Effective Field Theory for Density Functional Theory II

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

Web Resources

- These lectures are available in PDF form at
  http://www.physics.ohio-state.edu/~ntg/talks/
- Class notes for a two-quarter course on "Nuclear Many-Body Physics" given by Dick Furnstahl and Achim Schwenk are available at
  http://www.physics.ohio-state.edu/~ntg/880/
  (username: physics, password: 880.05)

References for Many-Body Physics

- A.L. Fetter and J.D. Walecka, “Quantum Theory of Many-Particle Systems.” Classic text, but pre-path integrals. Now available in an inexpensive (about $20) Dover reprint. Get it!
- J.W. Negele and H. Orland, “Quantum Many-Particle Systems.” Detailed and careful use of path integrals. Full of good physics but most of the examples are in the problems, so it can be difficult to learn from.
- N. Nagaosa, “Quantum Field Theory in Condensed Matter Physics.” Recent text, covers path integral methods and symmetry breaking.
- A.M. Tsvelik, “Quantum Field Theory in Condensed Matter Physics.” Good on one-dimensional systems.
- M. Stone, “The Physics of Quantum Fields.” A combined introduction to quantum field theory as applied to particle physics problems and to nonrelativistic many-body problems. Some very nice explanations.
- R.D. Mattuck, “A Guide to Feynman Diagrams in the Many-Body Problems.” This is a nice, intuitive guide to the meaning and use of Feynman diagrams.
- N. Goldenfeld, “Lectures on Phase Transitions and the Renormalization Group.” The discussion of scaling, dimensional analysis, and phase transitions is wonderful.
- G.D. Mahan, “Many-Particle Physics.” Standard, encyclopedic reference for condensed matter applications.
- P. Ring and P. Schuck, “The Nuclear Many-Body Problem.” Somewhat out of date, but still a good, encyclopedic guide to the nuclear many-body problem. Doesn’t discuss Green’s function methods much and no path integrals.
- K. Huang, “Statistical Mechanics.” Excellent choice for general treatment of statistical mechanics, with good sections on many-body physics.

Outline

DFT from Effective Actions

EFT for Dilute Fermi Systems

DFT via EFT

Summary II: DFT from EFT

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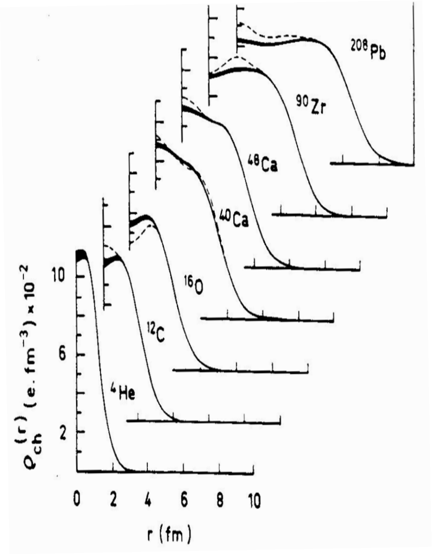
Density Functional Theory (DFT)

- Hohenberg-Kohn: There exists an energy functional $E_{v_{\rm ext}}[\rho]$ ...

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

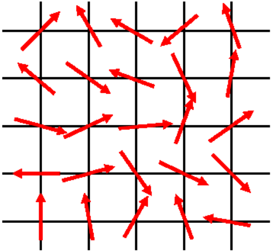
- $F_{\rm HK}$ is *universal* (same for any external $v_{\rm ext}$) $\Longrightarrow$ H_2 to DNA!
- Useful if you can approximate the energy functional
- Introduce orbitals and minimize energy functional $\Longrightarrow$ E_{gs}, ρ_{gs}



Thermodynamic Interpretation of DFT

- Consider a system of spins S_i on a lattice with interaction g
- The partition function has the information about the energy, magnetization of the system:

$$\mathcal{Z} = \mathrm{Tr}\, e^{-\beta g \sum_{\{i,j\}} S_i S_j}$$



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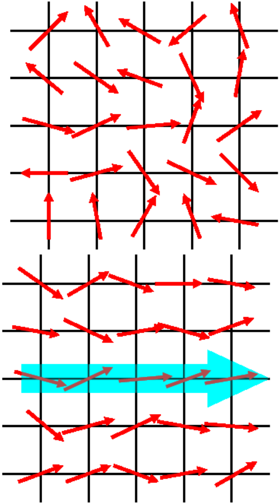
- The magnetization M is

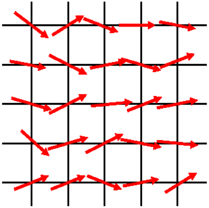
$$M = \left\langle \sum_i S_i \right\rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left[\left(\sum_i S_i \right) e^{-\beta g \sum_{\{i,j\}} S_i S_j} \right]$$



Add A Magnetic Probe Source H

- The source probes configurations near the ground state

$$\mathcal{Z}[H] = e^{-\beta F[H]} = \mathrm{Tr}\, e^{-\beta(g\sum_{\{i,j\}} S_i S_j - H\sum_i S_i)}$$



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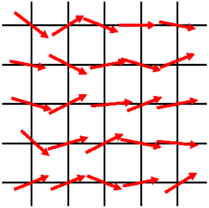

source magnet

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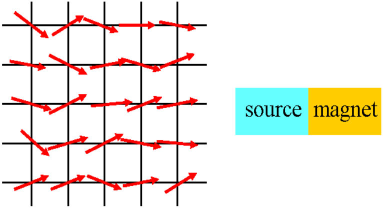

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$$M = \left\langle \sum_i S_i \right\rangle_H = -\frac{\partial F[H]}{\partial H}$$

- $F[H]$ is the Helmholtz free energy. Set $H = 0$ (or equal to a real external source) at the end

Legendre Transformation to Effective Action

- Find $H[M]$ by inverting

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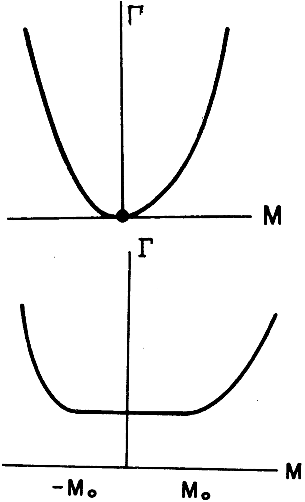
$$\Gamma[M] = F[H] + H\, M$$



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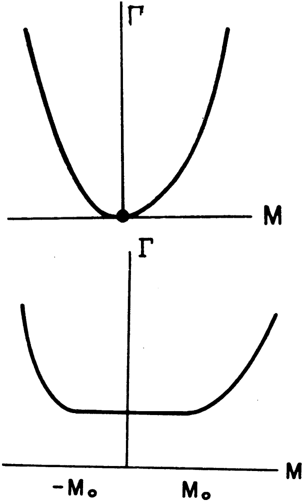
- The ground-state magnetization $M_{\rm gs}$ follows by minimizing $\Gamma[M]$:

$$H = \frac{\partial \Gamma[M]}{\partial M} \longrightarrow \left.\frac{\partial \Gamma[M]}{\partial M}\right|_{M_{\rm gs}} = 0$$



DFT as Effective Action

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

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

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

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

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

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

Partition Function in Zero Temperature Limit

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

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

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

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

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

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

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- Substitute and separate out the pieces:

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

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

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

Putting it all together . . .

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

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

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

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

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

Paths to the Effective Action Density Functional

1. Follow Coulomb Kohn-Sham DFT
   - Calculate uniform system as function of density
     $\Longrightarrow$ LDA functional + standard Kohn-Sham procedure
   - Add semi-empirical gradient expansion
2. RG approach [Polonyi/Schwenk] $\Longrightarrow$ Friday
3. Use auxiliary fields [Faussurier, Valiev/Fernando, Diehl/Wetterich]
   - Couple $\psi^\dagger\psi$ to auxiliary field φ; eliminate (part of) $(\psi^\dagger\psi)^2$
   - Source $J\varphi$; loop expansion about expectation value $\phi = \langle\varphi\rangle$
   - Kohn-Sham: Use freedom to require density unchanged
4. Inversion method [Fukuda et al., Valiev/Fernando]
   $\Longrightarrow$ systematic Kohn-Sham DFT
   - Relies on an order-by-order expansion $\Longrightarrow$ EFT power counting

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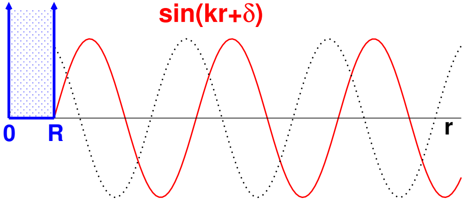
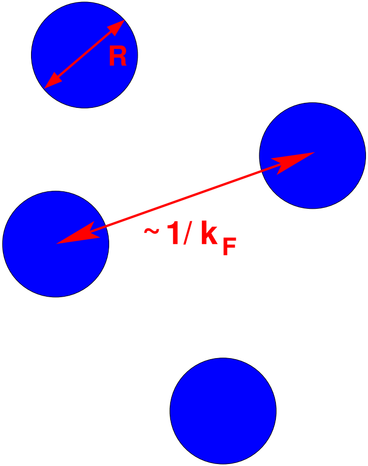
“Simple” Many-Body Problem: Hard Spheres

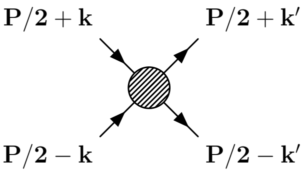
- Infinite potential at radius R

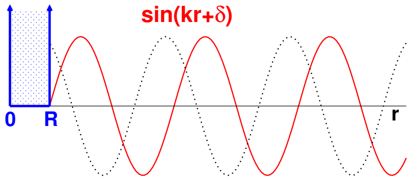




- Scattering length $a_0 = R$
- Dilute $\rho R^3 \ll 1 \Longrightarrow k_{\mathrm{F}} a_0 \ll 1$
- What is the energy/particle?
- Ref.: nucl-th/0004043

Quick Review of Scattering





- Relative motion with total $P=0$: $\psi(r) \xrightarrow{r\to\infty} e^{i\mathbf{k}\cdot\mathbf{r}} + f(k,\theta)\frac{e^{ikr}}{r}$
  where $k^2 = k'^2 = ME_k$ and $\cos\theta = \hat{k}\cdot\hat{k}'$
- Differential cross section is $d\sigma/d\Omega = |f(k,\theta)|^2$

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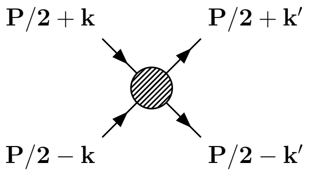

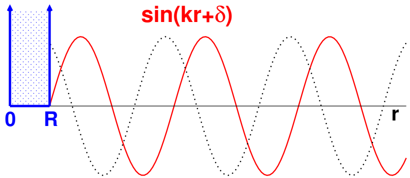

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  where $k^2 = k'^2 = ME_k$ and $\cos\theta = \hat{k}\cdot\hat{k}'$
- Differential cross section is $d\sigma/d\Omega = |f(k,\theta)|^2$
- Central $V \Longrightarrow$ partial waves:
  $f(k,\theta) = \sum_l (2l+1) f_l(k) P_l(\cos\theta)$

$$\text{where} \quad f_l(k) = \frac{e^{i\delta_l(k)}\sin\delta_l(k)}{k} = \frac{1}{k\cot\delta_l(k) - ik}$$

and the S-wave phase shift is defined by

$$u_0(r) \xrightarrow{r\to\infty} \sin[kr + \delta_0(k)] \quad \Longrightarrow \quad \delta_0(k) = -kR \text{ for hard sphere}$$

At Low Energies: Effective Range Expansion

- As first shown by Schwinger, $k^{l+1} \cot \delta_l(k)$ has a power series expansion. For $l = 0$:

$$k \cot \delta_0 = -\frac{1}{a_0} + \frac{1}{2} r_0 k^2 - P r_0^3 k^4 + \cdots$$

defines the *scattering length* a_0 and the *effective range* r_0

- While $r_0 \sim R$, the range of the potential, a_0 can be anything
  - if $a_0 \sim R$, it is called "natural"
  - $|a_0| \gg R$ (unnatural) is particularly interesting $\Longrightarrow$ cold atoms
- The effective range expansion for hard sphere scattering is:

$$k \cot(-kR) = -\frac{1}{R} + \frac{1}{3} R k^2 + \cdots \quad \Longrightarrow \quad a_0 = R \quad r_0 = 2R/3$$

so the low-energy effective theory is natural

EFT for “Natural” Short-Range Interaction

- A simple, general interaction is a sum of delta functions and derivatives of delta functions. In momentum space,

$$\langle \mathbf{k}|V_{\rm eft}|\mathbf{k}'\rangle = C_0 + \frac{1}{2}C_2(\mathbf{k}^2 + \mathbf{k}'^2) + C_2'\mathbf{k}\cdot\mathbf{k}' + \cdots$$

- Or, $\mathcal{L}_{\rm eft}$ has most general local (contact) interactions:

$$\mathcal{L}_{\rm eft} = \psi^\dagger\Big[i\frac{\partial}{\partial t} + \frac{\overrightarrow{\nabla}^2}{2M}\Big]\psi - \frac{C_0}{2}(\psi^\dagger\psi)^2 + \frac{C_2}{16}\big[(\psi\psi)^\dagger(\psi\overleftrightarrow{\nabla}^2\psi) + \text{ h.c.}\big]$$
$$+ \frac{C_2'}{8}(\psi\overleftrightarrow{\nabla}\psi)^\dagger\cdot(\psi\overleftrightarrow{\nabla}\psi) - \frac{D_0}{6}(\psi^\dagger\psi)^3 + \ldots$$

- Dimensional analysis $\Longrightarrow C_{2i} \sim \frac{4\pi}{M}R^{2i+1}\,, \quad D_{2i} \sim \frac{4\pi}{M}R^{2i+4}$

Effective Field Theory Ingredients

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

1. Use the most general $\mathcal{L}$ with low-energy dof’s consistent with global and local symmetries of underlying theory
   - $\mathcal{L}_{\rm eft} = \psi^\dagger \big[i\frac{\partial}{\partial t} + \frac{\overrightarrow{\nabla}^{\,2}}{2M} \big] \psi - \frac{C_0}{2}(\psi^\dagger\psi)^2 - \frac{D_0}{6}(\psi^\dagger\psi)^3 + \ldots$

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2. Declaration of regularization and renormalization scheme
   - natural $a_0 \Longrightarrow$ dimensional regularization and min. subtraction

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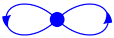
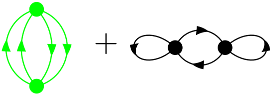
2. Declaration of regularization and renormalization scheme
   - natural $a_0 \Longrightarrow$ dimensional regularization and min. subtraction
3. Well-defined power counting $\Longrightarrow$ small expansion parameters
   - use the separation of scales $\Longrightarrow \dfrac{k_{\rm F}}{\Lambda}$ with $\Lambda \sim 1/R \Longrightarrow k_{\rm F} a_0$, etc.

$\mathcal{O}(k_{\rm F}^6)$:



$\mathcal{O}(k_{\rm F}^7)$:



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

Feynman Rules for EFT Vertices

$$\mathcal{L}_{\rm eft} = \psi^\dagger\Big[i\frac{\partial}{\partial t} + \frac{\overrightarrow{\nabla}^{2}}{2M}\Big]\psi - \frac{C_0}{2}(\psi^\dagger\psi)^2 + \frac{C_2}{16}\Big[(\psi\psi)^\dagger(\psi\overleftrightarrow{\nabla}^2\psi) + \text{ h.c.}\Big]$$

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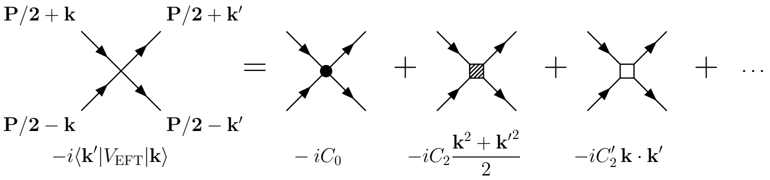
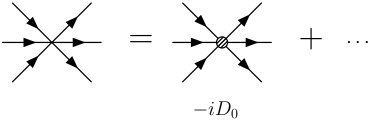




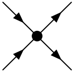
Renormalization

- Reproduce $f_0(k)$ in perturbation theory (Born series):

$$f_0(k) \propto a_0 - i a_0^2 k - (a_0^3 - a_0^2 r_0/2) k^2 + \mathcal{O}(k^3 a_0^4)$$

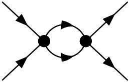
- Consider the leading potential $V_{\rm EFT}^{(0)}(\mathbf{x}) = C_0 \delta(\mathbf{x})$ or

$$\langle \mathbf{k} | V_{\rm eft}^{(0)} | \mathbf{k}' \rangle \Longrightarrow$$



$$\Longrightarrow C_0$$

- Choosing $C_0 \propto a_0$ gets the first term. Now $\langle \mathbf{k} | V G_0 V | \mathbf{k}' \rangle$:



$$\Longrightarrow C_0 M \int \frac{d^3 q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\epsilon} C_0 \longrightarrow \infty!$$

$\Longrightarrow$ Linear divergence!

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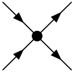

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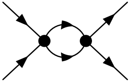


$$\Longrightarrow \int^{\Lambda_c} \frac{d^3q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\epsilon} \longrightarrow \frac{\Lambda_c}{2\pi^2} - \frac{ik}{4\pi} + \mathcal{O}(\frac{k^2}{\Lambda_c})$$

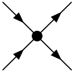
$\Longrightarrow$ If cutoff at Λ_c, then can absorb into C_0, but all powers of k^2

Renormalization

- Reproduce $f_0(k)$ in perturbation theory (Born series):

$$f_0(k) \propto a_0 - i a_0^2 k - (a_0^3 - a_0^2 r_0/2) k^2 + \mathcal{O}(k^3 a_0^4)$$

- Consider the leading potential $V_{\rm EFT}^{(0)}(\mathbf{x}) = C_0 \delta(\mathbf{x})$ or

$$\langle \mathbf{k} | V_{\rm eft}^{(0)} | \mathbf{k}' \rangle \Longrightarrow$$

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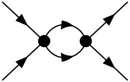
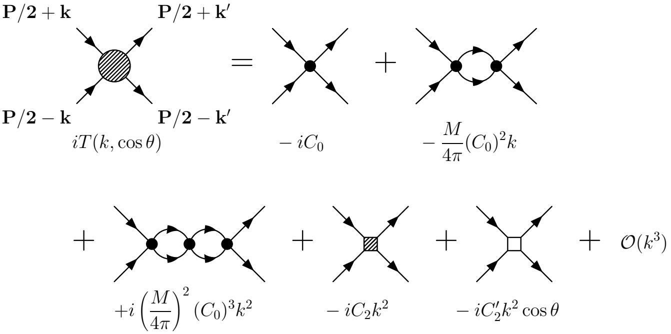


$$\Longrightarrow \int \frac{d^D q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\epsilon} \xrightarrow{D \to 3} -\frac{ik}{4\pi}$$

Dimensional regularization with minimal subtraction
$\Longrightarrow$ only one power of k!

- Dim. reg. + minimal subtraction $\Longrightarrow$ simple power counting:



- Matching:

$$C_0 = \frac{4\pi}{M} a_0 = \frac{4\pi}{M} R \;, \quad C_2 = \frac{4\pi}{M}\frac{a_0^2 r_0}{2} = \frac{4\pi}{M}\frac{R^3}{3} \;, \quad \cdots$$

- Recovers expansion order-by-order with diagrams

Noninteracting Fermi Sea at $T = 0$

- Put system in a large box ($V = L^3$) with periodic bc's
  - spin-isospin degeneracy ν (e.g., for nuclei, $\nu = 4$)
  - fill momentum states up to Fermi momentum $k_{\rm F}$

$$N = \nu \sum_{\mathbf{k}}^{k_{\rm F}} 1 \,, \qquad E = \nu \sum_{\mathbf{k}}^{k_{\rm F}} \frac{\hbar^2 k^2}{2M}$$

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$$N = \nu \frac{L}{2\pi} \int_{-k_{\rm F}}^{+k_{\rm F}} dk = \frac{\nu k_{\rm F}}{\pi} L \implies \rho = \frac{N}{L} = \frac{\nu k_{\rm F}}{\pi}; \quad \frac{E}{L} = \frac{1}{3} \frac{\hbar^2 k_{\rm F}^2}{2M} \rho$$

- In 3-D:

$$N = \nu \frac{V}{(2\pi)^3} \int^{k_{\rm F}} d^3k = \frac{\nu k_{\rm F}^3}{6\pi^2} V \implies \rho = \frac{N}{V} = \frac{\nu k_{\rm F}^3}{6\pi^2}; \quad \frac{E}{V} = \frac{3}{5} \frac{\hbar^2 k_{\rm F}^2}{2M} \rho$$

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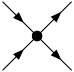
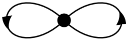
- Volume/particle $V/N = 1/\rho \sim 1/k_{\rm F}^3$, so spacing $\sim 1/k_{\rm F}$

Energy Density From Summing Over Fermi Sea

- Leading order $V^{(0)}_{\rm EFT}(\mathbf{x}) = C_0\delta(\mathbf{x}) \Longrightarrow V^{(0)}_{\rm EFT}(\mathbf{k},\mathbf{k}') = C_0$



$\Longrightarrow$



$$\mathcal{E}_{\rm LO} = \frac{C_0}{2}\nu(\nu-1)\left(\sum_{\mathbf{k}}^{k_{\rm F}} 1\right)^2 \propto a_0 k_{\rm F}^6$$

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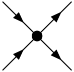
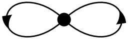
 $\Longrightarrow$ 

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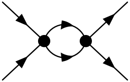
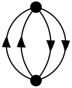
 $\Longrightarrow$ 

$$\mathcal{E}_{\mathrm{NLO}} \propto \int_{k_{\mathrm{F}}}^{\infty} \frac{d^3q}{(2\pi)^3}\frac{C_0^2}{k^2-q^2}$$

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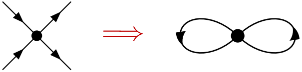

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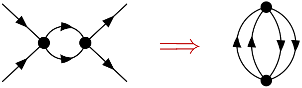


$$\mathcal{E}_{\rm NLO} \propto \int_{k_{\rm F}}^{\infty} \frac{d^3q}{(2\pi)^3}\frac{C_0^2}{k^2-q^2}$$

- Same renormalization fixes it! Particles $\longrightarrow$ holes

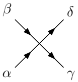
$$\int_{k_{\rm F}}^{\infty}\frac{1}{k^2-q^2} = \int_0^{\infty}\frac{1}{k^2-q^2} - \int_0^{k_{\rm F}}\frac{1}{k^2-q^2} \xrightarrow{D\to 3} -\int_0^{k_{\rm F}}\frac{1}{k^2-q^2} \propto a_0^2 k_{\rm F}^7$$

Feynman Rules for Energy Density at $T = 0$

- $T = 0$ Energy density $\mathcal{E}$ is sum of *Hugenholtz* diagrams
  - same vertices as free space (same renormalization!)
- Feynman rules:

1. Each line is assigned conserved $\widetilde{k} \equiv (k_0, \mathbf{k})$ and $[\omega_{\mathbf{k}} \equiv k^2/2M]$

$$iG_0(\widetilde{k})_{\alpha\beta} = i\delta_{\alpha\beta}\left(\frac{\theta(k - k_{\rm F})}{k_0 - \omega_{\mathbf{k}} + i\epsilon} + \frac{\theta(k_{\rm F} - k)}{k_0 - \omega_{\mathbf{k}} - i\epsilon}\right)$$

2. 

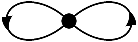
$\longrightarrow (\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})$ (if spin-independent)

3. After spin summations, $\delta_{\alpha\alpha} \rightarrow -\nu$ in every closed fermion loop.
4. Integrate $\int d^4k/(2\pi)^4$ with $e^{ik_0 0^+}$ for tadpoles
5. Symmetry factor $i/(S \prod_{l=2}^{l_{\rm max}}(l!)^k)$ counts vertex permutations and equivalent l–tuples of lines

Power Counting

- Power counting rules
  1. for every propagator (line): $M/k_{\rm F}^2$
  2. for every loop integration: $k_{\rm F}^5/M$
  3. for every n–body vertex with $2i$ derivatives: $k_{\rm F}^{2i}/M\Lambda^{2i+3n-5}$
- Diagram with V_{2i}^n n–body vertices scales as $(k_{\rm F})^\beta$ *only*:

$$\beta = 5 + \sum_{n=2}^{\infty}\sum_{i=0}^{\infty}(3n+2i-5)V_{2i}^n\,.$$

- e.g., $\mathcal{O}(k_{\rm F}^6)$:  $\Longrightarrow V_0^2 = 1$

$$\Longrightarrow \beta = 5 + (3\cdot 2 + 2\cdot 0 - 5)\cdot 1 = 6 \Longrightarrow \mathcal{O}(k_{\rm F}^6)$$

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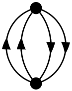
- e.g.,  $\Longrightarrow V_0^2 = 2$

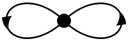
$$\Longrightarrow \beta = 5 + (3\cdot 2 + 2\cdot 0 - 5)\cdot 2 = 7 \Longrightarrow \mathcal{O}(k_{\mathrm{F}}^7)$$

$T = 0$ Energy Density from Hugenholtz Diagrams

$$\frac{E}{V} = \rho \frac{k_{\mathrm{F}}^2}{2M} \left[\frac{3}{5} \right.$$

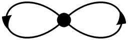
$$\left. \right]$$

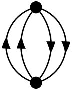
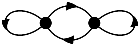
$T = 0$ Energy Density from Hugenholtz Diagrams

$\mathcal{O}(k_F^6)$: 

$$\frac{E}{V} = \rho \frac{k_F^2}{2M} \left[\frac{3}{5} + (\nu - 1) \frac{2}{3\pi} (k_F a_0) \right]$$

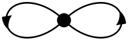
$T = 0$ Energy Density from Hugenholtz Diagrams

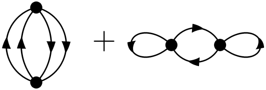
$\mathcal{O}(k_F^6)$: 

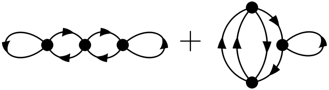
$\mathcal{O}(k_F^7)$:  + 

$$\frac{E}{V} = \rho \frac{k_F^2}{2M} \Big[\frac{3}{5} + (\nu - 1)\frac{2}{3\pi}(k_F a_0) + (\nu - 1)\frac{4}{35\pi^2}(11 - 2\ln 2)(k_F a_0)^2 \Big]$$

$T = 0$ Energy Density from Hugenholtz Diagrams

$\mathcal{O}(k_F^6)$: 

$\mathcal{O}(k_F^7)$: 

$\mathcal{O}(k_F^8)$: 

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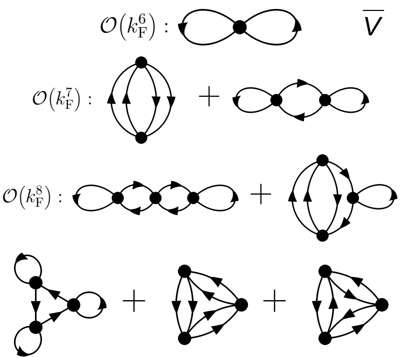

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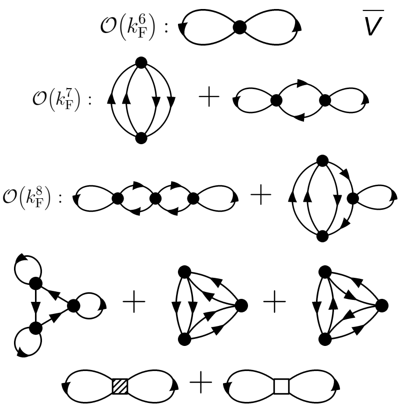

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Looks Like a Power Series in k_F! Is it?

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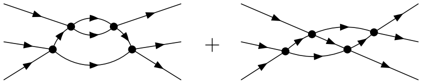
- New logarithmic divergences in 3–3 scattering



$$\propto (C_0)^4 \ln(k/\Lambda_c)$$

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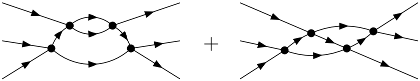

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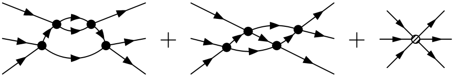
- Changes in Λ_c must be absorbed by 3-body coupling $D_0(\Lambda_c)$
  $\Longrightarrow D_0(\Lambda_c) \propto (C_0)^4 \ln(a_0\Lambda_c) + \text{const.}$ [Braaten & Nieto]

$\frac{d}{d\Lambda_c}$ [] $= 0 \Longrightarrow$ fixes coefficient!

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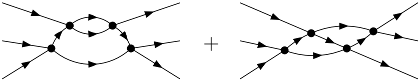

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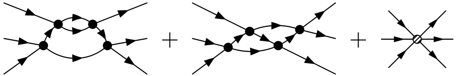
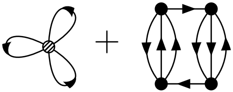
$\frac{d}{d\Lambda_c}\Big[$  $\Big] = 0 \Longrightarrow$ fixes coefficient!

- What does this imply for the energy density?

$\mathcal{O}(k_\mathrm{F}^9 \ln(k_\mathrm{F}))$:  $+ \ldots \propto (\nu-2)(\nu-1)\,(k_\mathrm{F}a_0)^4 \ln(k_\mathrm{F}a_0)$

Summary: Dilute Fermi System with Natural a_0

- The many-body energy density is perturbative in $k_F a_0$
  - efficiently reproduced by the EFT approach
- Power counting $\Longrightarrow$ error estimate from omitted diagrams
- Three-body forces are inevitable in a low-energy effective theory
  - and not unique $\Longrightarrow$ they depend on the two-body potential
- The case of a natural scattering length is under control for a uniform system
  - What if the scattering length is not natural?
  - What about a finite # of fermions in a trap? (Next!)

Outline

DFT from Effective Actions

EFT for Dilute Fermi Systems

DFT via EFT

Summary II: DFT from EFT

DFT as Effective Action

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

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

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

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

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

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

What can EFT do for DFT?

- Effective action as a path integral $\Longrightarrow$ construct $W[J]$, order-by-order in EFT expansion
  - For dilute system, same diagrams as before
  - But propagators (lines) are in the background field $J(\mathbf{x})$

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

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

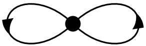
What can EFT do for DFT?

- Effective action as a path integral $\Longrightarrow$ construct $W[J]$, order-by-order in EFT expansion
  - For dilute system, same diagrams as before
  - But propagators (lines) are in the background field $J(\mathbf{x})$

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

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

- Apply to leading-order (LO) contribution: Hartree-Fock

LO : 

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

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

What can Power Counting do for DFT?

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

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

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

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

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

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

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

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

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- Start with exact expressions for Γ and ρ [note: β or $T = 1$]

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

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

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

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

Kohn-Sham Potential

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

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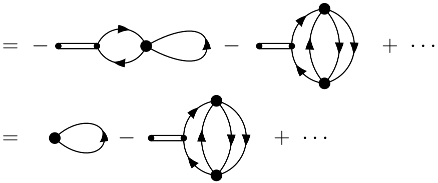

- New Feynman rules for $\Gamma_{\rm int} \Longrightarrow$ anomalous diagrams

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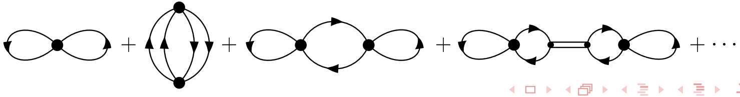

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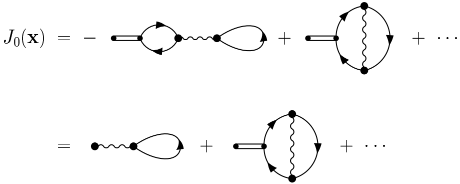

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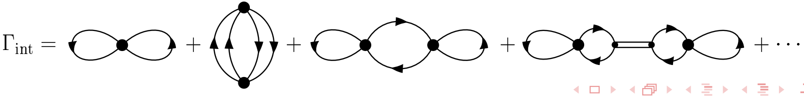

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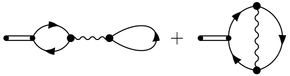
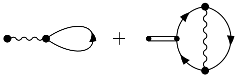
$J_0(\mathbf{x}) = -$  $+ \cdots$

$=$  $+ \cdots$

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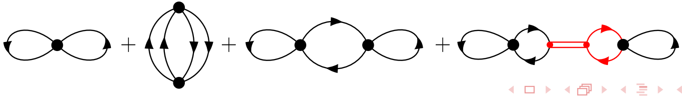
$\Gamma_{\text{int}} =$  $+ \cdots$

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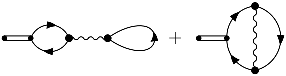
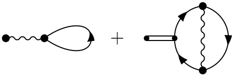
$J_0(\mathbf{x}) = -$  $+ \cdots$

$=$  $+ \cdots$

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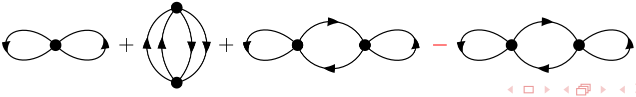
$\Gamma_{\rm int} =$  $+ \cdots$

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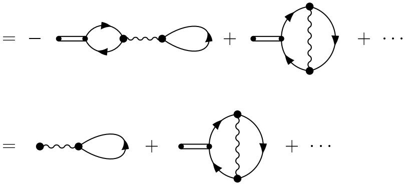

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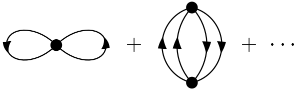

Now Source $J_0(\mathbf{x})$ is the Background Field

- Construct $W[J]$ and new diagrams for $\Gamma[\rho]$ order-by-order in an expansion (e.g., EFT power counting)
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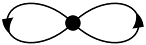
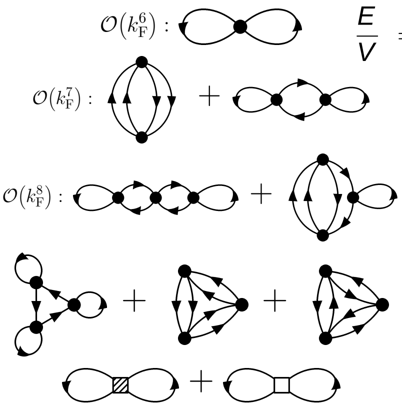
- E.g., apply to short-range LO contribution: Hartree-Fock

LO : 

$$\begin{aligned} W_1[J_0] &= \frac{1}{2}\nu(\nu-1)C_0\int d^3\mathbf{x}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,G^0_{\rm KS}(\mathbf{x},\mathbf{x};\omega)G^0_{\rm KS}(\mathbf{x},\mathbf{x};\omega') \\ &= -\frac{1}{2}\frac{(\nu-1)}{\nu}C_0\int d^3\mathbf{x}\,[\rho_{J_0}(\mathbf{x})]^2 \quad \text{where} \quad \rho_{J_0}(\mathbf{x}) \equiv \nu\sum_\alpha^{\epsilon_{\rm F}}|\psi_\alpha(\mathbf{x})|^2 \end{aligned}$$

$T = 0$ LDA Energy from Hugenholtz Diagrams

Uniform system: Each line is non-interacting propagator



$$\frac{E}{V} = \rho\frac{k_F^2}{2M}\left[\frac{3}{5} + (\nu-1)\frac{2}{3\pi}(k_F a_0)\right.$$

$$+ (\nu-1)\frac{4}{35\pi^2}(11 - 2\ln 2)(k_F a_0)^2$$

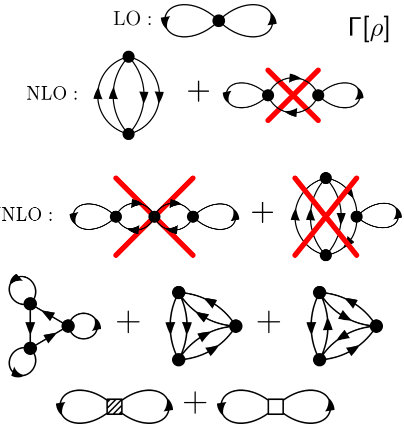
$$+ (\nu-1)\big(0.076 + 0.057(\nu-3)\big)(k_F a_0)^3$$

$$+ (\nu-1)\frac{1}{10\pi}(k_F r_0)(k_F a_0)^2$$

$$\left. + (\nu+1)\frac{1}{5\pi}(k_F a_p)^3 + \cdots\right]$$

$T = 0$ LDA Energy from Hugenholtz Diagrams

Now each line is propagator in $J_0(\mathbf{x})$ corresponding to $\rho(\mathbf{x})$



$$\Gamma[\rho] = \int d^3x \left[K(\mathbf{x}) + \frac{1}{2}\frac{(\nu-1)}{\nu}\frac{4\pi a_0}{M}[\rho(\mathbf{x})]^2 + d_1 \frac{a_0^2}{2M}[\rho(\mathbf{x})]^{7/3} + d_2\, a_0^3[\rho(\mathbf{x})]^{8/3} + d_3\, a_0^2\, r_0[\rho(\mathbf{x})]^{8/3} + d_4\, a_p^3[\rho(\mathbf{x})]^{8/3} + \cdots \right]$$

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- Follows immediately in the local density approximation (LDA)

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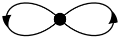

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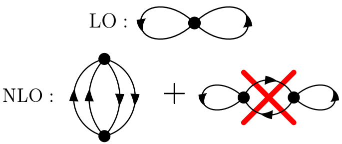

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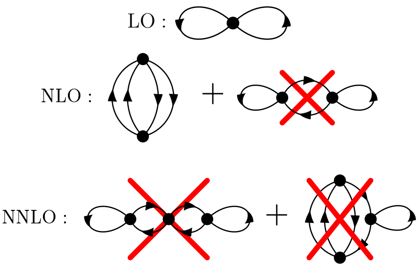

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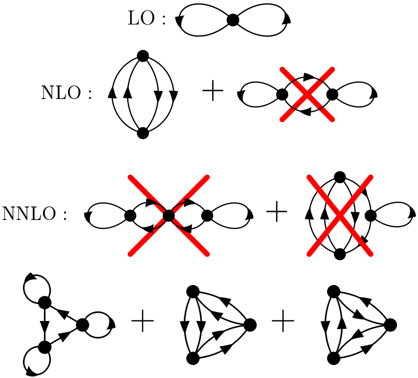

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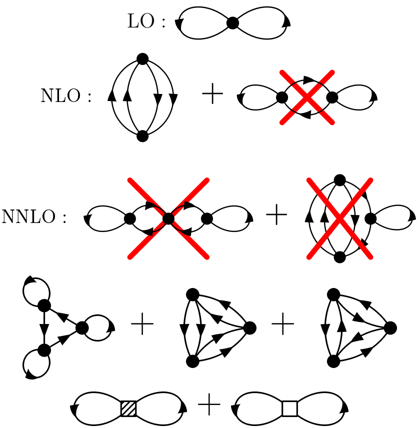

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Dilute Fermi Gas in a Harmonic Trap

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5. Repeat 2.–4. until changes are small (“self-consistent”)

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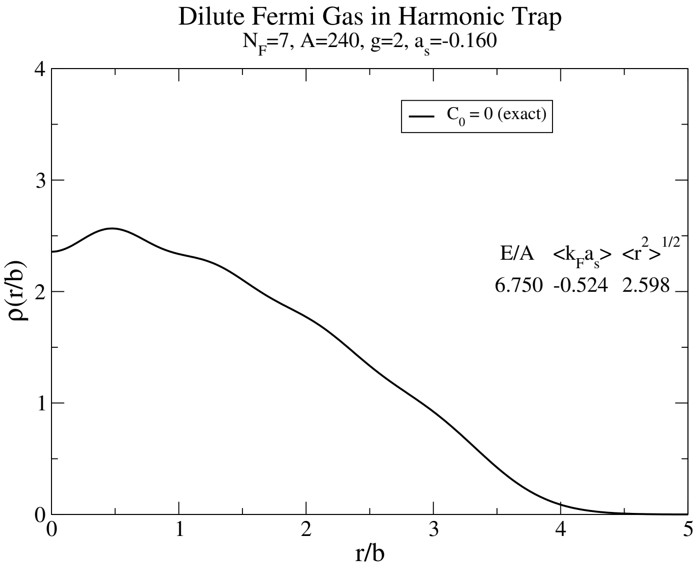
   - other observables are functionals of $\{\psi_\alpha, \epsilon_\alpha\}$
5. Repeat 2.–4. until changes are small (“self-consistent”)

Looks like a simple Hartree calculation!

Check Out An Example [nucl-th/0212071]



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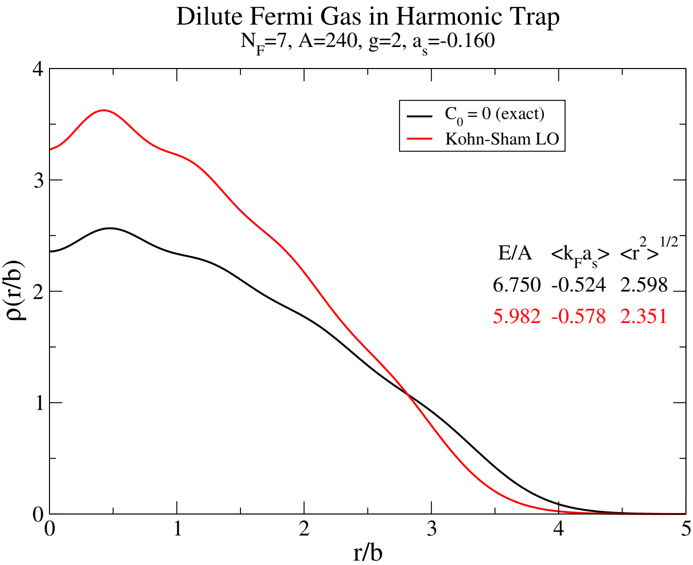

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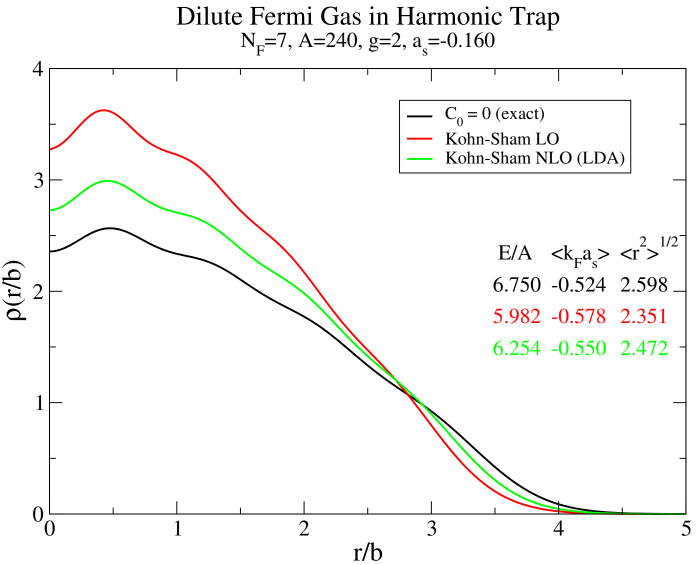

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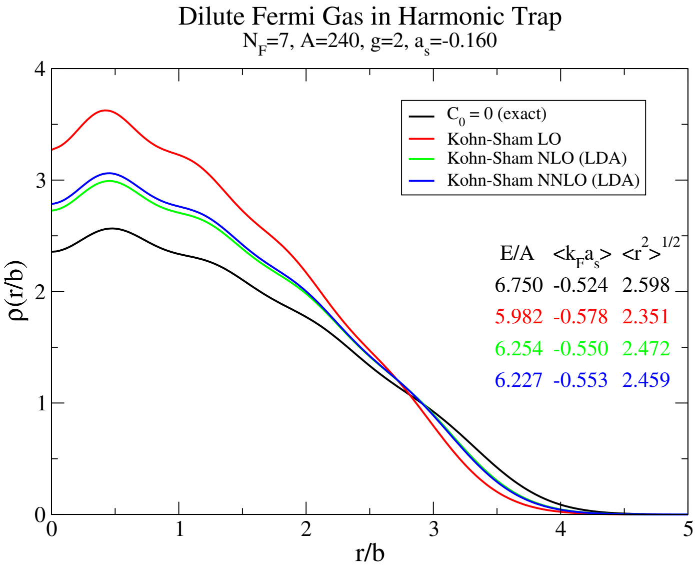

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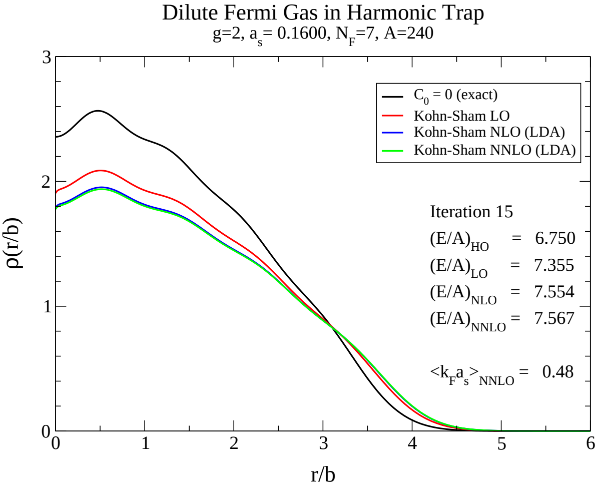

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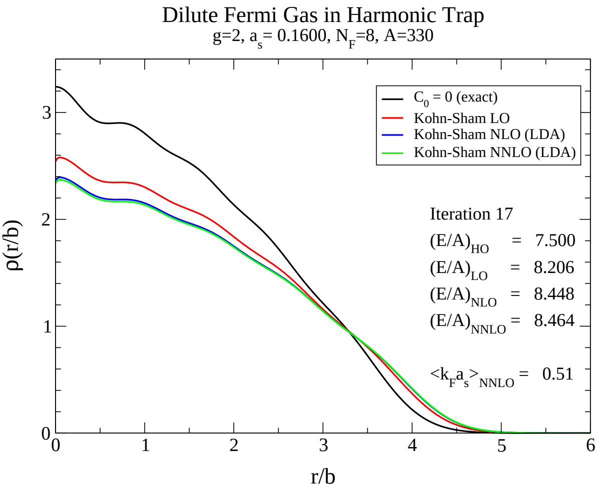

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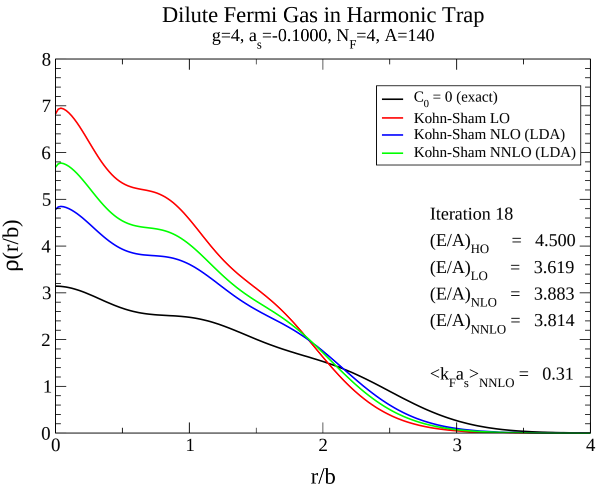

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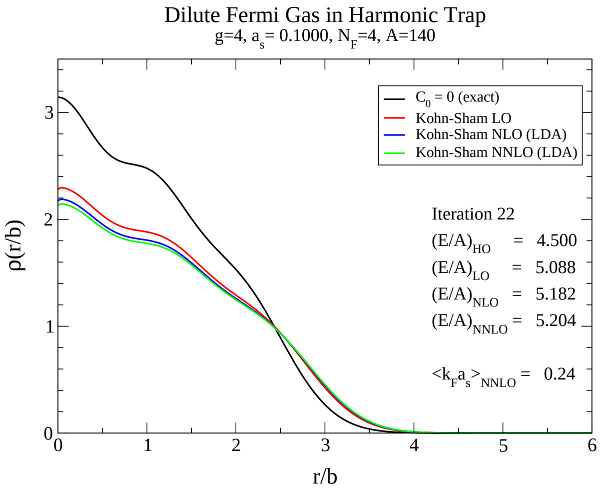
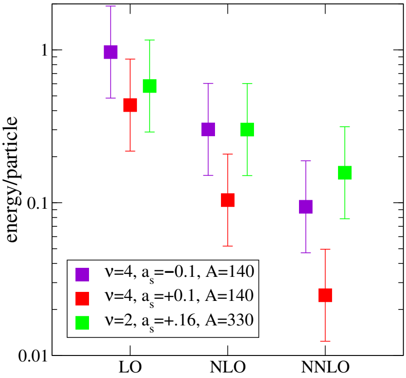


Power Counting Terms in Energy Functionals

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



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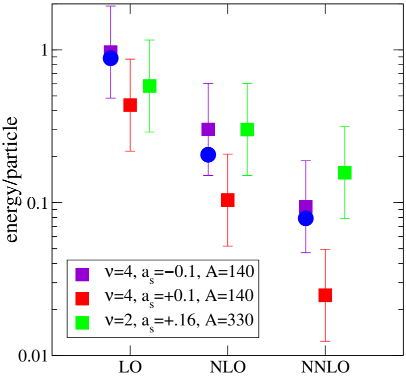

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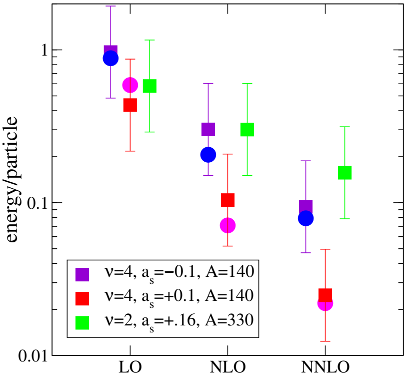

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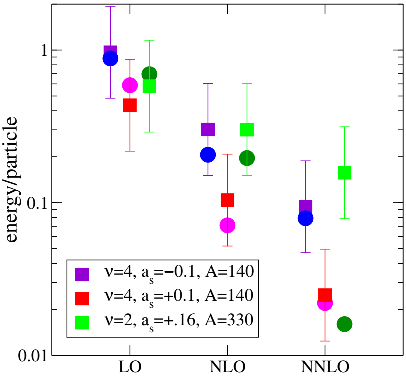

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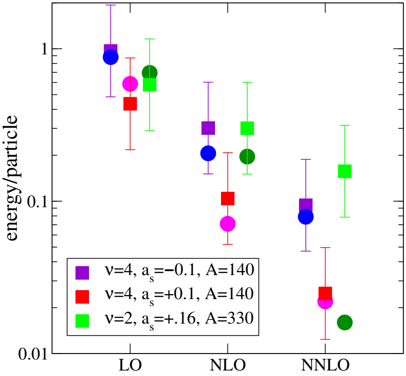
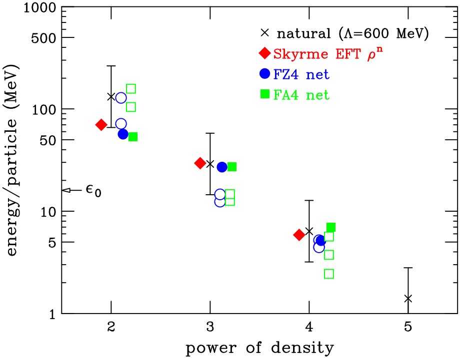




- Reasonable estimates $\Longrightarrow$ truncation errors understood

Outline

DFT from Effective Actions

EFT for Dilute Fermi Systems

DFT via EFT

Summary II: DFT from EFT

Summary II: DFT from EFT

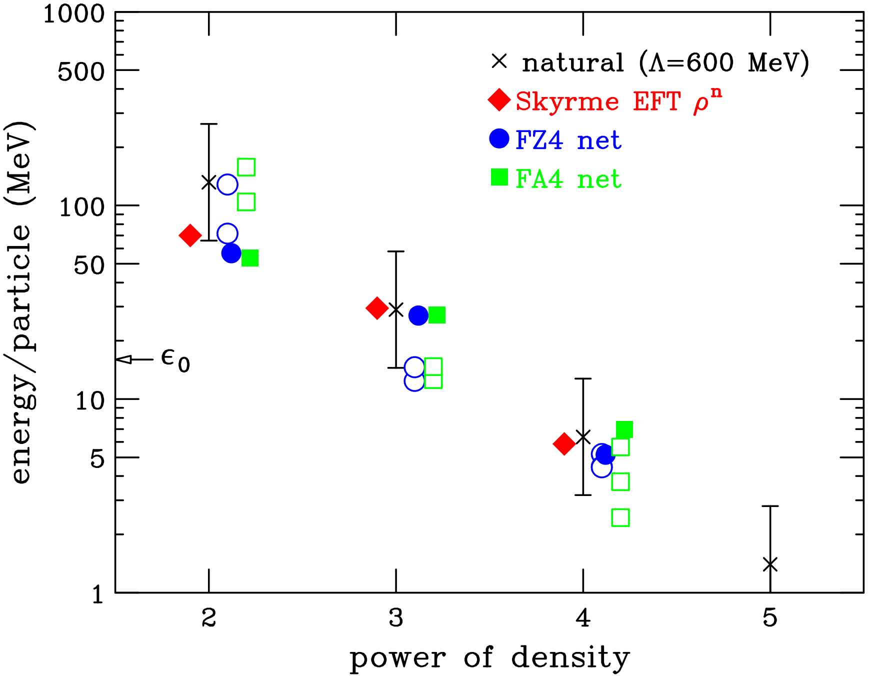
- Conventional DFT is one example of using effective actions
  - a different effective action may be better
- Kohn-Sham DFT from EFT expansion with inversion method
- EFT application to dilute Fermi system in a trap
  - well-defined expansion
  - power counting and error estimates for the finite system work

Next: Toward Nuclear DFT

- Skyrme functional depends on $\rho(\mathbf{x})$, $\tau(\mathbf{x})$, and $\mathbf{J}(\mathbf{x})$
  $\Longrightarrow$ How does that work?
- Can we calculate single-particle properties?
- How do we incorporate pairing?
- How do we use microscopic inter-nucleon interactions?

Effective Action as Energy Functional: Minkowski

Kohn-Luttinger-Ward Inversion Method



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

Outline

Effective Action as Energy Functional: Minkowski

Kohn-Luttinger-Ward Inversion Method

Effective Action as Energy Functional: Minkowski

back

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

Outline

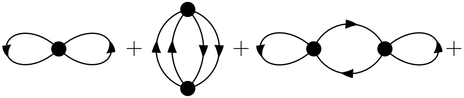
Effective Action as Energy Functional: Minkowski

Kohn-Luttinger-Ward Inversion Method

Kohn-Luttinger-Ward Theorem (1960)

- $T \to 0$ diagram expansion of $\Omega(\mu, V, T)$ in external $v(\mathbf{x})$
  $\Longrightarrow$ same as $F(N, V, T \equiv 0)$ with μ_0 and no "anomalous"

$$\Omega(\mu, V, T) = \Omega_0(\mu) \; + $$



$+ \cdots$

with $\mathcal{G}_0(\mu, T)$

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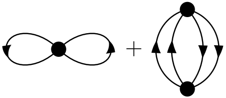

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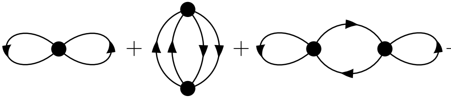

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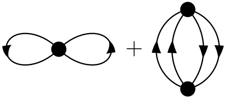

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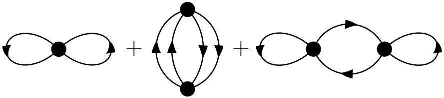

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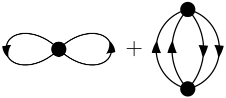

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Kohn-Luttinger Inversion Method [F & W, sec. 30]

- Find $F(N) = \Omega(\mu) + \mu N$ with $\mu(N)$ from $N(\mu) = -(\partial\Omega/\partial\mu)_{TV}$

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- Same pattern to all orders: μ_i determined by functions of μ_0

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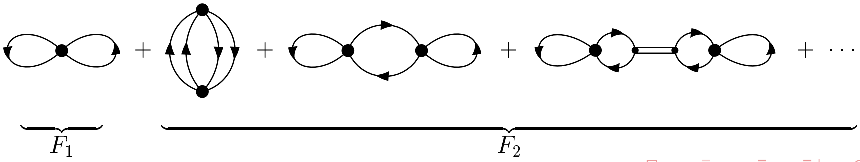

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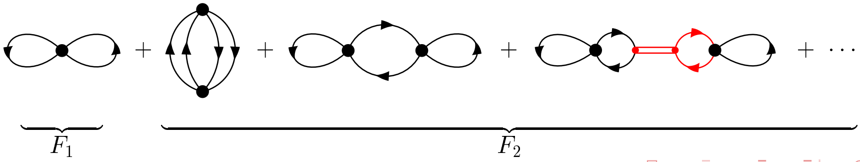

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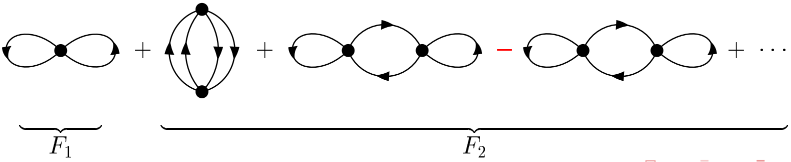

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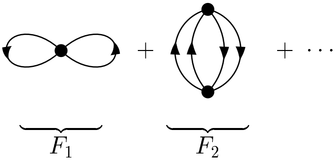

Generalizing the KLW Inversion Approach

back

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  - it has chemical potential μ_0 and external potential $v(\mathbf{x})$
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  - for a self-bound system (nucleus!), there is no [net] $v(\mathbf{x})$

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  1. $\mu N + J(\mathbf{x})\rho(\mathbf{x})$ with $J(\mathbf{x}) = \delta F[\rho]/\delta\rho(\mathbf{x}) \rightarrow 0$ in ground state

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  3. Add a source coupled to the *divergent* pair density
     $\Longrightarrow$ e.g., $j\langle \psi_\uparrow^\dagger\psi_\downarrow^\dagger + \psi_\downarrow\psi_\uparrow \rangle \Longrightarrow$ set j to zero in ground state

Generalizing the KLW Inversion Approach back

- Generalizations: Kohn-Sham DFT, other sources, pairing
  1. $\mu N + J(\mathbf{x})\rho(\mathbf{x})$ with $J(\mathbf{x}) = \delta F[\rho]/\delta\rho(\mathbf{x}) \rightarrow 0$ in ground state
  2. Add a source coupled to the kinetic energy density

$$+\eta(\mathbf{x})\tau(\mathbf{x}) \quad \text{where} \quad \tau(x) \equiv \langle \nabla\psi^\dagger \cdot \nabla\psi \rangle$$

$\Longrightarrow M^*(\mathbf{x})$ in the Kohn-Sham equation (cf. Skyrme)

$$\left[-\frac{\nabla^2}{2M} + v_{\mathrm{KS}}(\mathbf{x})\right]\psi_\alpha = \epsilon_\alpha\psi_\alpha \Longrightarrow \left[-\nabla\frac{1}{M^*(\mathbf{x})}\nabla + v_{\mathrm{KS}}(\mathbf{x})\right]\psi_\alpha = \epsilon_\alpha\psi_\alpha$$

  3. Add a source coupled to the *divergent* pair density
     $\Longrightarrow$ e.g., $j\langle\psi_\uparrow^\dagger\psi_\downarrow^\dagger + \psi_\downarrow\psi_\uparrow\rangle \Longrightarrow$ set j to zero in ground state
- Same inversion method, but use $[j]_{\mathrm{gs}} = j_0 + j_1 + j_2 + \cdots = 0$
  $\Longrightarrow$ find j_0 iteratively: from $[j_0]_{\mathrm{old}}$ find $[j_0]_{\mathrm{new}} = -j_1 - j_2 + \cdots$