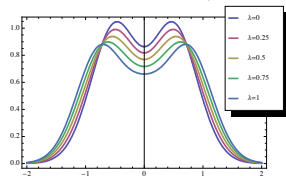
$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{2} V_{\text{low } k}$$

$\Gamma_\lambda[\rho]$  is the density functional

$$S_\lambda[\psi^\dagger, \psi] = \int \psi^\dagger \left[ \partial_t - \frac{1}{2m} \Delta + (1 - \lambda) U_\lambda \right] \psi + \frac{1}{2} \int \psi^\dagger \psi \lambda V_{\text{low } k} \psi^\dagger \psi$$

+ ( $\lambda V_{3N}$  will be included later)

- density basis expansion scales favorably to heavy nuclei
- allows for a calculation of ground-state energy and density from nuclear forces
- in production: results for  $^{16}\text{O}$



Example: RG flow of the ground-state density for 1d model ("smeared-out"  $\delta$ -function interaction)

# Energy Interpretation [back](#)

- 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)

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- Potential ambiguities in the renormalization
  - Arbitrary finite part of added counterterms  $\implies$  shift minima
  - Verschelde et al. claim not arbitrary
- Are the stationary points valid in any case?