DFT Pairing from Effective Actions

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Outline

Effective Actions and Pairing $\Longrightarrow$ Kohn-Sham DFT

Renormalization Issues

Open Questions

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Renormalization Issues

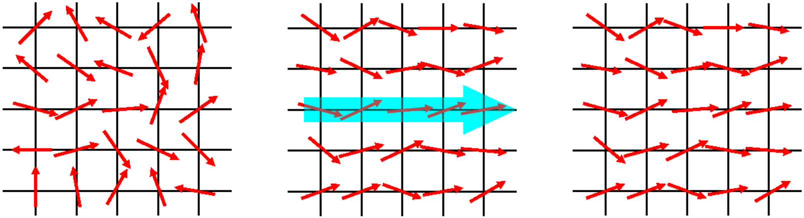
Open Questions

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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  - to leading order in the loop expansion (mean field) $\Longrightarrow$ BCS weak-coupling gap equation with gap Δ
- 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:

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

- Densities found by functional derivatives wrt J, j:

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

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

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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

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

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

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

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

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

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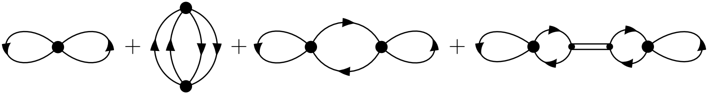
- Introduce single-particle orbitals and solve (cf. HFB)

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

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

Diagrammatic Expansion of W_i

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

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

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

  - Extra diagrams enforce inversion (here removes anomalous)

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

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

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

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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UV Divergences in Nonrelativistic and Relativistic Effective Actions

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

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

Divergences: Uniform Dilute Fermi System

- Generating functional with constant sources μ and j:

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

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

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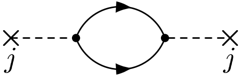
- New divergences because of $j \Longrightarrow$ e.g., expand to $\mathcal{O}(j^2)$

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

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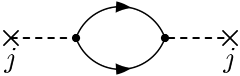
$W[\mu,j] = \cdots +$  $+ \cdots$

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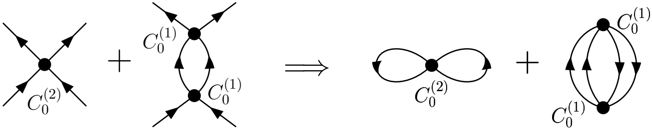
  - Recover DR/MS with $\Lambda=0$
- E.g., verify NLO renormalization $\Longrightarrow$ independent of Λ



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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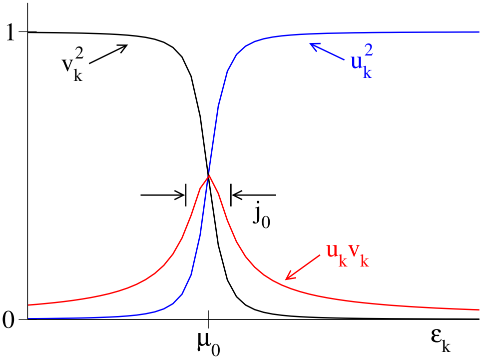

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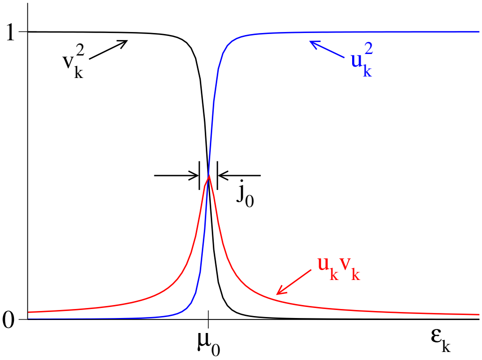

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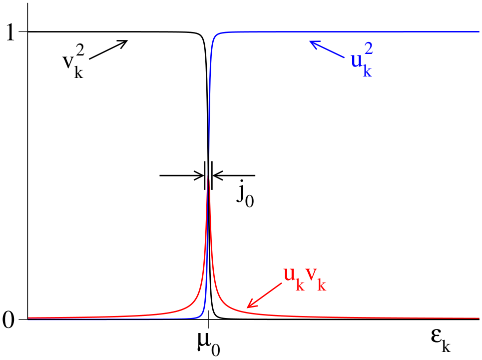

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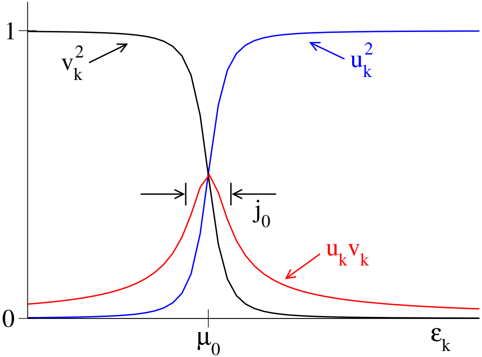

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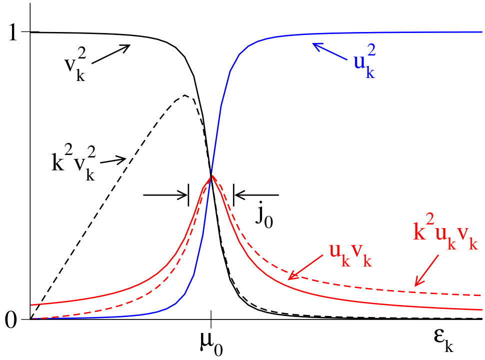

- j_0 plays role of constant gap

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

Kohn-Sham Non-Interacting System

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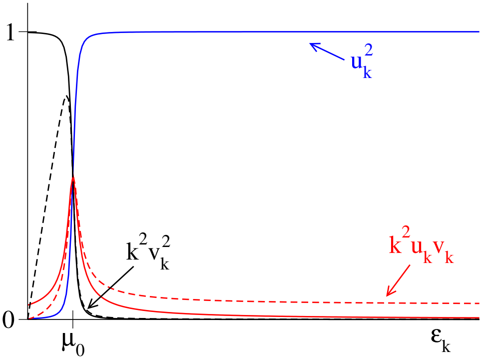

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- The basic DR/PDS integral in D dimensions, with $x \equiv j_0/\mu_0$, is

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

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

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

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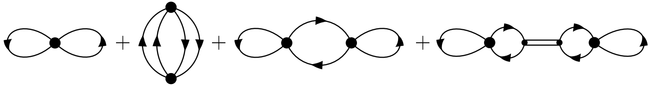
- The KS equation for the pair density ϕ fixes $\zeta^{(0)}$:

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

Calculating to n^{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

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

- 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!
  - Choose $\delta Z_j^{(n)}$ and $\zeta^{(n)}$ to convert ϕ_B to renormalized ϕ

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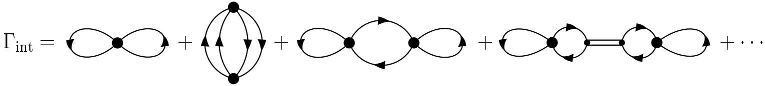

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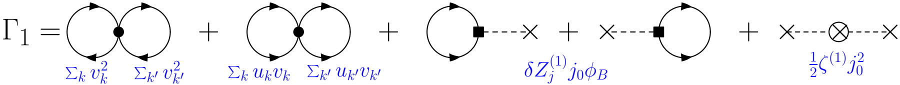
  - No freedom in choosing $C_0(\Lambda) \Longrightarrow \Lambda$'s must cancel!
  - Choose $\delta Z_j^{(n)}$ and $\zeta^{(n)}$ to convert ϕ_B to renormalized ϕ
- Leading order: Diagrams for $\Gamma_1[\rho,\phi] = W_1[\mu_0(\rho,\phi), j_0(\rho,\phi)]$



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

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 $x \equiv |j_0/\mu_0|$)

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

$\Longrightarrow$ if $k_{\mathrm{F}}a_s < 1$, $\dfrac{j_0}{\mu_0} = \dfrac{8}{e^2}e^{-\pi/2k_{\mathrm{F}}|a_s|}$ 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
  $\Longrightarrow$ same results as Papenbrock/Bertsch (plus HF term)

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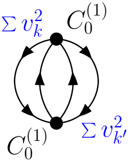
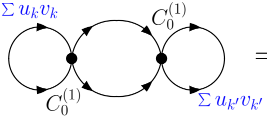
- To find the energy density, evaluate Γ at the stationary point $j_0 = -\frac{1}{2}|C_0^{(1)}|\phi$ with μ_0 fixed by the equation for ρ $\Longrightarrow$ same results as Papenbrock/Bertsch (plus HF term)
- Life gets more complicated at NLO
  - dependence of Γ_2 on ρ, ϕ is no longer explicit
  - analytic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

Γ_2 at Next-to-Leading Order (NLO)



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



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

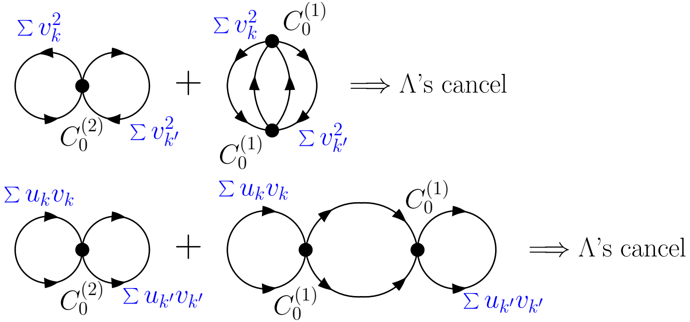
- UV divergences identified from

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

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

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:



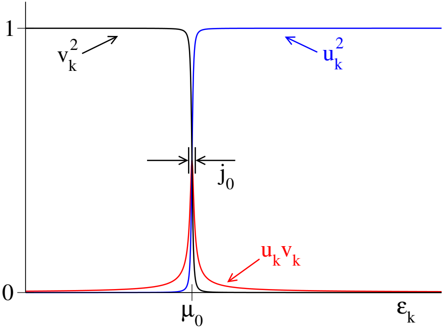
(Note that $\delta Z_j^{(1)}$ vertex takes $\phi_B \to \phi$)

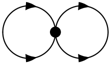
- How do we see cancellation of Λ's and evaluate renormalized results without analytic formulas? [but first . . .]

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 $T = 0$:

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



$$\Gamma_1 = $$ 

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

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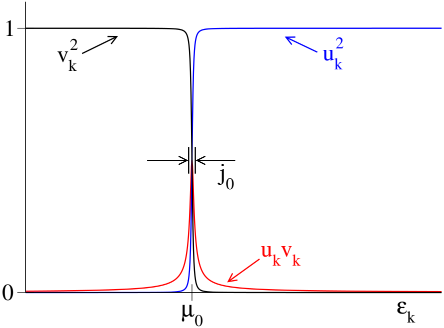
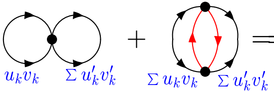
- NLO modifies exponent
  $\Longrightarrow$ changes prefactor
- $\Delta_{NLO} \approx \Delta_{LO}/(4e)^{1/3}$



$\Gamma_1 + \Gamma_2 =$ 

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

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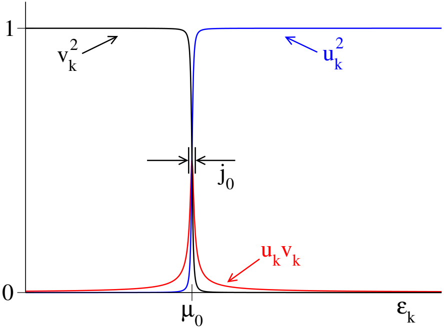
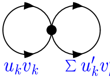
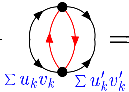


$\Gamma_1 + \Gamma_2 =$  $+$  $\Longrightarrow j_1 + j_2 = \frac{1}{2}|C_0|\left[1 - |C_0|\langle\Pi_0\rangle_{|\mathbf{k}|=|\mathbf{k}'|=k_{\rm F}}\right]\phi$

- 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)

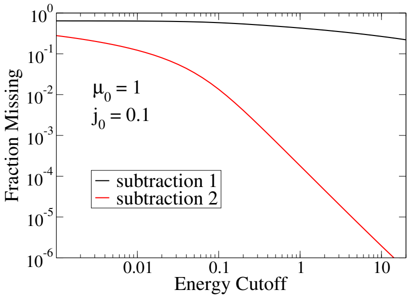
$$\phi(\mathbf{x}) = 2 \sum_i^{E_c} u_i(\mathbf{x})v_i(\mathbf{x}) - j_0(\mathbf{x}) \frac{M\, k_c(\mathbf{x})}{2\pi^2} \quad \text{with} \quad E_c = \frac{k_c^2(\mathbf{x})}{2M} + J(\mathbf{x}) - \mu_0$$

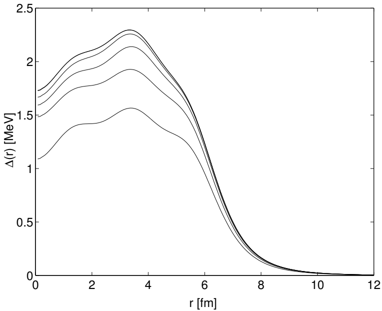
Bulgac Renormalization [Bulgac/Yu PRL 88 (2002) 042504]

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

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

- Compare convergence in uniform system, in nuclei with LDA





- How do we generalize this?

Outline

Effective Actions and Pairing $\Longrightarrow$ Kohn-Sham DFT

Renormalization Issues

Open Questions

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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  - Euclidean space (see Zinn-Justin)

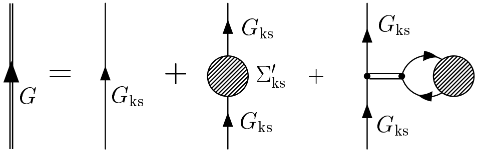
$$\frac{1}{\beta}\Gamma[\rho] = \langle \widehat{H}(J) \rangle_J - \int J\,\rho = \langle \widehat{H} \rangle_J$$

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

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



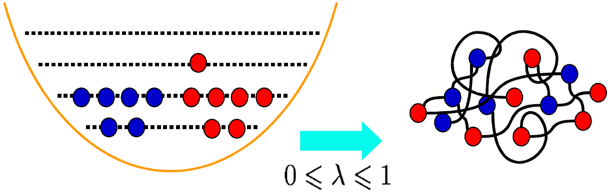
  - When do we need the "real" gap?
- What about broken symmetries?
  - E.g., number projection for pairing
  - How to accomodate within effective action framework?

Better Alternatives to Local Kohn-Sham?

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

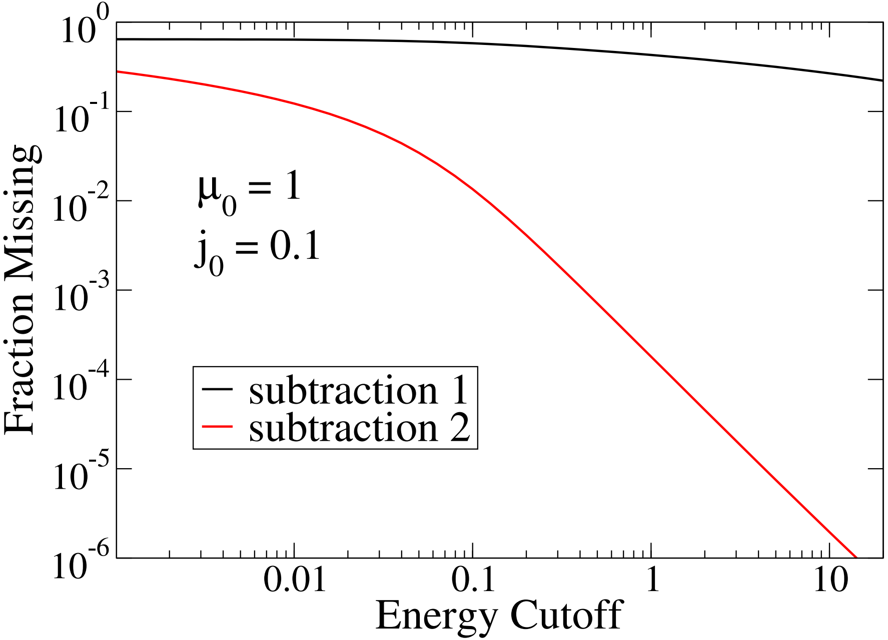
$$\widehat{H} \longrightarrow \widehat{H} - \int dx\, dx' \, [D^*(x,x')\psi_\uparrow(x)\psi_\downarrow(x') + \text{H.c.}]$$

  - 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)



Summary

- Effective action formalism generates Kohn-Sham DFT with local pairing fields $\Longrightarrow$ systematic expansion
- Renormalization is tricky, but consistent treatment possible
- 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?



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