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

- 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.
- 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.
- 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 Somewhat out of date, but still a good, encyclopedic guide to the nuclear many-body problem.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.
Outline

DFT from Effective Actions

EFT for Dilute Fermi Systems

DFT via EFT

Summary II: DFT from EFT
DFT from Effective Actions

EFT for Dilute Fermi Systems

DFT via EFT

Summary II: DFT from EFT
Density Functional Theory (DFT)

- Hohenberg-Kohn: There exists an energy functional $E_{\text{ext}}[\rho] \ldots$

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

- $F_{\text{HK}}$ is universal (same for any external $v_{\text{ext}}$) $\implies$ $H_2$ to DNA!

- Useful if you can approximate the energy functional

- Introduce orbitals and minimize energy functional $\implies E_{gs}, \rho_{gs}$
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:

$$Z = \text{Tr} \ e^{-\beta g \sum_{\{i,j\}} S_i S_j}$$
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:
  \[ Z = \text{Tr} \, e^{-\beta g \sum_{\{i,j\}} S_i S_j} \]
- The magnetization $M$ is
  \[
  M = \left\langle \sum_i S_i \right\rangle \\
  = \frac{1}{Z} \text{Tr} \left[ \left( \sum_i S_i \right) e^{-\beta g \sum_{\{i,j\}} S_i S_j} \right]
  \]
The source probes configurations near the ground state

\[ \mathcal{Z}[H] = e^{-\beta F[H]} = \text{Tr} \ e^{-\beta (g \sum_{\{i,j\}} S_i S_j - H \sum_i S_i)} \]
Add A Magnetic Probe Source $\mathcal{H}$

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- Variations of the source yield the magnetization

$$M = \left\langle \sum_i S_i \right\rangle_{\mathcal{H}} = -\frac{\partial F[\mathcal{H}]}{\partial H}$$
Add A Magnetic Probe Source $H$

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- Variations of the source yield the magnetization

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

- $F[H]$ 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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Legendre Transformation to Effective Action

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- Legendre transform to the Gibbs free energy
  \[ \Gamma[M] = F[H] + H M \]
Legendre Transformation to Effective Action

- Find $H[M]$ by inverting
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- Legendre transform to the Gibbs free energy
  \[ \Gamma[M] = F[H] + HM \]

- The ground-state magnetization $M_{gs}$ follows by minimizing $\Gamma[M]$: 
  \[ H = \frac{\partial \Gamma[M]}{\partial M} \rightarrow \left. \frac{\partial \Gamma[M]}{\partial M} \right|_{M_{gs}} = 0 \]
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:

$$Z[J] = e^{-W[J]} \sim \text{Tr} e^{-\beta(\hat{H} + J\hat{\rho})} \rightarrow \int \mathcal{D}[\psi^\dagger] \mathcal{D}[\psi] e^{-\int [\mathcal{L} + J\psi^\dagger\psi]}$$

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

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

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

$$\Gamma[\rho] = W[J] - \int J \rho \quad \text{and} \quad J(x) = -\frac{\delta \Gamma[\rho]}{\delta \rho(x)}$$
Partition Function in Zero Temperature Limit

- Consider Hamiltonian with time-independent source \( J(x) \):
  \[
  \hat{H}(J) = \hat{H} + \int J \psi^\dagger \psi
  \]

- If ground state is isolated (and bounded from below),
  \[
  e^{-\beta \hat{H}} = e^{-\beta E_0} \left[ |0\rangle \langle 0| + O\left(e^{-\beta(E_1-E_0)}\right) \right]
  \]

- As \( \beta \to \infty \), \( Z[J] \leftrightarrow \) ground state of \( \hat{H}(J) \) with energy \( E_0(J) \)
  \[
  Z[J] = e^{-W[J]} \sim \text{Tr} e^{-\beta (\hat{H}+J\hat{\rho})} \implies E_0(J) = \lim_{\beta \to \infty} -\frac{1}{\beta} \log Z[J] = \frac{1}{\beta} W[J]
  \]
Partition Function in Zero Temperature Limit

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- As \( \beta \to \infty \), \( Z[J] \longrightarrow \) ground state of \( \hat{H}(J) \) with energy \( E_0(J) \)
  \[
  Z[J] = e^{-W[J]} \sim \text{Tr} \ e^{-\beta(\hat{H}+J \hat{\rho})} \longrightarrow E_0(J) = \lim_{\beta \to \infty} -\frac{1}{\beta} \log Z[J] = \frac{1}{\beta} W[J]
  \]

- Substitute and separate out the pieces:
  \[
  E_0(J) = \langle \hat{H}(J) \rangle_J = \langle \hat{H} \rangle_J + \int J \langle \psi^\dagger \psi \rangle_J = \langle \hat{H} \rangle_J + \int J \rho(J)
  \]

- Expectation value of \( \hat{H} \) in ground state generated by \( J[\rho] \)
  \[
  \langle \hat{H} \rangle_J = E_0(J) - \int J \rho = \frac{1}{\beta} \Gamma[\rho]
  \]
Putting it all together . . .

\[ \frac{1}{\beta} \Gamma[\rho] = \langle \hat{H} \rangle_J \xrightarrow{J \to 0} E_0 \quad \text{and} \quad J(x) = -\frac{\delta \Gamma[\rho]}{\delta \rho(x)} \xrightarrow{J \to 0} \frac{\delta \Gamma[\rho]}{\delta \rho(x)} \bigg|_{\rho_{gs}(x)} = 0 \]

\[ \Rightarrow \text{For static } \rho(x), \Gamma[\rho] \propto \text{the DFT energy functional } F_{HK}! \]
Putting it all together . . .

\[ \frac{1}{\beta} \Gamma[\rho] = \langle \hat{H} \rangle \xrightarrow{J \to 0} E_0 \quad \text{and} \quad J(x) = -\frac{\delta \Gamma[\rho]}{\delta \rho(x)} \xrightarrow{J \to 0} \delta \frac{\delta \Gamma[\rho]}{\delta \rho(x)} \bigg|_{\rho_{\text{gs}}(x)} = 0 \]

\[ \quad \implies \quad \text{For static } \rho(x), \, \Gamma[\rho] \propto \text{the DFT energy functional } F_{\text{HK}}! \]

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

\[
\frac{1}{\beta} \Gamma[\rho] = \langle \hat{\mathcal{H}} \rangle \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_{\text{gs}}(x)} = 0
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⇒ For static \( \rho(x) \), \( \Gamma[\rho] \propto \) the DFT energy functional \( F_{\text{HK}} \)!

- The true ground state (with \( J = 0 \)) is a variational minimum
  - So more sources should be better! (e.g., \( \Gamma[\rho, \tau, J, \cdots] \))
- 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
  ⇒ 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
     \[ \Rightarrow \text{LDA functional + standard Kohn-Sham procedure} \]
   - Add semi-empirical gradient expansion

2. RG approach [Polonyi/Schwenk] \[ \Rightarrow \text{Friday} \]

3. Use auxiliary fields [Faussurier, Valiev/Fernando, Diehl/Wetterich]
   - Couple \( \psi^\dagger \psi \) to auxiliary field \( \varphi \); 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]
   \[ \Rightarrow \text{systematic Kohn-Sham DFT} \]
   - Relies on an order-by-order expansion \[ \Rightarrow \text{EFT power counting} \]
Outline

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Summary II: DFT from EFT
“Simple” Many-Body Problem: Hard Spheres

- Infinite potential at radius $R$
  \[ \sin(kr+\delta) \]
- Scattering length $a_0 = R$
- Dilute $\rho R^3 \ll 1 \implies k_F a_0 \ll 1$
- What is the energy/particle?
- Ref.: nucl-th/0004043
Quick Review of Scattering

\[ \frac{P}{2} + k \quad \frac{P}{2} + k' \]

\[ \frac{P}{2} - k \quad \frac{P}{2} - k' \]

- Relative motion with total \( P = 0 \): \( \psi(r) \xrightarrow{r \to \infty} e^{i k \cdot r} + f(k, \theta) \frac{e^{i k r}}{r} \)
  
  where \( k^2 = k'^2 = ME_k \) and \( \cos \theta = \hat{k} \cdot \hat{k}' \)

- Differential cross section is \( d\sigma / d\Omega = |f(k, \theta)|^2 \)
Quick Review of Scattering

Relative motion with total \( P = 0 \):
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Differential cross section is \( d\sigma/d\Omega = |f(k, \theta)|^2 \)

Central \( V \) \( \Longrightarrow \) partial waves:
\[
f(k, \theta) = \sum_l (2l + 1) f_l(k) P_l(\cos \theta)
\]
where
\[
f_l(k) = \frac{e^{i\delta_l(k)} \sin \delta_l(k)}{k} = \frac{1}{k \cot \delta_l(k) - ik}
\]
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 \( l = 0 \):

\[
k \cot \delta_0 = -\frac{1}{a_0} + \frac{1}{2} r_0 k^2 - Pr_0^3 k^4 + \cdots
\]

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 \( \Rightarrow \) cold atoms

The effective range expansion for hard sphere scattering is:

\[
k \cot(-kR) = -\frac{1}{R} + \frac{1}{3} Rk^2 + \cdots \quad \Rightarrow \quad a_0 = R \quad r_0 = 2R/3
\]

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,

\[ \langle k | V_{\text{eft}} | k' \rangle = C_0 + \frac{1}{2} C_2 (k^2 + k'^2) + C'_2 k \cdot k' + \cdots \]

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

\[ \mathcal{L}_{\text{eft}} = \psi^\dagger \left[ i \frac{\partial}{\partial t} + \frac{\nabla^2}{2M} \right] \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 + \frac{C_2}{16} (\psi^\dagger \psi^\dagger \nabla^2 \psi) + \text{h.c.} + \frac{C'_2}{8} (\psi \nabla \psi)^\dagger \cdot (\psi \nabla \psi) - \frac{D_0}{6} (\psi^\dagger \psi)^3 + \cdots \]

Dimensional analysis \( \implies \) \( C_{2i} \sim \frac{4\pi}{M} R^{2i+1} \), \( D_{2i} \sim \frac{4\pi}{M} R^{2i+4} \).
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

$$\mathcal{L}_{\text{eft}} = \psi^\dagger \left[ i \frac{\partial}{\partial t} + \frac{\nabla^2}{2M} \right] \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 - \frac{D_0}{6} (\psi^\dagger \psi)^3 + \ldots$$
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2. Declaration of regularization and renormalization scheme
   - natural $a_0 \rightarrow$ dimensional regularization and min. subtraction
Effective Field Theory Ingredients

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2. Declaration of regularization and renormalization scheme

- natural $a_0 \Rightarrow$ dimensional regularization and min. subtraction

3. Well-defined power counting $\Rightarrow$ small expansion parameters

- use the separation of scales $\Rightarrow \frac{k_F}{\Lambda}$ with $\Lambda \sim 1/R \Rightarrow k_F a_0$, etc.

$$\mathcal{O}(k_F^6) : \infty \quad \mathcal{O}(k_F^7) : \quad + \quad \infty$$

$$\mathcal{E} = \rho \frac{k_F^2}{2M} \left[ \frac{3}{5} + \frac{2}{3\pi} (k_F a_0) + \frac{4}{35\pi^2} (11 - 2 \ln 2) (k_F a_0)^2 + \cdots \right]$$
Feynman Rules for EFT Vertices

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

\[ + \frac{C'_2}{8} (\psi \nabla \psi)^\dagger \cdot (\psi \nabla \psi) - \frac{D_0}{6} (\psi^\dagger \psi)^3 + \ldots \]

P/2 + k' P/2 + k

P/2 - k P/2 - k'

\[ -i \langle k' | V_{\text{EFT}} | k \rangle \]

\[ -i C_0 \]

\[ -i C_2 \frac{k^2 + k'^2}{2} \]

\[ -i C'_2 k \cdot k' \]

\[ -i D_0 \]

\[ = \quad + \quad + \quad + \quad \ldots \]
Renormalization

- Reproduce $f_0(k)$ in perturbation theory (Born series):
  \[ f_0(k) \propto a_0 - ia_0^2 k - (a_0^3 - a_0^2 r_0/2)k^2 + O(k^3 a_0^4) \]

- Consider the leading potential $V^{(0)}_{\text{EFT}}(x) = C_0 \delta(x)$ or
  \[ \langle k | V_{\text{eft}}^{(0)} | k' \rangle \implies \quad \implies C_0 \]

- Choosing $C_0 \propto a_0$ gets the first term. Now $\langle k | V G_0 V | k' \rangle$:
  \[ \implies C_0 M \int \frac{d^3q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\epsilon} \quad C_0 \implies \infty! \]
  \[ \implies \text{Linear divergence!} \]
Renormalization

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- Choosing $C_0 \propto a_0$ gets the first term. Now $\langle k | V G_0 V | k' \rangle$:
  \[ \implies \int_{\Lambda_c} \frac{d^3q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\epsilon} \rightarrow \frac{\Lambda_c}{2\pi^2} - \frac{ik}{4\pi} + \mathcal{O}\left(\frac{k^2}{\Lambda_c}\right) \]

  \[ \implies \text{If cutoff at } \Lambda_c, \text{ then can absorb into } C_0, \text{ but all powers of } k^2 \]
Renormalization

- Reproduce $f_0(k)$ in perturbation theory (Born series):
  \[ f_0(k) \propto a_0 - ia_0^2 k - (a_0^3 - a_0^2 r_0/2)k^2 + \mathcal{O}(k^3 a_0^4) \]

- Consider the leading potential $V^{(0)}_{\text{EFT}}(x) = C_0 \delta(x)$ or
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- Choosing $C_0 \propto a_0$ gets the first term. Now $\langle k | V G_0 V | k' \rangle$:
  \[ \implies \int \frac{d^D q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\epsilon} \xrightarrow{D \to 3} - \frac{4\pi}{4\pi} \]

  Dimensional regularization with minimal subtraction
  \[ \implies \text{only one power of } k! \]
Dim. reg. + minimal subtraction $\implies$ simple power counting:

\[
\begin{align*}
\frac{P}{2} + k & \quad \frac{P}{2} + k' \\
\frac{P}{2} - k & \quad \frac{P}{2} - k' \\
\end{align*}
\]

\[iT(k, \cos \theta) = -iC_0 - \frac{M}{4\pi} (C_0)^2 k\]

\[+ \quad + \quad \quad + \quad \quad \quad + \quad \mathcal{O}(k^3)\]

\[+ i \left(\frac{M}{4\pi}\right)^2 (C_0)^3 k^2 \quad - iC_2 k^2 \quad - iC'_2 k^2 \cos \theta\]

Matching:

\[C_0 = \frac{4\pi}{M} a_0 = \frac{4\pi}{M} R, \quad C_2 = \frac{4\pi}{M} \frac{a_0^2 r_0}{2} = \frac{4\pi}{M} \frac{R^3}{3}, \quad \ldots\]

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 $\nu$ (e.g., for nuclei, $\nu = 4$)
  - fill momentum states up to Fermi momentum $k_F$

\[ N = \nu \sum_{k} k_F, \quad E = \nu \sum_{k} \frac{\hbar^2 k^2}{2M} \]
Noninteracting Fermi Sea at $T = 0$

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$$N = \nu \sum_{k} k_F, \quad E = \nu \sum_{k} \frac{\hbar^2 k^2}{2M}$$

- Use: $\int F(k) \, dk \approx \sum_i F(k_i) \Delta k_i = \sum_i F(k_i) \frac{2\pi}{L} \Delta n_i = \frac{2\pi}{L} \sum_i F(k_i)$
Noninteracting Fermi Sea at $T = 0$

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  - spin-isospin degeneracy $\nu$ (e.g., for nuclei, $\nu = 4$)
  - fill momentum states up to Fermi momentum $k_F$

$$N = \nu \sum_k \frac{k_F}{\nu} , \quad E = \nu \sum_k \frac{\hbar^2 k^2}{2M}$$

- Use: $\int F(k) \, dk \approx \sum_i F(k_i) \Delta k_i = \sum_i F(k_i) \frac{2\pi}{L} \Delta n_i = \frac{2\pi}{L} \sum_i F(k_i)$

- In 1-D:
  $$N = \nu \frac{L}{2\pi} \int_{-k_F}^{+k_F} dk = \frac{\nu k_F}{\pi} L \quad \Rightarrow \quad \rho = \frac{N}{L} = \frac{\nu k_F}{\pi} ; \quad \frac{E}{L} = \frac{1}{3} \frac{\hbar^2 k_F^2}{2M} \rho$$

- In 3-D:
  $$N = \nu \frac{V}{(2\pi)^3} \int d^3 k = \frac{\nu k_F^3}{6\pi^2} V \quad \Rightarrow \quad \rho = \frac{N}{V} = \frac{\nu k_F^3}{6\pi^2} ; \quad \frac{E}{V} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2M} \rho$$
Noninteracting Fermi Sea at $T = 0$

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

$$N = \nu \sum_k 1, \quad E = \nu \sum_k \frac{\hbar^2 k^2}{2M}$$

- Use: $\int F(k) \, dk \approx \sum_i F(k_i) \Delta k_i = \sum_i F(k_i) \frac{2\pi}{L} \Delta n_i = \frac{2\pi}{L} \sum_i F(k_i)$
- In 1-D:
  $$N = \nu \frac{L}{2\pi} \int_{-k_F}^{+k_F} dk = \nu \frac{k_F}{\pi} L \implies \rho = \frac{N}{L} = \frac{\nu k_F}{\pi}; \quad \frac{E}{L} = \frac{1}{3} \frac{\hbar^2 k_F^2}{2M} \rho$$

- In 3-D:
  $$N = \nu \frac{V}{(2\pi)^3} \int d^3k = \nu \frac{k_F^3}{6\pi^2} V \implies \rho = \frac{N}{V} = \frac{\nu k_F^3}{6\pi^2}; \quad \frac{E}{V} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2M} \rho$$

- Volume/particle $V/N = 1/\rho \sim 1/k_F^3$, so spacing $\sim 1/k_F$
Energy Density From Summing Over Fermi Sea

- Leading order $V_{\text{EFT}}^{(0)}(x) = C_0 \delta(x) \implies V_{\text{EFT}}^{(0)}(k, k') = C_0$

$$\epsilon_{\text{LO}} = \frac{C_0}{2} \nu(\nu - 1) \left( \sum_{k} 1 \right)^2 \propto a_0 k_F^6$$
Energy Density From Summing Over Fermi Sea

- **Leading order**: \( V_{\text{EFT}}^{(0)}(x) = C_0 \delta(x) \implies V_{\text{EFT}}^{(0)}(k, k') = C_0 \)

  \[ \implies \quad \epsilon_{\text{LO}} = \frac{C_0}{2} \nu (\nu - 1) \left( \sum_k 1 \right)^2 \propto a_0 k_F^6 \]

- At the next order, we get a linear divergence again:

  \[ \implies \quad \epsilon_{\text{NLO}} \propto \int_{k_F}^{\infty} \frac{d^3q}{(2\pi)^3} \frac{C_0^2}{k^2 - q^2} \]
Energy Density From Summing Over Fermi Sea

- Leading order $V_{\text{EFT}}^{(0)}(x) = C_0 \delta(x) \implies V_{\text{EFT}}^{(0)}(k, k') = C_0$

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  \[ \implies \quad \varepsilon_{\text{NLO}} \propto \int_{k_F}^{\infty} \frac{d^3q}{(2\pi)^3} \frac{C_0^2}{k^2 - q^2} \]

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

  \[ \int_{k_F}^{\infty} \frac{1}{k^2 - q^2} = \int_0^{\infty} \frac{1}{k^2 - q^2} - \int_0^{k_F} \frac{1}{k^2 - q^2} \xrightarrow{D \rightarrow 3} - \int_0^{k_F} \frac{1}{k^2 - q^2} \propto a_0^2 k_F^7 \]
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 $\tilde{k} \equiv (k_0, \mathbf{k})$ and $[\omega_k \equiv k^2/2M]$

$$iG_0(\tilde{k})_{\alpha\beta} = i\delta_{\alpha\beta}\left(\frac{\theta(k - k_F)}{k_0 - \omega_k + i\epsilon} + \frac{\theta(k_F - k)}{k_0 - \omega_k - i\epsilon}\right)$$

  2. $\beta \bigtriangledown \delta \longrightarrow (\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})$ (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 $e^{ik_00^+}$ for tadpoles

  5. Symmetry factor $i/(S \prod_{l=2}^{l_{\text{max}}}(l!)^k)$ counts vertex permutations and equivalent $l$–tuples of lines
Power Counting

- Power counting rules
  1. for every propagator (line): $M/k_F^2$
  2. for every loop integration: $k_F^5/M$
  3. for every $n$–body vertex with $2i$ derivatives: $k_F^{2i}/M\Lambda^{2i+3n-5}$

- Diagram with $V_{2i}^n$ $n$–body vertices scales as $(k_F)^\beta$ only:

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

- e.g., $O(k_F^6)$:

$$\beta = 5 + (3 \cdot 2 + 2 \cdot 0 - 5) \cdot 1 = 6 \Rightarrow O(k_F^6)$$
Power Counting

- Power counting rules
  1. for every propagator (line): $M/k_F^2$
  2. for every loop integration: $k_F^5/M$
  3. for every $n$–body vertex with $2i$ derivatives: $k_F^{2i}/M\Lambda^{2i+3n-5}$

- Diagram with $V_{2i}^n$ $n$–body vertices scales as $(k_F)^\beta$ only:

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

- e.g., $\quad \implies V_0^2 = 2$

$$\implies \beta = 5 + (3 \cdot 2 + 2 \cdot 0 - 5) \cdot 2 = 7 \implies O(k_F^7)$$
$T = 0$ Energy Density from Hugenholtz Diagrams

$$
\frac{E}{V} = \rho \frac{k_F^2}{2M} \left[ \frac{3}{5} \right]
$$
$T = 0$ Energy Density from Hugenholtz Diagrams

$$\mathcal{O}(k_F^6) : \quad \frac{E}{V} = \rho \frac{k_F^2}{2M} \left[ \frac{3}{5} + (\nu - 1) \frac{2}{3\pi} (k_F a_0) \right]$$
**T = 0 Energy Density from Hugenholtz Diagrams**

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

\[ O(k_F^6) : \]
\[ O(k_F^7) : \]
\[ O(k_F^8) : \]
$T = 0$ Energy Density from Hugenholtz Diagrams

$$\frac{E}{V} = \rho \frac{k_F^2}{2M} \left[ \frac{3}{5} + (\nu - 1) \frac{2}{3\pi} (k_F a_0) \right] + (\nu - 1) \frac{4}{35\pi^2} (11 - 2 \ln 2) (k_F a_0)^2 + (\nu - 1) (0.076 + 0.057(\nu - 3)) (k_F a_0)^3$$
\( T = 0 \) Energy Density from Hugenholtz Diagrams

\[
\frac{E}{V} = \frac{\rho k_F^2}{2M} \left[ \frac{3}{5} + (\nu - 1) \frac{2}{3\pi} (k_F a_0) \right] \\
+ (\nu - 1) \frac{4}{35\pi^2} (11 - 2\ln 2)(k_F a_0)^2 \\
+ (\nu - 1) (0.076 + 0.057(\nu - 3))(k_F a_0)^3 \\
+ (\nu - 1) \frac{1}{10\pi} (k_F r_0)(k_F a_0)^2 \\
+ (\nu + 1) \frac{1}{5\pi} (k_F a_p)^3 + \cdots
\]
Looks Like a Power Series in $k_F$! Is it?
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- New logarithmic divergences in 3–3 scattering

\[ \propto \left( C_0 \right)^4 \ln(\frac{k}{\Lambda_c}) \]
Looks Like a Power Series in $k_F$! Is it?

- New logarithmic divergences in 3–3 scattering

\[ \propto (C_0)^4 \ln(k/\Lambda_c) \]

- Changes in $\Lambda_c$ must be absorbed by 3-body coupling $D_0(\Lambda_c)$

\[ \implies D_0(\Lambda_c) \propto (C_0)^4 \ln(a_0 \Lambda_c) + \text{const.} \quad \text{[Braaten & Nieto]} \]

\[ \frac{d}{d\Lambda_c} \left[ \begin{array}{c}
\text{Diagrams}
\end{array} \right] = 0 \implies \text{fixes coefficient!} \]
Looks Like a Power Series in $k_F$! Is it?

- New logarithmic divergences in 3–3 scattering

\[ \propto (C_0)^4 \ln(k/\Lambda_c) \]

- Changes in $\Lambda_c$ must be absorbed by 3-body coupling $D_0(\Lambda_c)$

\[ \Rightarrow D_0(\Lambda_c) \propto (C_0)^4 \ln(a_0\Lambda_c) + \text{const.} \quad \text{[Braaten & Nieto]} \]

\[ \frac{d}{d\Lambda_c} \left[ \begin{array}{c} \text{diagrams} \end{array} \right] = 0 \Rightarrow \text{fixes coefficient!} \]

- What does this imply for the energy density?

\[ \mathcal{O}(k_F^0 \ln(k_F)) : \quad + \quad + \quad \ldots \propto (\nu-2)(\nu-1)(k_Fa_0)^4 \ln(k_Fa_0) \]
The many-body energy density is perturbative in $k_F a_0$
- efficiently reproduced by the EFT approach

Power counting $\Rightarrow$ error estimate from omitted diagrams

Three-body forces are inevitable in a low-energy effective theory
- and not unique $\Rightarrow$ 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:

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

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

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

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

$$\Gamma[\rho] = W[J] - \int J \rho \quad \text{and} \quad J(x) = -\frac{\delta \Gamma[\rho]}{\delta \rho(x)}$$
What can EFT do for DFT?

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

\[
G_0^0(x, x'; \omega) = \sum_\alpha \psi_\alpha(x) \psi^*_\alpha(x') \left[ \frac{\theta(\epsilon_\alpha - \epsilon_F)}{\omega - \epsilon_\alpha + i\eta} + \frac{\theta(\epsilon_F - \epsilon_\alpha)}{\omega - \epsilon_\alpha - i\eta} \right]
\]

where \( \psi_\alpha(x) \) satisfies:

\[
\left[ -\frac{\nabla^2}{2M} + v_{ext}(x) - J(x) \right] \psi_\alpha(x) = \epsilon_\alpha \psi_\alpha(x)
\]
What can EFT do for DFT?

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

$$G^0_J(x, x'; \omega) = \sum_{\alpha} \psi_\alpha(x) \psi^*_\alpha(x') \left[ \frac{\theta(\epsilon_\alpha - \epsilon_F)}{\omega - \epsilon_\alpha + i\eta} + \frac{\theta(\epsilon_F - \epsilon_\alpha)}{\omega - \epsilon_\alpha - i\eta} \right]$$

where $\psi_\alpha(x)$ satisfies:

$$\left[ -\frac{\nabla^2}{2M} + \nu_{\text{ext}}(x) - J(x) \right] \psi_\alpha(x) = \epsilon_\alpha \psi_\alpha(x)$$

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

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

$$= -\frac{1}{2} \frac{(\nu - 1)}{\nu} C_0 \int d^3x [\rho_J(x)]^2 \quad \text{where} \quad \rho_J(x) \equiv \nu \sum_{\alpha} |\psi_\alpha(x)|^2$$
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 $J(x) = J_0(x) + J_{LO}(x) + J_{NLO}(x) + \ldots$
  - Two conditions on $J_0$:

    $$\rho(x) = \frac{\delta W_0[J_0]}{\delta J_0(x)} \quad \text{and} \quad J_0(x)|_{\rho=\rho_{gs}} = \frac{\delta \Gamma_{\text{interacting}}[\rho]}{\delta \rho(x)}|_{\rho=\rho_{gs}}$$
What can Power Counting do for DFT?

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

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

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

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

- Interpretation: \( J_0 \) is the external potential that yields for a noninteracting system the exact density
  - This is the Kohn-Sham potential!
  - Two conditions involving \( J_0 \) \( \implies \) Self-consistency
**Kohn-Sham Via Inversion Method** *(cf. KLW [1960])*

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

  \[
  \mathcal{W}[J, \lambda] = \mathcal{W}_0[J] + \lambda \mathcal{W}_1[J] + \lambda^2 \mathcal{W}_2[J] + \cdots
  \]

  \[
  J[\rho, \lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots
  \]

  \[
  \Gamma[\rho, \lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots
  \]

- Start with exact expressions for $\Gamma$ and $\rho$  
  [note: $\beta$ or $T = 1$]

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

\[
\Rightarrow \text{plug in expansions with } \rho \text{ treated as order unity}
\]
Kohn-Sham Via Inversion Method (cf. KLW [1960])

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

  \[
  \mathcal{W}[J, \lambda] = \mathcal{W}_0[J] + \lambda \mathcal{W}_1[J] + \lambda^2 \mathcal{W}_2[J] + \cdots
  \]

  \[
  J[\rho, \lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots
  \]

  \[
  \Gamma[\rho, \lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots
  \]

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

  \[
  \Gamma_0[\rho] = \mathcal{W}_0[J_0] - \int d^4x \, J_0(x) \rho(x) \quad \Rightarrow \quad \rho(x) = \frac{\delta \mathcal{W}_0[J_0]}{\delta J_0(x)}
  \]

  \[
  \Rightarrow \text{Kohn-Sham system with the exact density! } J_0 \equiv V_{KS}
  \]
Kohn-Sham Via Inversion Method (cf. KLW [1960])

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

\[ \mathcal{W}[J, \lambda] = \mathcal{W}_0[J] + \lambda \mathcal{W}_1[J] + \lambda^2 \mathcal{W}_2[J] + \cdots \]

- assume
\[ J[\rho, \lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots \]

- derive
\[ \Gamma[\rho, \lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots \]

- Zeroth order is noninteracting system with potential $J_0(x)$
\[ \Gamma_0[\rho] = \mathcal{W}_0[J_0] - \int d^4 x \, J_0(x) \rho(x) \quad \implies \quad \rho(x) = \frac{\delta \mathcal{W}_0[J_0]}{\delta J_0(x)} \]

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

- Diagonalize $\mathcal{W}_0[J_0]$ by introducing KS orbitals $\implies$ sum of $\varepsilon_i$'s
Kohn-Sham Via Inversion Method (cf. KLW [1960])

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

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

\[ J[\rho, \lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots \]

\[ \Gamma[\rho, \lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots \]

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

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

\[ \implies \text{Kohn-Sham system with the exact density! } J_0 \equiv V_{KS} \]

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

- Find $J_0$ for the ground state via self-consistency loop:

\[ J_0 \rightarrow W_1 \rightarrow \Gamma_1 \rightarrow J_1 \rightarrow W_2 \rightarrow \Gamma_2 \rightarrow \cdots \implies J_0(x) = \sum_{i>0} \frac{\delta \Gamma_i[\rho]}{\delta \rho(x)} \]
Kohn-Sham Potential

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

\[
\text{since } J_0(x) = \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta \rho(x)}
\]

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

\[
J_0(x) = \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta \rho(x)} = \int \left( \frac{\delta \rho(x)}{\delta J_0(y)} \right)^{-1} \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta J_0(y)} = - \quad \infty \quad - \quad \infty + \cdots
\]

\[
= \quad \infty \quad - \quad \infty + \cdots
\]

- New Feynman rules for $\Gamma_{\text{int}} \longrightarrow$ anomalous diagrams

\[
\Gamma_{\text{int}} = \quad \infty \quad + \quad \infty \quad + \quad \infty \quad + \quad \infty \quad + \cdots
\]
Kohn-Sham Potential

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

$$J_0(x) = \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta \rho(x)}$$

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

$$J_0(x) = - \quad \quad + \quad \quad + \cdots$$

$$= \quad \quad + \quad \quad + \cdots$$

- New Feynman rules for $\Gamma_{\text{int}} \rightarrow$ anomalous diagrams

$$\Gamma_{\text{int}} = \quad + \quad + \quad + \cdots$$
Kohn-Sham Potential

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

$$J_0(x) = \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta \rho(x)}$$

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

$$J_0(x) = - \begin{array}{c}
\text{Diagram 1} \\
+ \text{Diagram 2} \\
+ \cdots
\end{array}$$

$$= \begin{array}{c}
\text{Diagram 1} \\
+ \text{Diagram 2} \\
+ \cdots
\end{array}$$

- New Feynman rules for $\Gamma_{\text{int}} \implies$ anomalous diagrams

$$\Gamma_{\text{int}} = \begin{array}{c}
\text{Diagram 1} \\
+ \text{Diagram 2} \\
+ \text{Diagram 3} \\
+ \text{Diagram 4} \\
+ \cdots
\end{array}$$
Kohn-Sham Potential

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

$$J_0(\mathbf{x}) = \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta \rho(\mathbf{x})}$$

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

\[
J_0(\mathbf{x}) = - \begin{array}{c}
  \text{Diagram 1}
\end{array} + \begin{array}{c}
  \text{Diagram 2}
\end{array} + \cdots
\]

\[
= \begin{array}{c}
  \text{Diagram 1}
\end{array} + \begin{array}{c}
  \text{Diagram 2}
\end{array} + \cdots
\]

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

\[
\Gamma_{\text{int}} = \begin{array}{c}
  \text{Diagram 1}
\end{array} + \begin{array}{c}
  \text{Diagram 2}
\end{array} + \begin{array}{c}
  \text{Diagram 3}
\end{array} - \begin{array}{c}
  \text{Diagram 4}
\end{array} + \cdots
\]
Kohn-Sham Potential

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

\[
J_0(x) = \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta \rho(x)}
\]

since $J_0(x) = \delta \Gamma_{\text{int}}[\rho] / \delta \rho(x)$

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

\[
J_0(x) = - \quad \text{Diagram 1} \quad + \quad \text{Diagram 2} \quad + \cdots
\]

\[
= \quad \text{Diagram 3} \quad + \quad \text{Diagram 4} \quad + \cdots
\]

- New Feynman rules for $\Gamma_{\text{int}}$ $\implies$ anomalous diagrams

\[
\Gamma_{\text{int}} = \quad \text{Diagram 5} \quad + \quad \text{Diagram 6} \quad + \cdots
\]
Now Source $J_0(x)$ is the Background Field

- Construct $W[J]$ and new diagrams for $\Gamma[\rho]$ order-by-order in an expansion (e.g., EFT power counting)
- Propagators (lines) are in the background field $J_0(x)$

$$G^0_{\text{KS}}(x, x'; \omega) = \sum_{\alpha} \psi_{\alpha}(x)\psi^*_{\alpha}(x') \left[ \frac{\theta(\epsilon_{\alpha} - \epsilon_F)}{\omega - \epsilon_{\alpha} + i\eta} + \frac{\theta(\epsilon_F - \epsilon_{\alpha})}{\omega - \epsilon_{\alpha} - i\eta} \right]$$

where $\psi_{\alpha}(x)$ satisfies:

$$\left[ -\frac{\nabla^2}{2M} + v(x) - J_0(x) \right] \psi_{\alpha}(x) = \epsilon_{\alpha} \psi_{\alpha}(x)$$
Now Source $J_0(x)$ is the Background Field

- Construct $W[J]$ and new diagrams for $\Gamma[\rho]$ order-by-order in an expansion (e.g., EFT power counting)
- Propagators (lines) are in the background field $J_0(x)$

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where $\psi_{\alpha}(x)$ satisfies: $[-\nabla^2 + v(x) - J_0(x)] \psi_{\alpha}(x) = \epsilon_{\alpha} \psi_{\alpha}(x)$

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

$$W_1[J_0] = \frac{1}{2} \nu(\nu - 1) C_0 \int d^3x \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} G^0_{KS}(x, x; \omega) G^0_{KS}(x, x; \omega')$$

$$= -\frac{1}{2} \frac{(\nu - 1)}{\nu} C_0 \int d^3x [\rho_{J_0}(x)]^2 \text{ where } \rho_{J_0}(x) \equiv \nu \sum_{\alpha} \vert \psi_{\alpha}(x) \vert^2$$
$T = 0$ LDA Energy from Hugenholtz Diagrams

Uniform system: Each line is non-interacting propagator

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

\[
+ (\nu - 1) (0.076 + 0.057(\nu - 3)) (k_F a_0)^3
\]

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

\[
+ (\nu + 1) \frac{1}{5\pi} (k_F a_\rho)^3 + \cdots
\]
$T = 0$ LDA Energy from Hugenholtz Diagrams

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

\[
\Gamma[\rho] = \int d^3x \left[ K(x) + \frac{1}{2} \frac{(\nu - 1)}{\nu} \frac{4\pi a_0}{M} [\rho(x)]^2 \right.
\]

\[
+ d_1 a_0^2 [\rho(x)]^{7/3}
\]

\[
+ d_2 a_0^3 [\rho(x)]^{8/3}
\]

\[
+ d_3 a_0^2 r_0 [\rho(x)]^{8/3}
\]

\[
+ d_4 a_0^3 [\rho(x)]^{8/3} + \ldots \]

Dick Furnstahl

EFT for DFT II
Kohn-Sham $J_0$ According to the EFT Expansion

- Follows immediately in the local density approximation (LDA)

$$J_0(x) = \begin{pmatrix} \end{pmatrix}$$
Kohn-Sham $J_0$ According to the EFT Expansion

- Follows immediately in the local density approximation (LDA)

$$ LO : \quad J_0(x) = - \frac{(\nu - 1)}{\nu} \frac{4\pi a_0}{M} \rho(x) $$
Kohn-Sham $J_0$ According to the EFT Expansion

- Follows immediately in the local density approximation (LDA)

\[
J_0(x) = -\frac{(\nu - 1)}{\nu} \frac{4\pi a_0}{M} \rho(x) - c_1 \frac{a_0^2}{2M} \left[\rho(x)\right]^{4/3}
\]
Kohn-Sham $J_0$ According to the EFT Expansion

- Follows immediately in the local density approximation (LDA)

\[ J_0(x) = - \frac{(\nu - 1)}{\nu} \frac{4\pi a_0}{M} \rho(x) \]

\[ - c_1 \frac{a_0^2}{2M} [\rho(x)]^{4/3} \]

LO: 

NLO: 

NNLO: 

Dick Furnstahl

EFT for DFT II
Kohn-Sham $J_0$ According to the EFT Expansion

- Follows immediately in the local density approximation (LDA)

\[
J_0(x) = \left[ -\frac{(\nu - 1)}{\nu} \frac{4\pi a_0}{M} \rho(x) \right.
- c_1 \frac{a_0^2}{2M} [\rho(x)]^{4/3}
- c_2 a_0^3 [\rho(x)]^{5/3}
\]
Kohn-Sham $J_0$ According to the EFT Expansion

- Follows immediately in the local density approximation (LDA)

$$J_0(x) = \left[ -\frac{(\nu - 1)}{\nu} \frac{4\pi a_0}{M} \rho(x) \right. $$

$$- c_1 \frac{a_0^2}{2M} [\rho(x)]^{4/3} $$

$$- c_2 a_0^3 [\rho(x)]^{5/3} $$

$$- c_3 a_0^2 r_0 [\rho(x)]^{5/3} $$

$$- c_4 a_0^3 [\rho(x)]^{5/3} + \cdots \right]$$
Dilute Fermi Gas in a Harmonic Trap

Iteration procedure:

1. Guess an initial density profile \( \rho(r) \) (e.g., Thomas-Fermi).
2. Evaluate local single-particle potential \( V_{KS}(r) \equiv v_{ext}(r) - J_0(r) \).
3. Solve for lowest \( \mathcal{A} \) states (including degeneracies): \( \{ \psi_\alpha, \epsilon_\alpha \} \)
   \[
   -\nabla^2 \frac{M}{2} + V_{KS}(r) \psi_\alpha(x) = \epsilon_\alpha \psi_\alpha(x),
   \]
4. Compute a new density \( \rho(r) = \sum_{\mathcal{A}} |\psi_\alpha(x)|^2 \) 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!
Dilute Fermi Gas in a Harmonic Trap

Iteration procedure:

1. Guess an initial density profile $\rho(r)$ (e.g., Thomas-Fermi)
Dilute Fermi Gas in a Harmonic Trap

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Dilute Fermi Gas in a Harmonic Trap

Iteration procedure:

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3. Solve for lowest $A$ states (including degeneracies): $\{\psi_\alpha, \epsilon_\alpha\}$

$$\left[-\frac{\nabla^2}{2M} + V_{KS}(r)\right] \psi_\alpha(x) = \epsilon_\alpha \psi_\alpha(x)$$
Dilute Fermi Gas in a Harmonic Trap

Iteration procedure:

1. Guess an initial density profile $\rho(r)$ (e.g., Thomas-Fermi)
2. Evaluate local single-particle potential $V_{\text{KS}}(r) \equiv v_{\text{ext}}(r) - J_0(r)$
3. Solve for lowest $A$ states (including degeneracies): $\{\psi_\alpha, \epsilon_\alpha\}$
   \[
   \left[-\frac{\nabla^2}{2M} + V_{\text{KS}}(r)\right] \psi_\alpha(x) = \epsilon_\alpha \psi_\alpha(x)
   \]
4. Compute a new density $\rho(r) = \sum_{\alpha=1}^{A} |\psi_\alpha(x)|^2$
   - other observables are functionals of $\{\psi_\alpha, \epsilon_\alpha\}$
Dilute Fermi Gas in a Harmonic Trap

Iteration procedure:

1. Guess an initial density profile $\rho(r)$ (e.g., Thomas-Fermi)
2. Evaluate local single-particle potential $V_{KS}(r) \equiv v_{ext}(r) - J_0(r)$
3. Solve for lowest $A$ states (including degeneracies): $\{\psi_\alpha, \epsilon_\alpha\}$
   \begin{equation}
   \left[-\frac{\nabla^2}{2M} + V_{KS}(r)\right] \psi_\alpha(x) = \epsilon_\alpha \psi_\alpha(x)
   \end{equation}
4. Compute a new density $\rho(r) = \sum_{\alpha=1}^A |\psi_\alpha(x)|^2$
   - other observables are functionals of $\{\psi_\alpha, \epsilon_\alpha\}$
5. Repeat 2.–4. until changes are small (“self-consistent”)
Dilute Fermi Gas in a Harmonic Trap

Iteration procedure:

1. Guess an initial density profile $\rho(r)$ (e.g., Thomas-Fermi)
2. Evaluate local single-particle potential $V_{KS}(r) \equiv v_{\text{ext}}(r) - J_0(r)$
3. Solve for lowest $A$ states (including degeneracies): $\{\psi_\alpha, \epsilon_\alpha\}$
   
   $$\left[-\frac{\nabla^2}{2M} + V_{KS}(r)\right] \psi_\alpha(x) = \epsilon_\alpha \psi_\alpha(x)$$

4. Compute a new density $\rho(r) = \sum_{\alpha=1}^{A} |\psi_\alpha(x)|^2$
   
   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]

Dilute Fermi Gas in Harmonic Trap
$N_F=7$, $A=240$, $g=2$, $a_s=-0.160$

$E/A <k_{F,a_s}> <r^2>^{1/2}$
$6.750$ $-0.524$ $2.598$

$C_0 = 0$ (exact)
Check Out An Example [nucl-th/0212071]

Dilute Fermi Gas in Harmonic Trap
\[ N_F = 7, \ A = 240, \ g = 2, \ a_s = -0.160 \]

\[ \frac{E}{A} \ < k_F a_s \ < r^2 \frac{1}{2} \]

\begin{align*}
6.750 & \quad -0.524 & \quad 2.598 \\
5.982 & \quad -0.578 & \quad 2.351
\end{align*}
Check Out An Example [nucl-th/0212071]

Dilute Fermi Gas in Harmonic Trap
$N_F=7$, $A=240$, $g=2$, $a_s=-0.160$

$E/A$ $<k_F a_s>$ $<r^2>^{1/2}$
6.750 $-0.524$ $2.598$
5.982 $-0.578$ $2.351$
6.254 $-0.550$ $2.472$
Check Out An Example [nucl-th/0212071]

Dilute Fermi Gas in Harmonic Trap

\[ N_F = 7, \ A = 240, \ g = 2, \ a_s = -0.160 \]

\begin{align*}
\text{E/A} & \quad \langle k_F a_s \rangle & \quad \langle r^2 \rangle^{1/2} \\
6.750 & \quad -0.524 & \quad 2.598 \\
5.982 & \quad -0.578 & \quad 2.351 \\
6.254 & \quad -0.550 & \quad 2.472 \\
6.227 & \quad -0.553 & \quad 2.459 \\
\end{align*}
Other Examples [nucl-th/0212071]

Dilute Fermi Gas in Harmonic Trap
\( g=2, a_s = 0.1600, N_F = 7, A = 240 \)

- \( C_0 = 0 \) (exact)
- Kohn-Sham LO
- Kohn-Sham NLO (LDA)
- Kohn-Sham NNLO (LDA)

Iteration 15
\[
\begin{align*}
(E/A)_{\text{HO}} &= 6.750 \\
(E/A)_{\text{LO}} &= 7.355 \\
(E/A)_{\text{NLO}} &= 7.554 \\
(E/A)_{\text{NNLO}} &= 7.567 \\
<k_F a_s>_{\text{NNLO}} &= 0.48
\end{align*}
\]
Other Examples [nucl-th/0212071]

Dilute Fermi Gas in Harmonic Trap
\( g=2, a_s = 0.1600, N_F = 8, A = 330 \)

- \( C_0 = 0 \) (exact)
- Kohn-Sham LO
- Kohn-Sham NLO (LDA)
- Kohn-Sham NNLO (LDA)

Iteration 17

- \( (E/A)_{\text{HO}} = 7.500 \)
- \( (E/A)_{\text{LO}} = 8.206 \)
- \( (E/A)_{\text{NLO}} = 8.448 \)
- \( (E/A)_{\text{NNLO}} = 8.464 \)

- \( \langle k_{F_s} a_s \rangle_{\text{NNLO}} = 0.51 \)
Other Examples [nucl-th/0212071]

Dilute Fermi Gas in Harmonic Trap
\( g=4, a_s=-0.1000, N_F=4, A=140 \)

\[ C_0 = 0 \text{ (exact)} \]

- Kohn-Sham LO
- Kohn-Sham NLO (LDA)
- Kohn-Sham NNLO (LDA)

Iteration 18

\[
\begin{align*}
(E/A)_{HO} &= 4.500 \\
(E/A)_{LO} &= 3.619 \\
(E/A)_{NLO} &= 3.883 \\
(E/A)_{NNLO} &= 3.814 \\
<k_{F_a}>_{NNLO} &= 0.31
\end{align*}
\]
Other Examples [nucl-th/0212071]

Dilute Fermi Gas in Harmonic Trap
\( g=4, a_s = 0.1000, N_F=4, A=140 \)

- \( C_0 = 0 \) (exact)
- Kohn-Sham LO
- Kohn-Sham NLO (LDA)
- Kohn-Sham NNLO (LDA)

Iteration 22
\[
\begin{align*}
(E/A)_{HO} &= 4.500 \\
(E/A)_{LO} &= 5.088 \\
(E/A)_{NLO} &= 5.182 \\
(E/A)_{NNLO} &= 5.204 \\
\langle k_F a_s \rangle_{NNLO} &= 0.24
\end{align*}
\]
Power Counting Terms in Energy Functionals

- Scale contributions according to average density or $\langle k_F \rangle$
Power Counting Terms in Energy Functionals

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

![Graph showing the relationship between energy per particle and orders of approximation (LO, NLO, NNLO) for different values of $n$, $a_s$, and $A$. The graph includes error bars and distinguishes between $n=4, a_s=-0.1, A=140$, $n=4, a_s=+0.1, A=140$, and $n=2, a_s=+0.16, A=330$.](image)
Power Counting Terms in Energy Functionals

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

![Graph showing energy per particle vs. order of approximation (LO, NLO, NNLO)]

Legend:
- $v=4, a_s=-0.1, A=140$
- $v=4, a_s=+0.1, A=140$
- $v=2, a_s=+0.16, A=330$
Power Counting Terms in Energy Functionals

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

![Graph showing energy per particle vs. order of approximation (LO, NLO, NNLO) for different parameters.]

Reasonable estimates \( \Rightarrow \) truncation errors understood
Power Counting Terms in Energy Functionals

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

- Reasonable estimates $\implies$ truncation errors understood

Dick Furnstahl
EFT for DFT II
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 $\rho(x)$, $\tau(x)$, and $J(x)$
  $\implies$ 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
Scale contributions according to average density or $\langle k_F \rangle$.

Reasonable estimates $\Rightarrow$ truncation errors understood.

- × natural ($\Lambda=600$ MeV)
- • Skyrme EFT $\rho^n$
- ○ FZ4 net
- □ FA4 net

**Diagram:**
- **Y-axis:** Energy/particle (MeV)
- **X-axis:** Power of density
- Symbols represent different models and experimental data points.

$\epsilon_0$ indicates the energy scale for the natural density.
Effective Action as Energy Functional: Minkowski

Kohn-Luttinger-Ward Inversion Method
Effective Action as Energy Functional: Minkowski

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

Effective Action as Energy Functional: Minkowski

Kohn-Luttinger-Ward Inversion Method
Kohn-Luttinger-Ward Theorem (1960)

- $T \rightarrow 0$ diagram expansion of $\Omega(\mu, V, T)$ in external $\nu(x)$
  $\implies$ same as $F(N, V, T = 0)$ with $\mu_0$ and no “anomalous”

\[
\Omega(\mu, V, T) = \Omega_0(\mu) + \quad + \quad + \quad + \quad + \quad + \cdots
\]

with $G_0(\mu, T)$

\[
T \rightarrow 0 \quad F(N, V, T = 0) = E_0(N) + \quad + \quad + \quad + \quad + \cdots
\]

with $G_0(\mu_0)$
Kohn-Luttinger-Ward Theorem (1960)

- $T \to 0$ diagram expansion of $\Omega(\mu, V, T)$ in external $\nu(x)$

\[ \Omega(\mu, V, T) = \Omega_0(\mu) + \cdots \]

\[ \text{with } G_0(\mu, T) \]

\[ \lim_{T \to 0} F(N, V, T = 0) = E_0(N) + \cdots \]

\[ \text{with } G_0(\mu_0) \]

- Uniform Fermi system, no external potential (degeneracy $\nu$):

\[ \mu_0(N) = (6\pi^2 N/\nu V)^{2/3} \equiv k_F^2/2M \equiv \epsilon_F^0 \]
Kohn-Luttinger-Ward Theorem (1960)

- $T \to 0$ diagram expansion of $\Omega(\mu, V, T)$ in external $\nu(x)$
  $\implies$ same as $F(N, V, T \equiv 0)$ with $\mu_0$ and no “anomalous”

\[
\Omega(\mu, V, T) = \Omega_0(\mu) + \bigoplus \bigoplus + \bigoplus + \cdots
\]

\[
\text{with } G_0(\mu, T)
\]

\[
\overset{T \to 0}{F(N, V, T = 0)} = E_0(N) + \bigoplus + \bigoplus + \cdots
\]

\[
\text{with } G_0(\mu_0)
\]

- Uniform Fermi system, no external potential (degeneracy $\nu$):
  \[
  \mu_0(N) = (6\pi^2 N / \nu V)^{2/3} \equiv k_F^2 / 2M \equiv \epsilon_F^0
  \]

- If symmetry of non-interacting and interacting systems same
Kohn-Luttinger Inversion Method [F & W, sec. 30]

- Find \( F(N) = \Omega(\mu) + \mu N \) with \( \mu(N) \) from \( N(\mu) = -\left( \frac{\partial \Omega}{\partial \mu} \right)_{TV} \)
Kohn-Luttinger Inversion Method [F & W, sec. 30]

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

expand about non-interacting (subscripts label expansion):

\[
\begin{align*}
\Omega(\mu) &= \Omega_0(\mu) + \Omega_1(\mu) + \Omega_2(\mu) + \cdots \\
\mu &= \mu_0 + \mu_1 + \mu_2 + \cdots \\
F(N) &= F_0(N) + F_1(N) + F_2(N) + \cdots
\end{align*}
\]
Kohn-Luttinger Inversion Method [F & W, sec. 30]

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

- expand about non-interacting (subscripts label expansion):

  \[
  \Omega(\mu) = \Omega_0(\mu) + \Omega_1(\mu) + \Omega_2(\mu) + \cdots \\
  \mu = \mu_0 + \mu_1 + \mu_2 + \cdots \\
  F(N) = F_0(N) + F_1(N) + F_2(N) + \cdots 
  \]

- invert $N = -(\partial\Omega(\mu) / \partial \mu)_{TV}$ order-by-order in expansion
Kohn-Luttinger Inversion Method [F & W, sec. 30]

- Find $F(N) = \Omega(\mu) + \mu N$ with $\mu(N)$ from $N(\mu) = -(\partial\Omega/\partial \mu)_{TV}$
- expand about non-interacting (subscripts label expansion):

$$\begin{align*}
\Omega(\mu) &= \Omega_0(\mu) + \Omega_1(\mu) + \Omega_2(\mu) + \cdots \\
\mu &= \mu_0 + \mu_1 + \mu_2 + \cdots \\
F(N) &= F_0(N) + F_1(N) + F_2(N) + \cdots
\end{align*}$$

- invert $N = -(\partial\Omega(\mu)/\partial \mu)_{TV}$ order-by-order in expansion
- $N$ appears in $0^{\text{th}}$ order only: $N = -[\partial\Omega_0/\partial \mu]_{\mu=\mu_0} \implies \mu_0(N)$
Kohn-Luttinger Inversion Method [F & W, sec. 30]

- Find $F(N) = \Omega(\mu) + \mu N$ with $\mu(N)$ from $N(\mu) = -(\partial \Omega / \partial \mu)_{TV}$
- expand about non-interacting (subscripts label expansion):
  
  $\Omega(\mu) = \Omega_0(\mu) + \Omega_1(\mu) + \Omega_2(\mu) + \cdots$
  
  $\mu = \mu_0 + \mu_1 + \mu_2 + \cdots$
  
  $F(N) = F_0(N) + F_1(N) + F_2(N) + \cdots$

- invert $N = -(\partial \Omega(\mu)/\partial \mu)_{TV}$ order-by-order in expansion
- $N$ appears in 0th order only: $N = -[\partial \Omega_0/\partial \mu]_{\mu=\mu_0} \implies \mu_0(N)$
- first order has two terms, which lets us solve for $\mu_1$:

  $0 = [\partial \Omega_1/\partial \mu]_{\mu=\mu_0} + \mu_1[\partial^2 \Omega_0/\partial \mu^2]_{\mu=\mu_0} \implies \mu_1 = -\frac{[\partial \Omega_1/\partial \mu]_{\mu=\mu_0}}{[\partial^2 \Omega_0/\partial \mu^2]_{\mu=\mu_0}}$
Kohn-Luttinger Inversion Method [F & W, sec. 30]

- Find $F(N) = \Omega(\mu) + \mu N$ with $\mu(N)$ from $N(\mu) = -\left(\partial \Omega / \partial \mu\right)_{TV}$
- expand about non-interacting (subscripts label expansion):
  
  $$
  \Omega(\mu) = \Omega_0(\mu) + \Omega_1(\mu) + \Omega_2(\mu) + \cdots \\
  \mu = \mu_0 + \mu_1 + \mu_2 + \cdots \\
  F(N) = F_0(N) + F_1(N) + F_2(N) + \cdots
  $$

- invert $N = -\left(\partial \Omega(\mu) / \partial \mu\right)_{TV}$ order-by-order in expansion
- $N$ appears in 0th order only: $N = -[\partial \Omega_0 / \partial \mu]_{\mu=\mu_0} \implies \mu_0(N)$
- first order has two terms, which lets us solve for $\mu_1$:

  $$
  0 = \left[\partial \Omega_1 / \partial \mu\right]_{\mu=\mu_0} + \mu_1 \left[\partial^2 \Omega_0 / \partial \mu^2\right]_{\mu=\mu_0} \implies \mu_1 = -\frac{\left[\partial \Omega_1 / \partial \mu\right]_{\mu=\mu_0}}{\left[\partial^2 \Omega_0 / \partial \mu^2\right]_{\mu=\mu_0}}
  $$

- Same pattern to all orders: $\mu_i$ determined by functions of $\mu_0$
Apply this inversion to $F = \Omega + \mu N$:

$$F(N) = \underbrace{\Omega_0(\mu_0) + \mu_0 N}_{F_0} + \underbrace{\Omega_1(\mu_0) + \mu_1 N + \mu_1 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0}}_{F_1} + \underbrace{\Omega_2(\mu_0) + \mu_2 N + \mu_2 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0}}_{F_2} + \mu_1 \left[ \frac{\partial \Omega_1}{\partial \mu} \right]_{\mu=\mu_0} + \frac{1}{2} \mu_1^2 \left[ \frac{\partial^2 \Omega_0}{\partial \mu^2} \right]_{\mu=\mu_0} + \cdots$$
Apply this inversion to $F = \Omega + \mu N$:

$$F(N) = \Omega_0(\mu_0) + \mu_0 N + \Omega_1(\mu_0) + \mu_1 N + \mu_1 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0}$$

$$+ \Omega_2(\mu_0) + \mu_2 N + \mu_2 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0} + \mu_1 \left[ \frac{\partial \Omega_1}{\partial \mu} \right]_{\mu=\mu_0} + \frac{1}{2} \mu_1^2 \left[ \frac{\partial^2 \Omega_0}{\partial \mu^2} \right]_{\mu=\mu_0} + \cdots$$

$\mu_i$ always cancels from $F_i$ for $i \geq 1$:

$$F(N) = F_0(N) + \Omega_1(\mu_0) + \Omega_2(\mu_0) - \frac{1}{2} \left[ \frac{\partial \Omega_1/\partial \mu}{\partial \mu} \right]_{\mu=\mu_0}^2 + \cdots$$
Apply this inversion to \( F = \Omega + \mu N \):

\[
F(N) = F_0(N) + \Omega_1(\mu_0) + \mu_1 N + \mu_1 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0} + \mu_2 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0} + \mu_0 \left[ \frac{\partial \Omega_1}{\partial \mu} \right]_{\mu=\mu_0} + \frac{1}{2} \mu_1^2 \left[ \frac{\partial^2 \Omega_0}{\partial \mu^2} \right]_{\mu=\mu_0} + \cdots
\]

\( \mu_i \) always cancels from \( F_i \) for \( i \geq 1 \):

\[
F(N) = F_0(N) + \Omega_1(\mu_0) + \Omega_2(\mu_0) - \frac{1}{2} \left[ \frac{\partial \Omega_1}{\partial \mu} \right]_{\mu=\mu_0}^2 + \cdots
\]
Apply this inversion to $F = \Omega + \mu N$:

$$F(N) = \underbrace{\Omega_0(\mu_0) + \mu_0 N + \Omega_1(\mu_0) + \mu_1 N + \mu_1 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0}}_{F_0}$$

$$+ \underbrace{\Omega_2(\mu_0) + \mu_2 N + \mu_2 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0} + \mu_1 \left[ \frac{\partial \Omega_1}{\partial \mu} \right]_{\mu=\mu_0} + \frac{1}{2} \mu_1^2 \left[ \frac{\partial^2 \Omega_0}{\partial \mu^2} \right]_{\mu=\mu_0}}_{F_1}$$

$$+ \underbrace{\mu_i \text{ always cancels from } F_i \text{ for } i \geq 1:}_{F_2}$$

$$F(N) = F_0(N) + \underbrace{\Omega_1(\mu_0) + \Omega_2(\mu_0) - \frac{1}{2} \left[ \frac{\partial \Omega_1}{\partial \mu} \right]_{\mu=\mu_0}^2}_{F_1}$$

$$- \underbrace{\frac{1}{2} \left[ \frac{\partial^2 \Omega_0}{\partial \mu^2} \right]_{\mu=\mu_0}}_{F_2}$$

$$+ \cdots$$
Apply this inversion to $F = \Omega + \mu N$:

$$F(N) = \Omega_0(\mu_0) + \mu_0 N + \Omega_1(\mu_0) + \mu_1 N + \mu_1 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0} F_0$$

$$+ \Omega_2(\mu_0) + \mu_2 N + \mu_2 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0} + \mu_1 \left[ \frac{\partial \Omega_1}{\partial \mu} \right]_{\mu=\mu_0} + \frac{1}{2} \mu_1^2 \left[ \frac{\partial^2 \Omega_0}{\partial \mu^2} \right]_{\mu=\mu_0} F_1$$

$$+ \Omega_2(\mu_0) + \mu_2 N + \mu_2 \left[ \frac{\partial \Omega_1}{\partial \mu} \right]_{\mu=\mu_0} + \frac{1}{2} \mu_1^2 \left[ \frac{\partial^2 \Omega_0}{\partial \mu^2} \right]_{\mu=\mu_0} F_2$$

$\mu_i$ always cancels from $F_i$ for $i \geq 1$:

$$F(N) = F_0(N) + \Omega_1(\mu_0) + \Omega_2(\mu_0) - \frac{1}{2} \left[ \frac{\partial \Omega_1}{\partial \mu} \right]^2_{\mu=\mu_0} + \cdots$$
Generalizing the KLO Inversion Approach

- Zeroth order is non-interacting system $\implies$ easy to solve
  - It has chemical potential $\mu_0$ and external potential $v(x)$
  - $\implies$ fill levels up to $\mu_0$, which is known by counting up to $N$
Zeroth order is non-interacting system $\Rightarrow$ easy to solve
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Generalizing the KLW Inversion Approach

Generalizations: Kohn-Sham DFT, other sources, pairing

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

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  3. Add a source coupled to the *divergent* pair density
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- Same inversion method, but use \( [j]_{\text{gs}} = j_0 + j_1 + j_2 + \cdots = 0 \)
  \[ \rightarrow \text{find } j_0 \text{ iteratively: from } [j_0]_{\text{old}} \text{ find } [j_0]_{\text{new}} = -j_1 - j_2 + \cdots \]