Density Functional Theory
from
Effective Field Theory

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The Big Picture (adapted from Richter @INPC2004)
Problems with Extrapolations

- Mass formulas and energy functionals do well where there is data, but elsewhere ...
Density Functional Theory (DFT)

- Dominant application: inhomogeneous electron gas
- Interacting point electrons in static potential of atomic nuclei
- “Ab initio” calculations of atoms, molecules, crystals, surfaces
- HF is good starting point, DFT/LDA is better, DFT/GGA is best

![Atomization Energies of Hydrocarbon Molecules](image)

- **Hartree-Fock**
- **DFT Local Spin Density Approximation**
- **DFT Generalized Gradient Approximation**
Density Functional Theory (DFT)

- Hohenberg-Kohn: There exists an energy functional $E_v[\rho] \ldots$

$$E_v[\rho] = F_{HK}[\rho] + \int d^3 x \, v(x) \rho(x)$$

- $F_{HK}$ is universal (same for any external $v$) $\implies$ $H_2$ to DNA!
- Useful if you can approximate the energy functional
- Introduce orbitals and minimize energy functional $\implies E_{gs}, \rho_{gs}$
Kohn-Sham DFT

$V_{HO} \equiv \text{Non-interacting density in } V_{KS}$

Find Kohn-Sham potential $V_{KS}(x)$ from $\delta E_v[^{\rho}]/\delta \rho(x)$

Solve self-consistently
Kohn-Sham DFT

- Interacting density in $V_{HO}$ $\equiv$ Non-interacting density in $V_{KS}$
- Orbitals $\{\phi_i(x)\}$ in local potential $V_{KS}(\rho, x)$

$$ [-\nabla^2/2m + V_{KS}(x)]\phi_i = \epsilon_i \phi_i \implies \rho(x) = \sum_{i=1}^{N} |\phi_i(x)|^2 $$

- Find Kohn-Sham potential $V_{KS}(x)$ from $\delta E_v[\rho]/\delta \rho(x)$
- Solve self-consistently
Questions about DFT and Nuclear Structure

- How is Kohn-Sham DFT more than mean field?
  - Where are the approximations? How do we truncate?
  - How do we include long-range effects (correlations)?
- What can you calculate in a DFT approach?
  - What about single-particle properties? Excited states?
- How does pairing work in DFT?
  - Can we (should we) decouple $pp$ and $ph$?
  - Are higher-order contributions important?
- What about broken symmetries? (translation, rotation, . . .)
- How do we connect to the free NN· · · N interaction?
  - What about chiral EFT or low-momentum interactions/RG?
Outline

EFT-Based Kohn-Sham DFT from Effective Actions

Adding Sources: Kinetic Energy Density and Pairing

Matching to NN and NNN and . . .

Summary
Outline

EFT-Based Kohn-Sham DFT from Effective Actions

Adding Sources: Kinetic Energy Density and Pairing

Matching to NN and NNN and . . .

Summary
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
  \[
  M = \left< \sum_i S_i \right> \\
  = \frac{1}{Z} \text{Tr} \left[ \left( \sum_i S_i \right) e^{-\beta g \sum_{\{i,j\}} S_i S_j} \right]
  \]
Add A Magnetic Probe Source $H$

- The source probes configurations near the ground state

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

- 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

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

- Legendre transform to the Gibbs free energy

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

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

$$H = \frac{\partial \Gamma[M]}{\partial M} \to \left. \frac{\partial \Gamma[M]}{\partial M} \right|_{M_{gs}} = 0$$
DFT as Analogous Legendre Transformation

In analogy to the spin system, add source \( J(x) \) coupled to density operator \( \hat{\rho}(x) \equiv \psi^\dagger(x)\psi(x) \) to the partition function:

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

- In analogy to the spin system, add source $J(x)$ coupled to density operator $\hat{\rho}(x) \equiv \psi^\dagger(x)\psi(x)$ to the partition function:
  \[
  Z[J] = e^{-W[J]} \sim \text{Tr} \ e^{-\beta(\hat{H}+J\hat{\rho})} \rightarrow \int \mathcal{D}[\psi^\dagger]\mathcal{D}[\psi] \ e^{-\int[\mathcal{L}+J\psi^\dagger\psi]}
  \]

- The density $\rho(x)$ in the presence of $J(x)$ is
  \[
  \rho(x) \equiv \langle \hat{\rho}(x) \rangle_J = \frac{\delta W[J]}{\delta J(x)}
  \]
DFT as Analogous Legendre Transformation

- In analogy to the spin system, add source $J(x)$ coupled to density operator $\hat{\rho}(x) \equiv \psi^\dagger(x)\psi(x)$ to the partition function:

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

- The density $\rho(x)$ in the presence of $J(x)$ is

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

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

$$\Gamma[\rho] = W[J] - \int J \rho \quad \text{with} \quad J(x) = -\frac{\delta \Gamma[\rho]}{\delta \rho(x)} \rightarrow \frac{\delta \Gamma[\rho]}{\delta \rho(x)} \bigg|_{\rho_{gs}(x)} = 0$$

$$\Rightarrow \text{For static } \rho(x), \ \Gamma[\rho] \propto \text{the DFT energy functional } F_{HK}!$$
A Bestiary of Effective Actions

- Couple source to local Lagrangian field, e.g., $J(x) \phi(x)$
  - $\Gamma[\phi]$ where $\phi(x) = \langle \phi(x) \rangle \implies$ 1PI effective action
  - Arises from fermion $\mathcal{L}$'s by introducing auxiliary fields
  - Kohn-Sham via special saddlepoint evaluation (?)
A Bestiary of Effective Actions

- Couple source to local Lagrangian field, e.g., $J(x)\varphi(x)$
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  - Kohn-Sham via special saddlepoint evaluation (?)

- Couple $J$ to non-local composite op, e.g., $J(x, x')\varphi(x)\varphi(x')$
  - $\Gamma[G, \phi] \implies 2$PI effective action [CJT]
A Bestiary of Effective Actions

- Couple source to local Lagrangian field, e.g., $J(x)\varphi(x)$
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- Couple $J$ to non-local composite op, e.g., $J(x, x')\varphi(x)\varphi(x')$
  - $\Gamma[G, \phi] \implies$ 2PI effective action [CJT]
- Source coupled to local composite operator, e.g., $J(x)\varphi^2(x)$
  - 1.5PI effective action? Almost:
  - Kohn-Sham from inversion method
  - Problem from new divergences $\implies J^n$ counterterms
    - “Sentenced to death” by Banks and Raby; reprieve?
    - energy interpretation? variational?
Where Does Kohn-Sham $V_{KS}$ Come From?

- Interacting density in $V_{HO} \equiv$ Non-interacting density in $V_{KS}$
- Orbitals $\{\phi_i(x)\}$ in local potential $V_{KS}(\rho, x)$

$$
\left[-\nabla^2/2m + V_{KS}(x)\right] \phi_i = \varepsilon_i \phi_i \implies \rho(x) = \sum_{i=1}^{N} |\phi_i(x)|^2
$$

- Find Kohn-Sham potential $V_{KS}(x)$ from $\delta E_{\nu}[\rho]/\delta \rho(x)$
- Solve self-consistently

Dick Furnstahl  DFT from EFT
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)

\[
\mathcal{W}[J, \lambda] = \mathcal{W}_0[J] + \lambda \mathcal{W}_1[J] + \lambda^2 \mathcal{W}_2[J] + \cdots
\]
\[
J[\rho, \lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots
\]
\[
\Gamma[\rho, \lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots
\]
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 $J_0(x)$

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

$$\Rightarrow$$ 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)

\[ W[J, \lambda] = W_0[J] + \lambda W_1[J] + \lambda^2 W_2[J] + \cdots \]
\[ J[\rho, \lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \cdots \]
\[ \Gamma[\rho, \lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \cdots \]

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

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

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

- Diagonalize $W_0[J_0]$ by introducing KS orbitals \( \Rightarrow \) 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)

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

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

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

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

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

\[\implies\] 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
- Find $J_0$ for the ground state via self-consistency loop:

\[
J_0 \rightarrow \mathcal{W}_1 \rightarrow \Gamma_1 \rightarrow J_1 \rightarrow \mathcal{W}_2 \rightarrow \Gamma_2 \rightarrow \cdots \implies J_0(x) = \sum_{i>0} \frac{\delta \Gamma_i[\rho]}{\delta \rho(x)}
\]
New Feynman Rules

- Conventional diagrammatic expansion of propagator:

\[ \begin{array}{c}
\text{\includegraphics[width=0.9\textwidth]{feynman_diagram}}
\end{array} \]

\[ \Rightarrow \Sigma(x, x'; \omega) \]

- Non-local, state-dependent \( \Sigma^*(x, x'; \omega) \) vs. local \( J_0(x) \):

\[ J_0(x) = \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta \rho(x)} = \int \left( \frac{\delta \rho(x)}{\delta J_0(y)} \right)^{-1} \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta J_0(y)} = \begin{array}{c}
\text{\includegraphics[width=0.9\textwidth]{feynman_diagram}}
\end{array} \]

\[ \Rightarrow \text{“inverse density-density correlator”} \]

- New Feynman rules \( \Gamma_{\text{int}} \):

\[ \Gamma_{\text{int}} = \begin{array}{c}
\text{\includegraphics[width=0.9\textwidth]{feynman_diagram}}
\end{array} \]
New Feynman Rules

- Conventional diagrammatic expansion of propagator:

\[
\begin{align*}
\Gamma_\text{int}[\rho] &= \int \left( \frac{\delta \rho(x)}{\delta J_0(y)} \right)^{-1} \delta \Gamma_\text{int}[\rho] \\
&= - \quad - \quad + \quad + \quad + \quad \Rightarrow \Sigma^*(x, x'; \omega)
\end{align*}
\]

- Non-local, state-dependent \(\Sigma^*(x, x'; \omega)\) vs. local \(J_0(x)\):

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

- New Feynman rules \(\Gamma_\text{int} \quad \Rightarrow \quad \text{“inverse density-density correlator”}\)
New Feynman Rules

- Conventional diagrammatic expansion of propagator:

\[
\begin{align*}
&= \cdots \quad \Rightarrow \quad \Sigma^*(x, x'; \omega)
\end{align*}
\]

- Non-local, state-dependent \( \Sigma^*(x, x'; \omega) \) vs. local \( J_0(x) \):

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

\[
= \cdots
\]

- New Feynman rules \( \Rightarrow \) “inverse density-density correlator”

\[
\Gamma_{\text{int}} = \cdots
\]
New Feynman Rules

- Conventional diagrammatic expansion of propagator:

\[
\begin{align*}
\cdots &= + + + \cdots \\
&= + \sum^\infty \delta \Gamma_{\text{int}}[\rho] = \int \left( \frac{\delta \rho(x)}{\delta \rho(y)} \right)^{-1} \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta \rho(y)} = - + \cdots \\
&= + \delta \Gamma_{\text{int}}[\rho] = \int \left( \frac{\delta \rho(x)}{\delta J_0(y)} \right)^{-1} \frac{\delta \Gamma_{\text{int}}[\rho]}{\delta J_0(y)} = - + \cdots \\
\end{align*}
\]

- Non-local, state-dependent \( \Sigma^*(x, x'; \omega) \) vs. local \( J_0(x) \):

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

- New Feynman rules \( \implies \) “inverse density-density correlator”

\[
\Gamma_{\text{int}} = + + \cdots \\
\]
"Simple" Many-Body Problem: Hard Spheres

- Infinite potential at radius $R$
  
  \[ \sin(kr + \delta) \]

- Scattering length $a_0 = R$

- Dilute $nR^3 \ll 1 \implies k_F a_0 \ll 1$

- What is the energy / particle?
In Search of a Perturbative Expansion

For free-space scattering at momentum $k \ll 1/R$, should get perturbative expansion in $kR$ for scattering amplitude:

$$f_0(k) \propto \frac{1}{k \cot \delta(k) - ik} \rightarrow a_0 - ia_0^2k - (a_0^3 - a_0^2r_0/2)k^2 + O(k^3 a_0^3)$$

with $a_0 = R$ and $r_0 = 2R/3$ for hard-core spheres.

Perturbation theory in the hard-core potential won’t work:

$$\langle k | V | k' \rangle \propto \int dx \: e^{ik \cdot x} \: V(x) \: e^{-ik' \cdot x} \rightarrow \infty$$

Standard solution: Solve nonperturbatively, then expand.

EFT approach: $k \ll 1/R$ means we probe at low resolution

$$\rightarrow$$ replace potential with a simpler but general interaction
Nonrelativistic EFT for “Natural” Dilute Fermions

- 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:

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

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

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

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

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

- Dimensional analysis \( \Rightarrow C_{2i} \sim \frac{4\pi}{M} R^{2i+1}, \quad D_{2i} \sim \frac{4\pi}{M} R^{2i+4} \)
Renormalization

- Reproduce: $f_0(k) \propto a_0 - ia_0^2 k - (a_0^3 - a_0^2 r_0/2) k^2 + \mathcal{O}(k^3 a_0^3)$

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

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

- Reproduce: \( f_0(k) \propto a_0 - ia_0^2 k - (a_0^3 - a_0^2 r_0/2)k^2 + \mathcal{O}(k^3 a_0^3) \)

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

\[
\langle k | V_\text{eft}^{(0)} | k' \rangle \quad \implies \quad \begin{array}{c}
\text{Diagram} \\
\end{array} \quad \implies \quad C_0
\]

- Choosing \( C_0 \propto a_0 \) gets the first term. Now \( \langle k | V G_0 V | k' \rangle \):

\[
\implies \int \frac{d^3q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\epsilon} \quad \longrightarrow \quad \infty!
\]

\( \implies \text{Linear divergence!} \)
Renormalization

- Reproduce: \( f_0(k) \propto a_0 - ia_0^2 k - (a_0^3 - a_0^2 r_0/2) k^2 + O(k^3 a_0^3) \)
- Consider the leading potential \( V_{\text{EFT}}^{(0)}(x) = C_0 \delta(x) \) or

\[
\langle k | V_{\text{eft}}^{(0)} | k' \rangle \quad \implies \quad \frac{1}{(2\pi)^3} \int d^3 q \quad \frac{1}{k^2 - q^2 + i\epsilon} \quad \implies \quad \frac{\Lambda_c}{2\pi^2} - \frac{ik}{4\pi} + O(k^2/\Lambda_c)
\]

- Choosing \( C_0 \propto a_0 \) gets the first term. Now \( \langle k | V G_0 V | k' \rangle \):

\[
\implies \quad \text{If cutoff at } \Lambda_c, \text{ can absorb into } V^{(0)}, \text{ but all powers of } k^2
Renormalization

- Reproduce: \( f_0(k) \propto a_0 - ia_0^2k - (a_0^3 - a_0^2r_0/2)k^2 + O(k^3a_0^3) \)

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

\[
\langle k | V_{\text{eft}}^{(0)} | k' \rangle \implies \quad \quad \implies \quad C_0
\]

- Choosing \( C_0 \propto a_0 \) gets the first term. Now \( \langle k | VG_0V | k' \rangle \):

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

Dimensional regularization with minimal subtraction
\implies only one power of \( k \)!
Dim. reg. + minimal subtraction $\implies$ simple power counting:

$\frac{P}{2} + k \quad \frac{P}{2} + k' \quad \frac{P}{2} - k \quad \frac{P}{2} - k' \quad iT(k, \cos \theta) = \quad + \quad +$ \quad $-iC_0 \quad - \frac{M}{4\pi} (C_0)^2 k$

$+ i \left( \frac{M}{4\pi} \right)^2 (C_0)^3 k^2 \quad -iC_2 k^2 \quad -iC_0^2 k^2 \cos \theta$

Matching:

$C_0 = \frac{4\pi}{M} a_0 = \frac{4\pi}{M} R , \quad C_2 = \frac{4\pi}{M} \frac{a_0^2 r_0}{2} = \frac{4\pi}{M} \frac{R^3}{3} , \quad \ldots$
Dim. reg. + minimal subtraction $\implies$ simple power counting:

\[
\begin{align*}
\frac{P}{2} + k & \quad \frac{P}{2} + k' \\
\frac{P}{2} - k & \quad \frac{P}{2} - k' \\
iT(k, \cos \theta) & \quad -iC_0 & \quad -\frac{M}{4\pi}(C_0)^2k \\
\end{align*}
\]

\[
\begin{align*}
+i \left(\frac{M}{4\pi}\right)^2(C_0)^3k^2 & \quad -iC_2k^2 & \quad -iC'_2k^2 \cos \theta \\
\end{align*}
\]

Matching:

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

Recover effective range expansion order-by-order with perturbative diagrammatic expansion:

- one power of $k$ per diagram
- estimate truncation error from dimensional analysis
Now Sum Over Fermions in the Fermi Sea

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

\[ \Rightarrow \quad \propto a_0 k_F^6 \]
Now Sum Over Fermions in the Fermi Sea

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

  \[
  \begin{align*}
  &\xrightarrow{\text{\textbullet}} \quad \infty \quad \propto a_0 k_F^6 \\
  \end{align*}
  \]

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

  \[
  \begin{align*}
  &\xrightarrow{\text{\textbullet}} \quad \int_{k_F}^{\infty} \frac{d^3q}{(2\pi)^3} \frac{1}{k^2 - q^2} \\
  \end{align*}
  \]
Now Sum Over Fermions in the Fermi Sea

- Leading order $V^{(0)}_{\text{EFT}}(x) = C_0 \delta(x)$

  \[ \implies \quad \propto a_0 k_F^6 \]

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

  \[ \implies \quad \propto \int_{k_F}^{\infty} \frac{d^3q}{(2\pi)^3} \frac{1}{k^2 - q^2} \]

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

  \[ \int_{k_F}^{\infty} \frac{1}{k^2 - q^2} = \int_0^{\infty} \frac{1}{k^2 - q^2} - \int_0^{k_F} \frac{1}{k^2 - q^2} \xrightarrow{D \rightarrow 3} - \int_0^{k_F} \frac{1}{k^2 - q^2} \propto a_0^2 k_F^7 \]
$T = 0$ Energy Density from Hugenholtz Diagrams
\( T = 0 \) Energy Density from Hugenholtz Diagrams

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

\[
\mathcal{O}(k_F^6) : \quad E/V = \frac{\rho k_F^2}{2M} \left[ \frac{3}{5} + (\nu - 1) \frac{2}{3\pi} (k_F a_0) \right] \\
\mathcal{O}(k_F^7) : \quad + \quad (\nu - 1) \frac{4}{35\pi^2} (11 - 2\ln 2) (k_F a_0)^2
\]
$T = 0$ Energy Density from Hugenholtz Diagrams

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

\[
\mathcal{O}(k_F^6) : \quad & \quad \mathcal{O}(k_F^7) : \quad \mathcal{O}(k_F^8) : \\
E \quad V = \rho \frac{k_F^2}{2M} \left[ \frac{3}{5} + (\nu - 1) \frac{2}{3\pi} (k_F a_0) \right] \\
& \quad + (\nu - 1) \frac{4}{35\pi^2} (11 - 2\ln 2) (k_F a_0)^2 \\
& \quad + (\nu - 1) (0.076 + 0.057(\nu - 3)) (k_F a_0)^3
\]
$T = 0$ Energy Density from Hugenholtz Diagrams

$$\mathcal{O}(k_F^6) : \quad \mathcal{O}(k_F^7) : \quad \mathcal{O}(k_F^8) : \quad \mathcal{O}(k_F^9) : \quad \mathcal{O}(k_F^{10}) :$$

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

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

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

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

$$+ (\nu + 1) \frac{1}{5\pi} (k_F a_0)^3 + \cdots$$
$T = 0$ Energy Density from Hugenholtz Diagrams

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

\[ + \left. d_1 \frac{a_0^2}{2M} \left[ \rho(x) \right]^{7/3} \right. \]

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

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

\[ + \left. d_4 a_p^3 \left[ \rho(x) \right]^{8/3} + \cdots \right] \]
Kohn-Sham $J_0$ According to the EFT Expansion

- Simplifying with 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

(Generic) Iteration procedure:

1. Guess an initial density profile $\rho(r)$ (e.g., Thomas-Fermi)
2. Evaluate local single-particle potential $V_{KS}(r) \equiv v(r) - J_0(r)$
3. Solve for lowest $N$ 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 $\rho(r) = \sum_{\alpha=1}^{N} |\psi_\alpha(x)|^2$
   - other observables are functionals of $\{\psi_\alpha, \epsilon_\alpha\}$
5. Repeat 2.–4. until changes are small (“self-consistent”)

Looks like a Skyrme Hartree-Fock calculation! [But no $M^*(r)$]
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

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

\[
\begin{array}{ccc}
E/A & <k_F a_s> & \langle r^2 \rangle^{1/2} \\
6.750 & -0.524 & 2.598 \\
5.982 & -0.578 & 2.351 \\
\end{array}
\]
Check Out An Example [nucl-th/0212071]

Dilute Fermi Gas in Harmonic Trap

$N_F=7$, $A=240$, $g=2$, $a_s=-0.160$

\[
\begin{array}{ccc}
E/A & \langle k_F a_s \rangle & \langle r^2 \rangle^{1/2} \\
6.750 & -0.524 & 2.598 \\
5.982 & -0.578 & 2.351 \\
6.254 & -0.550 & 2.472 \\
\end{array}
\]
Check Out An Example [nucl-th/0212071]

Dilute Fermi Gas in Harmonic Trap

$N_F = 7$, $A = 240$, $g = 2$, $a_s = -0.160$

Diagram showing the density $\rho(r/b)$ as a function of $r/b$ for different approximations:
- $C_0 = 0$ (exact)
- Kohn-Sham LO
- Kohn-Sham NLO (LDA)
- Kohn-Sham NNLO (LDA)

Results:

- $E/A$ $<k_F a_s>$ $<r^2>^{1/2}$
  - 6.750 $-0.524$ $2.598$
  - 5.982 $-0.578$ $2.351$
  - 6.254 $-0.550$ $2.472$
  - 6.227 $-0.553$ $2.459$
Power Counting Terms in Energy Functionals

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

![Graph showing energy per particle at LO, NLO, and NNLO for different values of $n$, $a_s$, and $A$.]
Power Counting Terms in Energy Functionals

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

![Graph showing energy per particle vs. LO, NLO, NNLO for different parameters]
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 $\langle k_F \rangle$
Power Counting Terms in Energy Functionals

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

![Graph showing energy/particle vs. power of density for different values of $n$, $a_s$, and $A$.]

- Reasonable estimates $\implies$ truncation errors understood

Dick Furnstahl
DFT from EFT
EFT-Based Kohn-Sham DFT from Effective Actions

Adding Sources: Kinetic Energy Density and Pairing

Matching to NN and NNN and . . .

Summary
Variational Energy and the Effective Action

- Consider Hamiltonian including time-independent $H$:
  \[ \mathcal{H}(H) = g \sum_{\{i,j\}} S_i S_j - H \sum_i S_i \]

- In large $\beta$ limit, $Z \rightarrow$ ground state of $\mathcal{H}(H)$ with energy
  \[ E(H) = \lim_{\beta \rightarrow \infty} -\frac{1}{\beta} \log Z[H] \]

- Separating out the pieces:
  \[ E(H) = \langle \mathcal{H}(H) \rangle_H = \langle \mathcal{H} \rangle_H - H \langle \sum_i S_i \rangle_H = \langle \mathcal{H} \rangle_H - HM \]

- Thus as $T \rightarrow 0$, the effective action
  \[ \Gamma(M) = E(H) + HM = \langle \mathcal{H} \rangle_H \]

  \[ \rightarrow \text{expectation value of } \mathcal{H} \text{ in ground state generated by } H \]

- The true ground state (with $H = 0$) is variational minimum!
Beyond Kohn-Sham LDA: Kinetic Energy Density

- Coulomb meta-GGA DFT $\implies E[\rho, \tau(\rho)]$ with $\tau \equiv \langle \nabla \psi^\dagger \cdot \nabla \psi \rangle$
  
  - But $\tau$ is expanded in terms of $\rho$
    
    $$
    \tau(x) = \frac{3}{5} (3\pi^2)^{2/3} \rho^{5/3} + \frac{1}{36} \frac{(\nabla \rho)^2}{\rho} + \cdots
    $$

  $\implies$ same Kohn-Sham equation

  $$
  J_0(x) = \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(x)} \implies \left[ -\frac{\nabla^2}{2M} + J_0(x) \right] \psi_\alpha = \epsilon_\alpha \psi_\alpha
  $$
Beyond Kohn-Sham LDA: Kinetic Energy Density

- **Coulomb meta-GGA DFT** \[\iff E[\rho, \tau(\rho)]\] with \[\tau \equiv \langle \nabla \psi^\dagger \cdot \nabla \psi \rangle\]
  - But \(\tau\) is expanded in terms of \(\rho\)
    \[
    \tau(x) = \frac{3}{5} (3\pi^2)^{2/3} \rho^{5/3} + \frac{1}{36} \frac{(\nabla \rho)^2}{\rho} + \cdots
    \]
    \[\implies\] same Kohn-Sham equation
    \[
    J_0(x) = \frac{\delta E_{\text{int}}[\rho]}{\delta \rho(x)} \implies \left[ -\frac{\nabla^2}{2M} + J_0(x) \right] \psi_\alpha = \epsilon_\alpha \psi_\alpha
    \]

- In Skyrme HF, \(\rho\) and \(\tau\) are treated independently in \(E[\rho, \tau, J]\)
  \[
  E[\rho, \tau, J] = \int d^3x \left\{ \frac{1}{2M} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho \tau \\
  + \frac{1}{64} (9t_1 - 5t_2) (\nabla \rho)^2 - \frac{3}{4} W_0 \rho \nabla \cdot J + \frac{1}{32} (t_1 - t_2) J^2 \right\}
  \]
To do this in DFT/EFT, add to Lagrangian $+ \eta(x) \nabla \psi^\dagger \nabla \psi$

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

Two Kohn-Sham potentials:

$$J_0(x) = \frac{\delta \Gamma_{\text{int}}[\rho, \tau]}{\delta \rho(x)} \quad \text{and} \quad \eta_0(x) = \frac{\delta \Gamma_{\text{int}}[\rho, \tau]}{\delta \tau(x)}$$
To do this in DFT/EFT, add to Lagrangian $+ \eta(x) \nabla \psi^\dagger \nabla \psi$

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

Two Kohn-Sham potentials:

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

Quadratic part of Lagrangian in $W_0$ diagonalized:

$$\int d^4x \left[ i \partial_t + \frac{\nabla^2}{2M} - v(x) + J_0(x) - \nabla \cdot \eta_0(x) \nabla \right] \psi$$

Kohn-Sham equation $\implies$ defines $1/2M^*(x) \equiv 1/2M - \eta_0(x)$
First Step: HF Diagrams With $\nabla$’s  [nucl-th/0408014]

- Consider bowtie diagrams from vertices with derivatives:

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

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

$$E_{\text{int}}[\rho] = \ldots + C_2 \left[ \frac{\left( \frac{6\pi^2}{\nu} \right)^2}{\rho^{8/3}} + 3 C'_2 \left( \frac{6\pi^2}{\nu} \right)^2 \frac{1}{\rho^{8/3}} \right] + \ldots$$

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

$$E_{\text{int}}[\rho, \tau] = \ldots + C_2 \left[ \rho \tau + \frac{3}{4} (\nabla \rho)^2 \right] + 3 C'_2 \left[ \rho \tau - \frac{1}{4} (\nabla \rho)^2 \right] + \ldots$$
First Step: HF Diagrams With $\nabla$’s  \[\text{[nucl-th/0408014]}\]

- Consider bowtie diagrams from vertices with derivatives:

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

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

\[
\mathcal{E}_{\text{int}}[\rho] = \ldots + \frac{C_2}{8} \left[ \frac{3}{5} \left( \frac{6\pi^2}{\nu} \right)^{2/3} \rho^{8/3} \right] + \frac{3C'_2}{8} \left[ \frac{3}{5} \left( \frac{6\pi^2}{\nu} \right)^{2/3} \rho^{8/3} \right] + \ldots
\]
First Step: HF Diagrams With $\nabla$’s  

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

$\nabla$ + $\nabla$

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

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

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

$$\mathcal{E}_{\text{int}}[\rho, \tau] = \ldots + \frac{C_2}{8} \left[ \rho \tau + \frac{3}{4} (\nabla \rho)^2 \right] + \frac{3 C'_2}{8} \left[ \rho \tau - \frac{1}{4} (\nabla \rho)^2 \right] + \ldots$$
Power Counting Estimates Work for Gradients!

ν = 2, a_s = 0.16, A = 240

ν = 4, a_s = 0.10, A = 140
Kohn-Sham LDA $\rho$ vs. $\rho_T$ [Anirban Bhattacharyya]

\[ \rho = \text{Kohn-Sham LDA} \]

\[ \rho_T = \text{DFT from EFT} \]

\[ n = 2, N_F = 7, A = 240 \]

\[ a_s = 0.16, r_s = 2a_s / 3 \]
Kohn-Sham LDA $\rho$ vs. $\rho_\tau$: Differences

<table>
<thead>
<tr>
<th>$a_p = a_s$</th>
<th>$E/A$</th>
<th>$\sqrt{\langle r^2 \rangle}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>7.66</td>
<td>2.87</td>
</tr>
<tr>
<td>$\rho_\tau$</td>
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<td>3.10</td>
</tr>
<tr>
<td>$\rho_\tau$</td>
<td>8.30</td>
<td>3.09</td>
</tr>
</tbody>
</table>

$v=2$, $N_F=7$, $A=240$

$a_s=0.16$, $r_s=2a_s/3$
Effective mass $M^*$ related to single-particle levels

$\nu=2$, $N_F=7$, $A=240$

$a_s=0.16$, $r_s=2a_s/3$
Effective Mass and the Single-Particle Spectrum

Uniform system:
\[ \varepsilon^\rho_{\mathbf{k}} - \varepsilon^{\rho\tau}_{\mathbf{k}} = \frac{\pi}{\nu} [(\nu - 1)a_s^2 r_s + 2(\nu + 1)a_p^3] \frac{k_F^2 - k^2}{2M} \rho \]
Comparing Skyrme and Dilute Functionals

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

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

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

$$E[\rho, \tau] = \int d^3 x \left\{ \frac{\tau}{2M} + \frac{3}{8} C_0 \rho^2 + \frac{1}{16} (3C_2 + 5C'_2) \rho \tau + \frac{1}{64} (9C_2 - 5C'_2) (\nabla \rho)^2 + \frac{c_1}{2M} C_0^2 \rho^{7/3} + \frac{c_2}{2M} C_0^3 \rho^{8/3} + \frac{1}{16} D_0 \rho^3 + \cdots \right\}$$
Comparing Skyrme and Dilute Functionals

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

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

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

\[
E[\rho, \tau] = \int d^3 x \left\{ \frac{\tau}{2M} + \frac{3}{8} C_0 \rho^2 + \frac{1}{16} (3C_2 + 5C'_2) \rho \tau \\
+ \frac{1}{64} (9C_2 - 5C'_2) (\nabla \rho)^2 + \frac{C_1}{2M} C_0^2 \rho^{7/3} + \frac{C_2}{2M} C_0^3 \rho^{8/3} + \frac{1}{16} D_0 \rho^3 + \cdots \right\}
\]

- Same functional as dilute Fermi gas with \( t_i \leftrightarrow C_i \)
  - equivalent \( a_s \approx -2-3 \) fm but |\( k_F a_p \), \( k_F r_s \)| < 1 (with \( a_p < 0 \))
  - missing non-analytic terms, NNN, \ldots
Pairing in DFT/EFT from Effective Action

- Natural framework for spontaneous symmetry breaking
  - e.g., test for zero-field magnetization $M$ in a spin system
  - introduce an external field $H$ to break rotational symmetry
  - Legendre transform Helmholtz free energy $F(H)$:

  \[
  M = -\frac{\partial F(H)}{\partial H} \implies \Gamma[M] = F[H(M)] + MH(M)
  \]

- since $H = \frac{\partial \Gamma}{\partial M}$, minimize $\Gamma$ to find ground state
Generalizing Effective Action to Include Pairing

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

$$Z[J, j] = e^{-W[J,j]} = \int D(\psi^\dagger \psi) \ e^{- \int d^4x \ [\mathcal{L} + J(x)\psi_\alpha^\dagger \psi_\alpha + j(x)(\psi_\uparrow^\dagger \psi_\downarrow^\uparrow + \psi_\downarrow \psi_\uparrow^\dagger)]}$$
Generalizing Effective Action to Include Pairing

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

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

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

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

$$\phi(x) \equiv \langle \psi_\uparrow^\dagger(x) \psi_\downarrow^\dagger(x) + \psi_\downarrow(x) \psi_\uparrow(x) \rangle_{J,j} = \frac{\delta W[J, j]}{\delta j(x)} \bigg|_j$$
Generalizing Effective Action to Include Pairing

1. Generating functional with sources \( J, j \) coupled to densities:

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

2. Densities found by functional derivatives wrt \( J, j \):

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

\[
\phi(x) \equiv \langle \psi^\dagger_\uparrow(x)\psi^\dagger_\downarrow(x) + \psi_\downarrow(x)\psi_\uparrow(x) \rangle_{J, j} = \frac{\delta W[J, j]}{\delta j(x)} \Big|_j
\]

3. Effective action \( \Gamma[\rho, \phi] \) by functional Legendre transformation:

\[
\Gamma[\rho, \phi] = W[J, j] - \int d^4x \ J(x)\rho(x) - \int d^4x \ j(x)\phi(x)
\]
• $\Gamma[\rho, \phi] \propto$ ground-state (free) energy functional $E[\rho, \phi]$
  • at finite temperature, the proportionality constant is $\beta$
\( \Gamma[\rho, \phi] \propto \) ground-state (free) energy functional \( E[\rho, \phi] \)

- at finite temperature, the proportionality constant is \( \beta \)
- The sources are given by functional derivatives wrt \( \rho \) and \( \phi \)

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

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

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

- This is Hohenberg-Kohn DFT extended to pairing!
\[ \Gamma[\rho, \phi] \propto \text{ground-state (free) energy functional} \ E[\rho, \phi] \]

- at finite temperature, the proportionality constant is \( \beta \)

- The sources are given by functional derivatives wrt \( \rho \) and \( \phi \)

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

- but the sources are zero in the ground state

\[ \implies \text{determine ground-state } \rho(x) \text{ and } \phi(x) \text{ by stationarity:} \]

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

- This is Hohenberg-Kohn DFT extended to pairing!

- We need a method to carry out the inversion
  - For Kohn-Sham DFT, apply inversion methods
  - We need to renormalize!
Kohn-Sham Inversion Method Revisited

- Order-by-order matching in EFT expansion parameter $\lambda$

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

- 0th order is Kohn-Sham system with potentials $J_0(x)$ and $j_0(x)$
  
  $\implies$ yields the exact densities $\rho(x)$ and $\phi(x)$

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

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

where

\[
h_0(x) \equiv -\frac{\nabla^2}{2M} + V(x) - J_0(x)
\]

with conventional orthonormality relations for $u_i, v_i$
Diagrammatic Expansion of $W_i$

- Same diagrams, but with Nambu-Gor’kov Green’s functions

\[
\Gamma_{\text{int}} = \sum [\text{diagrams}] + \sum [\text{diagrams}] + \sum [\text{diagrams}] + \sum [\text{diagrams}] + \cdots
\]

\[
iG = \begin{pmatrix}
\langle T \psi_\uparrow(x) \psi_\uparrow^\dagger(x') \rangle_0 & \langle T \psi_\uparrow(x) \psi_\downarrow(x') \rangle_0 \\
\langle T \psi_\downarrow^\dagger(x) \psi_\uparrow^\dagger(x') \rangle_0 & \langle T \psi_\uparrow^\dagger(x) \psi_\downarrow(x') \rangle_0
\end{pmatrix}
\equiv \begin{pmatrix}
iG_{ks}^0 & iF_{ks}^0 \\
iF_{ks}^0 & -iG_{ks}^0
\end{pmatrix}
\]

- In frequency space, the Green’s functions are

\[
iG_{ks}^0(x, x'; \omega) = \sum_i \frac{u_i(x) u_i^*(x')}{\omega - E_i + i\eta} + \frac{v_i(x') v_i^*(x)}{\omega + E_i - i\eta}
\]

\[
iF_{ks}^0(x, x'; \omega) = -\sum_i \frac{u_i(x) v_i^*(x')}{\omega - E_i + i\eta} - \frac{u_i(x') v_i^*(x)}{\omega + E_i - i\eta}
\]
Kohn-Sham Self-Consistency Procedure

- Same iteration procedure as in Skyrme or RMF with pairing
- In terms of the orbitals, the fermion density is

\[ \rho(x) = 2 \sum_i |v_i(x)|^2 \]

and the pair density is (warning: divergent!)

\[ \phi(x) = \sum_i [u_i^*(x)v_i(x) + u_i(x)v_i^*(x)] \]

- The chemical potential \( \mu_0 \) is fixed by \( \int \rho(x) = A \)
- Diagrams for \( \tilde{\Gamma}[\rho, \phi] = -E[\rho, \phi] \) (with LDA+) yields KS potentials

\[ J_0(x) \bigg|_{\rho=\rho_{gs}} = \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho, \phi]}{\delta \rho(x)} \bigg|_{\rho=\rho_{gs}} \quad \text{and} \quad j_0(x) \bigg|_{\phi=\phi_{gs}} = \frac{\delta \tilde{\Gamma}_{\text{int}}[\rho, \phi]}{\delta \phi(x)} \bigg|_{\phi=\phi_{gs}} \]
Divergences: Uniform System

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

$$e^{-W} = \int D(\psi^\dagger, \psi) \, e^{-\int d^4x \left[ \psi_\alpha^\dagger \left( \frac{\partial}{\partial \tau} - \frac{\nabla^2}{2M} - \mu \right) \psi_\alpha + \frac{c_0}{2} \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow + j(\psi_\uparrow \psi_\downarrow + \psi_\downarrow^\dagger \psi_\uparrow^\dagger) \right]}$$

- cf. adding integration over auxiliary field $\int D(\Delta^*, \Delta) \, e^{-\frac{1}{|c_0|} \int |\Delta|^2}$

$$\implies$$ shift variables to eliminate $\psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow$ for $\Delta^* \psi_\uparrow \psi_\downarrow$

Dick Furnstahl  DFT from EFT
Divergences: Uniform System

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

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

- cf. adding integration over auxiliary field $\int D(\Delta^*, \Delta) \ e^{-\frac{1}{|C_0|} \int |\Delta|^2}$

$\implies$ shift variables to eliminate $\psi^\dagger_\uparrow \psi^\dagger_\downarrow \psi_\downarrow \psi^\dagger_\uparrow$ for $\Delta^* \psi^\dagger \psi$

- New divergences because of $j$ $\implies$ e.g., expand to $O(j^2)$

\[
W[\mu, j] = \cdots + \underbrace{\cdots}_{j} \underbrace{\cdots}_{j} + \cdots
\]

- Same linear divergence as in 2-to-2 scattering
Divergences: Uniform System

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

$$e^{-W} = \int D(\psi^\dagger \psi) \ e^{-\int d^4x \ [\psi_\alpha^\dagger \left(\frac{\partial}{\partial \tau} - \frac{\nabla^2}{2M} - \mu\right) \psi_\alpha + \frac{C_0}{2} \psi^\dagger_\uparrow \psi^\dagger_\downarrow \psi_\downarrow \psi^\uparrow \psi^\dagger_\uparrow + j (\psi^\dagger_\uparrow \psi_\downarrow + \psi^\dagger_\downarrow \psi^\uparrow) + \frac{1}{2} \xi j^2]} \]$$

- cf. adding integration over auxiliary field $\int D(\Delta^*, \Delta) \ e^{-\frac{1}{|C_0|} \int |\Delta|^2}$

$$\implies \text{shift variables to eliminate } \psi^\dagger_\uparrow \psi^\dagger_\downarrow \psi_\downarrow \psi^\uparrow \text{ for } \Delta^* \psi^\dagger_\uparrow \psi_\downarrow$$

- New divergences because of $j \implies$ e.g., expand to $O(j^2)$

$$W[\mu, j] = \cdots + \underbrace{\cdots}_{j} \underbrace{\cdots}_{j} + \cdots$$

- Same linear divergence as in 2-to-2 scattering

- Strategy: Add counterterm $\frac{1}{2} \xi j^2$ to $\mathcal{L}$

  - additive to $W$ (cf. $|\Delta|^2$) $\implies$ no effect on scattering

  - Energy interpretation? Finite part?
**Kohn-Sham Non-interacting System**

- Canonical Bogoliubov transformation solves exactly

\[
W_0[\mu_0, j_0] = \int \frac{d^3 k}{(2\pi)^3} (\xi_k - E_k) + \frac{1}{2} \zeta^{(0)} j_0^2
\]

where \( \xi_k \equiv \epsilon_k^0 - \mu_0 \) and \( E_k \equiv \sqrt{\xi_k^2 + j_0^2} \)

- Kohn-Sham potential \( j_0 \) plays the role of a constant gap

\[
\rho = 2 \sum_k v_k^2 \rightarrow \int \frac{d^3 k}{(2\pi)^3} \left( 1 - \frac{\xi_k}{E_k} \right)
\]

\[
\phi = 2 \sum_k u_k v_k \rightarrow - \int \frac{d^3 k}{(2\pi)^3} \frac{j_0}{E_k} + \zeta^{(0)} j_0
\]
Observables With Kohn-Sham Pairing

- To find the energy density, evaluate $\Gamma$ at the stationary point:

$$
\frac{E}{V} = (\Gamma_0 + \Gamma_1)|_{j_0 = -\frac{1}{2}|C_0|\phi} = \int \frac{d^3k}{(2\pi)^3} \left[ \xi_k - E_k + \frac{1}{2} \frac{j_0^2}{E_k} \right] + \left[ \mu_0 - \frac{1}{4} |C_0| \rho \right] \rho
$$

with

$$
\rho = \int \frac{d^3k}{(2\pi)^3} \left( 1 - \frac{\xi_k}{E_k} \right) \quad \text{and} \quad \phi = - \int \frac{d^3k}{(2\pi)^3} \frac{j_0}{E_k} + \zeta^{(0)} j_0
$$

- Explicitly finite and dependence on $\zeta^{(0)}$ cancels out
- Recover normal state from $j_0 \to 0$:

$$
\frac{E}{V} \to \frac{3}{5} \mu_0 \rho - \frac{1}{4} |C_0| \rho^2 \quad \text{and} \quad \rho \to \frac{1}{3\pi^2} k_F^3 \quad \text{and} \quad \mu_0 \to \frac{k_F^2}{2M}
$$
Higher Order: Induced Interaction

- As $j_0 \to 0$, $u_k v_k$ peaks at $\mu_0$
As $j_0 \to 0$, $u_k v_k$ peaks at $\mu_0$.
As $j_0 \rightarrow 0$, $u_k v_k$ peaks at $\mu_0$
Higher Order: Induced Interaction

- As \( j_0 \to 0 \), \( u_k v_k \) peaks at \( \mu_0 \)
- Leading order \( T = 0 \):
  \[
  \Delta_{LO}/\mu_0 = \frac{8}{e^2} \left( \frac{1}{N(0)} \right) |C_0| \\
  = \frac{8}{e^2} e^{\pi/2|a_s|} 
  \]

\[
\Gamma_1 = \sum_k u_k v_k + CTC + \cdots \implies \dot{j}_1 = \frac{\delta \Gamma_1}{\delta \phi} = \frac{1}{2} |C_0| \phi
\]
Higher Order: Induced Interaction

- As \( j_0 \to 0 \), \( u_k v_k \) peaks at \( \mu_0 \)
- Leading order \( T = 0 \):
  \[
  \Delta_{LO}/\mu_0 = \frac{8}{e^2} e^{-1/N(0)}|C_0| = \frac{8}{e^2} e^{-\pi/2k_F|a_s|}
  \]
- NLO modifies exponent
  \( \implies \) changes prefactor
- \( \Delta_{NLO} \approx \Delta_{LO}/(4e)^{1/3} \)

\[
\Gamma_1+\Gamma_2 = \sum_{k} u_k v_k + \sum_{k} u_k' v_k' \implies j_1+j_2 = \frac{1}{2}|C_0| \left[ 1 - |\langle 0 | \prod_0 | k = k' = k_F \rangle| \right] \phi
\]
On-Going and Future Challenges
On-Going and Future Challenges

- Long-range effects

- Long-range forces (e.g., pion exchange)

\[ J_0(x) = - \quad + \quad + \cdots \]

- Non-localities from near-on-shell particle-hole excitations

\[ + \quad + \quad + \quad + \cdots \]
On-Going and Future Challenges

- Long-range effects
- Gradient expansions

- Semiclassical expansions used in Coulomb DFT
- Density matrix expansion
- Gradient expansion techniques for (one-loop) effective actions
- First step: beachball diagram
On-Going and Future Challenges

- Long-range effects
- Gradient expansions
- Restoring broken symmetries

- Translational and rotational invariance, particle number
- Not addressed in Coulomb DFT
- Effective action $\implies$ zero modes
  - cf. soliton zero modes
  - Fadeev-Popov games?
- Energy functional for the intrinsic density?
  [Engel, Furnstahl, Schwenk]
On-Going and Future Challenges

- Long-range effects
- Gradient expansions
- Restoring broken symmetries
- Auxiliary field Kohn-Sham Theory

Auxiliary fields correspond to non-dynamical meson fields
Apply saddlepoint evaluation requiring density to be unchanged
Faussier and Valiev/Fernando formalism, but no higher-order calculations yet
How to separate ph and pp for pairing?
Revisit large $N$ expansion?
On-Going and Future Challenges

- Long-range effects
- Gradient expansions
- Restoring broken symmetries
- Auxiliary field Kohn-Sham Theory
- Covariant DFT: Dilute system

- Controlled laboratory for finite system
  - IR with short-range only $\Rightarrow$ simple!
  - Compare to heavy baryon EFT
  - Focus on spin-orbit
  - Three-body forces?

- Covariant pairing
  - Induced interaction

- Time-dependent Kohn-Sham theory
  - Higher order in effective action formalism
  - Kohn-Sham part $\Rightarrow$ RPA
  - Point-coupling version?
Outline

EFT-Based Kohn-Sham DFT from Effective Actions

Adding Sources: Kinetic Energy Density and Pairing

Matching to NN and NNN and . . .

Summary
Skyrme Looks Like a Perturbative Functional!

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

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

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

$$E[\rho, \tau] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8} C_0 \rho^2 + \frac{1}{16} (3C_2 + 5C_2') \rho \tau + \frac{1}{64} (9C_2 - 5C_2') (\nabla \rho)^2 + \frac{C_1}{2M} C_0^2 \rho^{7/3} + \frac{C_2}{2M} C_0^3 \rho^{8/3} + \frac{1}{16} D_0 \rho^3 + \cdots \right\}$$
Skyrme Looks Like a Perturbative Functional!

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

- Dilute \( \rho \tau \) energy density functional for \( \nu = 4 \) (\( V_{\text{external}} = 0 \))
  \[
  E[\rho, \tau] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8} C_0 \rho^2 + \frac{1}{16} (3C_2 + 5C_2') \rho \tau \\
  + \frac{1}{64} (9C_2 - 5C_2')(\nabla \rho)^2 + \frac{c_1}{2M} C_0^2 \rho^{7/3} + \frac{c_2}{2M} C_0^3 \rho^{8/3} + \frac{1}{16} D_0 \rho^3 + \cdots \right\}
  \]

- But isn’t nuclear matter very non-perturbative?
Sources of Nonperturbative Physics for NN

1. Strong short-range repulsion ("hard core")
2. Iterated tensor interaction
3. Near zero-energy bound states
Sources of Nonperturbative Physics for NN

1. Strong short-range repulsion ("hard core")
2. Iterated tensor interaction
3. Near zero-energy bound states

Consequences:
- In Coulomb DFT, Hartree-Fock gives dominate contribution
  \(\implies\) correlations are small corrections \(\implies\) DFT works!
- cf. NN interactions \(\implies\) correlations \(\gg\) HF \(\implies\) DFT fails??
Sources of Nonperturbative Physics for NN

1. Strong short-range repulsion ("hard core")
2. Iterated tensor interaction
3. Near zero-energy bound states

Consequences:
- In Coulomb DFT, Hartree-Fock gives dominate contribution ➞ correlations are small corrections ➞ DFT works!
- cf. NN interactions ➞ correlations ≫ HF ➞ DFT fails??

However . . .
- the first two depend on the resolution ➞ cutoff dependent
- third one is affected by Pauli blocking
Hans Bethe in review of nuclear matter (1971):

“The theory must be such that it can deal with any nucleon-nucleon (NN) force, including hard or ‘soft’ core, tensor forces, and other complications. It ought not to be necessary to tailor the NN force for the sake of making the computation of nuclear matter (or finite nuclei) easier, but the force should be chosen on the basis of NN experiments (and possibly subsidiary experimental evidence, like the binding energy of \( H^3 \)).”
EFT and RG Make Physics Easier

- There’s an old vaudeville joke about a doctor and patient . . .
EFT and RG Make Physics Easier

- There’s an old vaudeville joke about a doctor and patient . . .

**Patient:** Doctor, doctor, it hurts when I do this!
EFT and RG Make Physics Easier

There’s an old vaudeville joke about a doctor and patient . . .

Patient: Doctor, doctor, it hurts when I do this!
Doctor: Then don’t do that.
EFT and RG Make Physics Easier

- There’s an old vaudeville joke about a doctor and patient . . .

**Patient:** Doctor, doctor, it hurts when I do this!
**Doctor:** Then don’t do that.

- Weinberg’s Third Law of Progress in Theoretical Physics:
  “You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you’ll be sorry!”
Gameplan: Exploit Variable Cutoff Potential

Bogner, Kuo, Schwenk

\[ T = V_\Lambda + q \leq \Lambda \]

- **Require** \( \frac{dT}{d\Lambda} = 0 \)
  \[ \implies \text{renormalization group equation for } V_\Lambda \]
- **Run from** \( \Lambda_B = 25 \text{ fm}^{-1} \) to \( \Lambda = 2 \text{ fm}^{-1} \sim E_{\text{lab}} \approx 350 \text{ MeV} \)

Dick Furnstahl

DFT from EFT
Gameplan: Exploit Variable Cutoff Potential

Bogner, Kuo, Schwenk

\[ T = V_{\Lambda} + q \leq \Lambda \]

- **Require** \( \frac{dT}{d\Lambda} = 0 \)
  \( \Rightarrow \) renormalization group equation for \( V_{\Lambda} \)

- **Run from** \( \Lambda_B = 25 \text{ fm}^{-1} \) to
  \( \Lambda = 2 \text{ fm}^{-1} \sim E_{\text{lab}} \doteq 350 \text{ MeV} \)
Gameplan: Exploit Variable Cutoff Potential

Bogner, Kuo, Schwenk

\[ T = V_\Lambda + \sum_{q \leq \Lambda} \]

- Require \( \frac{dT}{d\Lambda} = 0 \)
  \( \rightarrow \) renormalization group equation for \( V_\Lambda \)
- Run from \( \Lambda_B = 25 \text{ fm}^{-1} \) to \( \Lambda = 2 \text{ fm}^{-1} \sim E_{\text{lab}} \approx 350 \text{ MeV} \)

\[ V_{\text{NN}}(k,k) \quad \text{[fm]} \]

Dick Furnstahl  
DFT from EFT
Gameplan: Exploit Variable Cutoff Potential

Bogner, Kuo, Schwenk

\[ T \begin{pmatrix} -k' & +k' \\ -k & +k \end{pmatrix} = V_\Lambda \begin{pmatrix} -k' & +k' \\ -k & +k \end{pmatrix} + q \leq \Lambda \]

- Require \( \frac{dT}{d\Lambda} = 0 \)
  \(
  \Rightarrow \text{renormalization group equation for } V_\Lambda
  \)

- Run from \( \Lambda_B = 25 \text{ fm}^{-1} \) to \( \Lambda = 2 \text{ fm}^{-1} \sim E_{\text{lab}} = 350 \text{ MeV} \)

- Same long distance physics
  \( \Rightarrow \) collapse to “\( V_{\text{low } k} \)”!
NN Scattering in Free-Space and the Medium

\[ V(k,k) = V_{\text{NN}}(\text{Argonne v18}) + (\text{VGV})_{k_F=0} \]

Dick Furnstahl
DFT from EFT
NN Scattering in Free-Space and the Medium

Argonne V18

"V_{low k} (\Lambda = 2.1 \text{ fm}^{-1})"
NN Scattering in Free-Space and the Medium

\[ I_{\text{med}} = \quad + \quad + \quad + \cdots \]

Argonne V18

\[ V(k,k) \text{ and } V_{\text{GV}}(k,k) [\text{fm}] \]

- \( V = V_{\text{NN}} \) (Argonne v18)
- \( (V_{\text{GV}})_{k_F=0} \)
- \( (V_{\text{GV}})_{k_F=1.35 \text{ fm}^{-1}}[P=0] \)
- \( (V_{\text{GV}})_{k_F=1.35 \text{ fm}^{-1}}[P=2k_F] \)

“\( V_{\text{low } k} \) \( (\Lambda = 2.1 \text{ fm}^{-1}) \)

\[ V(k,k) \text{ and } V_{\text{GV}}(k,k) [\text{fm}] \]

- \( V = V_{\text{low } k} \) (\( \Lambda = 2.1 \text{ fm}^{-1} \))
- \( (V_{\text{GV}})_{k_F=0} \)
NN Scattering in Free-Space and the Medium

\[ I_{\text{med}} = \begin{array}{c}
\begin{array}{c}
\text{Cross term}
\end{array} + \begin{array}{c}
\text{Graphical term}
q > k_f
\end{array} + \begin{array}{c}
\text{Graphical term}
q, q' > k_f
\end{array} + \cdots
\end{array}\]

Argonne V18

\[ V = V_{\text{NN}} \quad (\text{Argonne v18}) \]

\[ (VGV)_{k_F=0} \]

\[ (VGV)_{k_F=1.35 \text{ fm}^{-1}}[P=0] \]

\[ (VGV)_{k_F=1.35 \text{ fm}^{-1}}[P=2k_F] \]

"V_{low k}" (\( \Lambda = 2.1 \text{ fm}^{-1} \))

\[ V = V_{\text{low k}} (\Lambda = 2.1 \text{ fm}^{-1}) \]

\[ (VGV)_{k_F=0} \]

\[ (VGV)_{k_F=1.35 \text{ fm}^{-1}}[P=0] \]

\[ (VGV)_{k_F=1.35 \text{ fm}^{-1}}[P=2k_F] \]
Covergence of the Born Series for Scattering

- Consider whether the Born series converges for given $z$

\[ T(z) = V + V \frac{1}{z - H_0} V + V \frac{1}{z - H_0} V \frac{1}{z - H_0} V + \cdots \]

- If bound state $|b\rangle$, series must diverge at $z = E_b$, where

\[ (H_0 + V)|b\rangle = E_b|b\rangle \quad \Rightarrow \quad V|b\rangle = (E_b - H_0)|b\rangle \]
Covergence of the Born Series for Scattering

Consider whether the Born series converges for given $z$

$$T(z) = V + V \frac{1}{z - H_0} V + V \frac{1}{z - H_0} V \frac{1}{z - H_0} V + \cdots$$

If bound state $|b\rangle$, series must diverge at $z = E_b$, where

$$(H_0 + V)|b\rangle = E_b|b\rangle \implies V|b\rangle = (E_b - H_0)|b\rangle$$

For fixed $E_b$, generalize to find eigenvalue $\eta_\nu$ [Weinberg]

$$\frac{1}{E_b - H_0} V|b\rangle = |b\rangle \implies \frac{1}{E_b - H_0} V|\Gamma_\nu\rangle = \eta_\nu |\Gamma_\nu\rangle$$

From $T$ applied to eigenstate, divergence for $|\eta_\nu| \geq 1$:

$$T(E_b)|\Gamma_\nu\rangle = V|\Gamma_\nu\rangle(1 + \eta_\nu + \eta_\nu^2 + \cdots)$$

$$\implies T \text{ diverges if bound state at } E_b \text{ for } V/\eta_\nu \text{ with } |\eta_\nu| \geq 1$$
Weinberg Eigenvalues as Function of Cutoff

- Deuteron $\rightarrow$ attractive eigenvalue $\eta_\nu$
  - $\Lambda \downarrow \rightarrow$ unchanged
- Hard core $\rightarrow$ repulsive eigenvalue $\eta_\nu$
  - $\Lambda \downarrow \rightarrow$ reduced

$$^3S_1 (E_{cm} = -2.223 \text{ MeV})$$

![Graph showing the variation of $\eta_\nu$ with cutoff $\Lambda$](image)
Weinberg Eigenvalues as Function of Cutoff

- Deuteron $\implies$ **attractive** eigenvalue $\eta_\nu$
  - $\Lambda \downarrow \implies$ unchanged
- Hard core $\implies$ **repulsive** eigenvalue $\eta_\nu$
  - $\Lambda \downarrow \implies$ reduced
- In medium: both reduced
  - $\eta_\nu \ll 1$ for $\Lambda \approx 2 \text{ fm}^{-1}$
  $\implies$ perturbative (in pp)

\[
^3S_1 \quad (E_{cm} = -2.223 \text{ MeV})
\]

- free space, $\eta > 0$
- free space, $\eta < 0$
- $k_f = 1.35 \text{ fm}^{-1}$, $\eta > 0$
- $k_f = 1.35 \text{ fm}^{-1}$, $\eta < 0$
Weinberg Eigenvalues as Function of Density

$^{3}S_1$ with Pauli blocking

$\Lambda = 8.0 \text{ fm}^{-1}$
Weinberg Eigenvalues as Function of Density

\[ \eta_v(B_d) \]

-3 \quad 0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1 \quad 1.2 \quad 1.4

\( k_f [\text{fm}^{-1}] \)

\( 3S_1 \) with Pauli blocking

\( \Lambda = 8.0 \text{ fm}^{-1} \)

\( \Lambda = 4.0 \text{ fm}^{-1} \)
Weinberg Eigenvalues as Function of Density

\[ ^3S_1 \text{ with Pauli blocking} \]

\[ \eta_v(B_d) \]

\[ k_f \text{ [fm}^{-1}] \]

\[ \Lambda = 8.0 \text{ fm}^{-1} \]
\[ \Lambda = 4.0 \text{ fm}^{-1} \]
\[ \Lambda = 3.0 \text{ fm}^{-1} \]
Weinberg Eigenvalues as Function of Density

\[ \eta_{v(B_d)} \]

with Pauli blocking

\[ \Lambda = 8.0 \text{ fm}^{-1} \]
\[ \Lambda = 4.0 \text{ fm}^{-1} \]
\[ \Lambda = 3.0 \text{ fm}^{-1} \]
\[ \Lambda = 2.0 \text{ fm}^{-1} \]
Why is In-Medium $T$ Perturbative for $V_{\text{low } k}$?

- Phase space in pp-channel strongly suppressed:
  \[
  \int_{k_F}^{\infty} q^2 \, dq \frac{V_{NN}(k', q) \, V_{NN}(q, k)}{k^2 - q^2}
  \]
  vs.
  \[
  \int_{k_F}^{\Lambda} q^2 \, dq \frac{V_{\text{low } k}(k', q) \, V_{\text{low } k}(q, k)}{k^2 - q^2}
  \]

- Tames hard core, tensor, and bound state

\[\Lambda: |P/2 \pm k| > k_F \, \text{and} \, |k| < \Lambda\]

\[F: |P/2 \pm k| < k_F\]
Nuclear Matter with NN Ladders Only

- Brueckner ladders order-by-order
- Repulsive core $\implies$ series diverges

Graph showing:
- 1st order
- 2nd order pp ladder
- 3rd order pp ladder

Argonne $v_{18}$
Nuclear Matter with NN Ladders Only

- Brueckner ladders order-by-order
- Repulsive core $\Rightarrow$ series diverges
- $V_{\text{low } k}$ converges

![Graph showing E/A vs. $k_f$ for different orders and ladders.]

Dick Furnstahl  DFT from EFT
Nuclear Matter with NN Ladders Only

- Brueckner ladders order-by-order
- Repulsive core $\Rightarrow$ series diverges
- $V_{\text{low } k}$ converges
- No saturation in sight!

![Graph](image-url)
Soft Potentials in History

- There were active attempts to transform away hard cores and soften the tensor interaction in the late sixties and early seventies.

- But the requiem for soft potentials was given by Bethe:
  
  "Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."

Dick Furnstahl

DFT from EFT
Soft Potentials in History

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- But the requiem for soft potentials was given by Bethe:
  
  "Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."

- But the story is not complete: three-nucleon forces (3NF)!
\( V_{\text{low } k} \) with Chiral 3NF

- **Ideal**: Start with chiral NN + 3NF EFT and run \( \Lambda \downarrow \)

- **Possible now**: Run NN and fit 3NF EFT at each \( \Lambda \)
  

  - two-pion-exchange \( c_i \)'s from NN PSA fit
  - two free parameters fit to \(^3\text{H}\) and \(^4\text{He}\) binding energies
  - ratio 2NF/3NF consistent with chiral counting
First Pass at 3NF for Nuclear Matter

[Bogner, rjf, Schwenk]

- First order: Hartree-Fock

$$\Delta E_{HF} = V_{lowk}$$

- 2nd order: Do 2nd order pp ladder with $V_{eff}$

$$V_{eff} = V_{lowk} + V_{3N}$$
(Preliminary) Nuclear Matter with NN and NNN

Hartree-Fock

\[ \text{E/A [MeV]} \]

\[ \Lambda = 1.6 \text{ fm}^{-1} \]
\[ \Lambda = 1.9 \text{ fm}^{-1} \]
\[ \Lambda = 2.1 \text{ fm}^{-1} \]
\[ \Lambda = 2.3 \text{ fm}^{-1} \]

\[ k_f [\text{fm}^{-1}] \]

\[ L = 1.6 \text{ fm}^{-1} \]
\[ L = 1.9 \text{ fm}^{-1} \]
\[ L = 2.1 \text{ fm}^{-1} \]
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(Preliminary) Nuclear Matter with NN and NNN

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- \[ \Lambda = 2.1 \text{ fm}^{-1} \]
- \[ \Lambda = 2.3 \text{ fm}^{-1} \]

\[ k_f \text{ [fm}^{-1}] \]

“\( \approx \) 2nd Order”

\[ E/A \text{ [MeV]} \]

- \[ \Lambda = 1.6 \text{ fm}^{-1} \]
- \[ \Lambda = 1.9 \text{ fm}^{-1} \]
- \[ \Lambda = 2.1 \text{ fm}^{-1} \]
- \[ \Lambda = 2.3 \text{ fm}^{-1} \]
\textbf{\Large Dependence of Perturbation Theory}

- Convergence degraded for $\Lambda > 2.5 \text{ fm}^{-1}$
- Iterated tensor force excites strongly to $q \sim 2.5–3.0 \text{ fm}^{-1}$

<table>
<thead>
<tr>
<th>旧</th>
<th>新</th>
</tr>
</thead>
<tbody>
<tr>
<td>One Hamiltonian for all problems and energy/length scales</td>
<td>Infinite # of low-energy potentials; different resolutions ⇒ different dof’s, Hamiltonian</td>
</tr>
<tr>
<td>Find the “best” potential</td>
<td>There is no best potential ⇒ use a convenient one! ⇒ vary Λ (NNN changes!!!)</td>
</tr>
<tr>
<td>Two-body data may be sufficient; many-body forces as last resort</td>
<td>Many-body data needed and many-body forces inevitable</td>
</tr>
<tr>
<td>Hide divergences</td>
<td>Exploit Λ dependence; optimize renormalization</td>
</tr>
<tr>
<td>Choose diagrams by “art”</td>
<td>Power counting determines diagrams and truncation error</td>
</tr>
</tbody>
</table>
Outline

EFT-Based Kohn-Sham DFT from Effective Actions

Adding Sources: Kinetic Energy Density and Pairing

Matching to NN and NNN and . . .

Summary
Summary and Selected On-Going Topics

- Effective action $\Rightarrow$ framework for Kohn-Sham DFT
  - EFT provides systematic expansions
  - Connect to full Green’s function $\Rightarrow$ single-particle properties
  - Exploit renormalization (e.g., pair density)
- In progress . . .
  - Pairing for finite systems
  - Long-range effects in functionals
  - Restoring broken symmetries
- Matching to NN + NNN + . . .
  - Chiral EFT $\xrightarrow{\text{RG}} V_{\text{low } k}$ is perturbative in pp channel
  - What about ph?
  - Is the expansion in many-body forces under control?
Kohn-Luttinger Inversion Method

How is the Full $G$ Related to $G_{ks}$?

More Pairing Stuff
Outline

Kohn-Luttinger Inversion Method

How is the Full $G$ Related to $G_{ks}$?

More Pairing Stuff
Kohn-Luttinger-Ward Theorem (1960)

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

\[
\Omega(\mu, V, T) = \Omega_0(\mu) + \infty + \infty + \infty + \cdots
\]
with $G_0(\mu, T)$

\[
T \rightarrow 0 \quad F(N, V, T = 0) = E_0(N) + \infty + \infty + \cdots
\]
with $G_0(\mu_0)$
Kohn-Luttinger-Ward Theorem (1960)

- $T \to 0$ diagram expansion of $\Omega(\mu, V, T)$ in external $\nu(x)$
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\[
\Omega(\mu, V, T) = \Omega_0(\mu) + \cdots
\]

with $G_0(\mu, T)$

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

with $G_0(\mu_0)$

- Uniform Fermi system, no external potential (degeneracy $\nu$):
  \[
  \mu_0(N) = \left(6\pi^2 N/\nu V\right)^{2/3} \equiv k_F^2/2M \equiv \epsilon_F^0
  \]
Kohn-Luttinger-Ward Theorem (1960)

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

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

with $G_0(\mu, T)$

$$\frac{T \to 0}{\implies} F(N, V, T = 0) = E_0(N) + \cdots$$

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):

\[
\Omega(\mu) = \Omega_0(\mu) + \Omega_1(\mu) + \Omega_2(\mu) + \cdots
\]
\[
\mu = \mu_0 + \mu_1 + \mu_2 + \cdots
\]
\[
F(N) = F_0(N) + F_1(N) + F_2(N) + \cdots
\]
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  \]
- invert \( N = -(\partial \Omega(\mu) / \partial \mu)_{TV} \) order-by-order in expansion
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  \]
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- $N$ 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]

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\[
\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*}
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- invert \( N = -(\partial \Omega(\mu) / \partial \mu)_{TV} \) order-by-order in expansion
- \( N \) appears in 0\(^{th}\) 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 \( \mu_1 \):

\[
0 = [\partial \Omega_1 / \partial \mu]_{\mu=\mu_0} + \mu_1 [\partial^2 \Omega_0 / \partial \mu^2]_{\mu=\mu_0} \implies \mu_1 = - \frac{[\partial \Omega_1 / \partial \mu]_{\mu=\mu_0}}{[\partial^2 \Omega_0 / \partial \mu^2]_{\mu=\mu_0}}
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  \]
- Same pattern to all orders: \( \mu_i \) determined by functions of \( \mu_0 \)
Apply this inversion to $F = \Omega + \mu N$:

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

$$+ \Omega_2(\mu_0) + \mu_2 N + \mu_2 \left[ \frac{\partial \Omega_0}{\partial \mu} \right]_{\mu=\mu_0} + \mu_1 \left[ \frac{\partial \Omega_1}{\partial \mu} \right]_{\mu=\mu_0} + \frac{1}{2} \mu_1^2 \left[ \frac{\partial^2 \Omega_0}{\partial \mu^2} \right]_{\mu=\mu_0} + \cdots$$
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$\mu_i$ always cancels from $F_i$ for $i \geq 1$:

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

\[ F_1 \quad F_2 \]
Apply this inversion to $F = \Omega + \mu N$:

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

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

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Generalizing the KGW Inversion Approach

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

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  - it has chemical potential $\mu_0$ and external potential $\nu(x)$
  - $\implies$ fill levels up to $\mu_0$, which is known by counting up to $N$
- But we still have a hard problem in finite systems
  - finding density $\rho(x)$ in non-uniform system is complicated
  - $\implies$ it is not the density of the non-interacting system
Generalizing the KLV Inversion Approach

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- But we still have a hard problem in finite systems
  - finding density $\rho(x)$ in non-uniform system is complicated
    $\implies$ it is *not* the density of the non-interacting system
  - for a self-bound system (nucleus!), there is no [net] $\nu(x)$
Generalizing the KLW Inversion Approach

- Generalizations: Kohn-Sham DFT, other sources, pairing
- $\mu N + J(x)\rho(x)$ with $J(x) = \delta F[\rho]/\delta \rho(x) \rightarrow 0$ in ground state
Generalizing the KLW Inversion Approach

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

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

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

\[
\left[-\frac{\nabla^2}{2M} + v_{KS}(x)\right] \psi_\alpha = \epsilon_\alpha \psi_\alpha \implies \left[-\nabla \frac{1}{M^*(x)} \nabla + v_{KS}(x)\right] \psi_\alpha = \epsilon_\alpha \psi_\alpha
\]
**Generalizing the KLW Inversion Approach**

- Generalizations: Kohn-Sham DFT, other sources, pairing
  1. $\mu N + J(x)\rho(x)$ with $J(x) = \delta F[\rho]/\delta \rho(x) \to 0$ in ground state
  2. Add a source coupled to the kinetic energy density
     
     $+ \eta(x)\tau(x)$ where $\tau(x) \equiv \langle \nabla \psi^\dagger \cdot \nabla \psi \rangle$

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

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

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

- Generalizations: Kohn-Sham DFT, other sources, pairing
  1. $\mu N + J(x)\rho(x)$ with $J(x) = \delta F[\rho]/\delta \rho(x) \rightarrow 0$ in ground state
  2. Add a source coupled to the kinetic energy density
     $$+ \eta(x)\tau(x) \text{ where } \tau(x) \equiv \langle \nabla \psi^{\dagger} \cdot \nabla \psi \rangle$$
     $$\implies M^*(x) \text{ in the Kohn-Sham equation (cf. Skyrme)}$$

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

- Add a source coupled to the \textit{divergent} pair density
  $$\implies \text{e.g., } j\langle \psi^{\dagger \uparrow} \psi^{\dagger \downarrow} + \psi_{\downarrow} \psi^{\uparrow} \rangle \implies \text{set } j \text{ to zero in ground state}$$

- Same inversion method, but use $[j]_{gs} = j_0 + j_1 + j_2 + \cdots = 0$
  $$\implies \text{find } j_0 \text{ iteratively: from } [j_0]_{\text{old}} \text{ find } [j_0]_{\text{new}} = -j_1 - j_2 + \cdots$$
Outline

Kohn-Luttinger Inversion Method

How is the Full $G$ Related to $G_{ks}$?

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

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

$$Z[J, \xi] = e^{iW[J, \xi]} = \int D\psi D\psi^\dagger \ e^{i \int d^4x \ [L + J(x)\psi^\dagger(x)\psi(x) + \int d^4x' \ \psi(x)\xi(x, x')\psi^\dagger(x')]}$$
How is the Full $G$ Related to $G_{ks}$? [nucl-th/0410105]

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

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

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

$$G(x, x') = \frac{\delta W}{\delta \xi} \bigg|_J = \frac{\delta \Gamma}{\delta \xi} \bigg|_{\rho} = G_{ks}(x, x') + G_{ks} \left[ \frac{1}{i} \frac{\delta \Gamma_{int}}{\delta G_{ks}} + \frac{\delta \Gamma_{int}}{\delta \rho} \right] G_{ks}$$
How Do $G$ and $G_{ks}$ Yield the Same Density?

• **Claim:** $\rho_{ks}(x) = -i \nu G^0_{KS}(x, x^+) \text{ equals } \rho(x) = -i \nu G(x, x^+)$

• **Start with**

\[
\begin{align*}
G & = G_{ks} + \Sigma'_{ks} + G_{ks} \\
\end{align*}
\]
How Do $G$ and $G_{ks}$ Yield the Same Density?

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

Start with

Simple diagrammatic demonstration:

Densities agree by construction!
How Do $G$ and $G_{ks}$ Yield the Same Density?

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

- Start with

- Simple diagrammatic demonstration:

- Densities agree by construction!

- But other quantities may differ . . .
Outline

Kohn-Luttinger Inversion Method

How is the Full $G$ Related to $G_{ks}$?

More Pairing Stuff
Renormalizing the “Gap” Equation

- Leading-order (LO) calculation requires $\Gamma_1[\rho, \phi]$

$$\Gamma_1: \quad \begin{array}{c}
\begin{array}{c}
\circ \quad \circ \\
\bigcirc \\
\bigcirc
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\circ \quad \circ \\
\bigcirc \\
\bigcirc
\end{array}
\end{array} + CTC \quad \Longrightarrow
$$

$$j_1 = \frac{\delta \Gamma_1}{\delta \phi} \sim C_0 \text{Tr} F + CTC$$

- Choose LO counterterms (“CTC”) so that $\Gamma_1$ is a function of $\rho$ and the renormalized $\phi$ only
Renormalizing the “Gap” Equation

- Leading-order (LO) calculation requires $\Gamma_1[\rho, \phi]$
  
  \[ \Gamma_1: \quad \begin{array}{c} \circ \quad \bullet \quad \circ \end{array} + \begin{array}{c} \circ \quad \circ \quad \bullet \end{array} + CTC \quad \Rightarrow \]
  
  \[ j_1 = \frac{\delta \Gamma_1}{\delta \phi} \sim C_0 \text{Tr } F + CTC \]

- Choose LO counterterms (“CTC”) so that $\Gamma_1$ is a function of $\rho$ and the renormalized $\phi$ only

- “Gap” equation from $j = j_0 + j_1 = 0 \quad \Rightarrow \text{linear divergence}$
  
  \[ j_0 = -j_1 = -\frac{1}{2} |C_0| \phi \text{ uniform} = \frac{1}{2} |C_0| j_0 \left( \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{(\epsilon_k^0 - \mu_0)^2 + j_0^2}} - \zeta^{(0)} \right) \]
Renormalizing the “Gap” Equation

- Leading-order (LO) calculation requires $\Gamma_1[\rho, \phi]$
  
  $\Gamma_1: \begin{array}{c} \hline \hline \end{array} + \begin{array}{c} \hline \hline \end{array} + \text{CTC} \implies j_1 = \delta \Gamma_1/\delta \phi \sim C_0 \text{Tr } F + \text{CTC}$

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- Conventional: Subtract equation for $a_s$ to eliminate $C_0$

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

- DR/PDS $\implies$ explicit $\Lambda$ to “check” for cutoff dependence
  - cf. Papenbrock & Bertsch DR/MS calculation $\implies$ $\Lambda = 0$

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

- Basic free-space integral $\implies$ beachball renormalization in $\Gamma_2$:

$$\left(\frac{\Lambda}{2}\right)^{3-D} \int \frac{d^D u}{(2\pi)^D} \frac{1}{t^2 - u^2 + i\epsilon} \xrightarrow{\text{PDS}} -\frac{1}{4\pi} (\Lambda + it)$$

$$\implies$$ independent of $\Lambda$
The basic DR/PDS integral in $D$ dimensions, with $x \equiv j_0/\mu_0$, is

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

$$+ (-)^{\beta+1} \frac{M^{3/2}}{\sqrt{2\pi}} \left[\mu_0^2(1 + x^2)\right]^{(\beta+1)/2} P_0^{\beta+1/2} \left(\frac{-1}{\sqrt{1 + x^2}}\right)$$
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$$+ (-1)^{\beta+1} \frac{M^{3/2}}{\sqrt{2\pi}} [\mu_0^2(1 + x^2)]^{(\beta+1)/2} P_{\beta+1/2}^0 \left( \frac{-1}{\sqrt{1 + x^2}} \right)$$

Check the density equation $\implies \Lambda$ dependence cancels:

$$\rho = \int \frac{d^3k}{(2\pi)^3} \left( 1 - \frac{\epsilon^0_k - \mu_0}{E_k} \right) = 0 - I(1) + \mu_0 I(0)$$
Dimensional Regularization and Pairing

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

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- The gap equation implies $\zeta^{(0)}$ is naturally taken from $1/C_0(\Lambda)$:

$$\frac{1}{|C_0(\Lambda)|} = \frac{1}{2} I(0) \quad \text{or} \quad \frac{1}{|C_0|} = \frac{1}{2} \left(I(0) - \zeta^{(0)}\right)$$
Anomalous Density in Finite Systems

- How do we renormalize the pair density in a finite system?
  \[ \phi(\mathbf{x}) = \sum_i [u_i^*(\mathbf{x})v_i(\mathbf{x}) + u_i(\mathbf{x})v_i^*(\mathbf{x})] \to \infty \]

- cf. scalar density \( \rho_s = \sum_i \overline{\psi}(\mathbf{x})\psi(\mathbf{x}) \) for solitons or relativistic nuclei
Anomalous Density in Finite Systems

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- In the uniform limit, \( \phi \) can be defined with a subtraction

\[
\phi = \int^{k_c} d^3k (2\pi)^3 \ j_0 \left( \frac{1}{\sqrt{(\epsilon_k^0 - \mu_0)^2 + j_0^2}} - \frac{1}{\epsilon_k^0} \right) \to \text{finite}
\]
Anomalous Density in Finite Systems

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- In the uniform limit, \( \phi \) can be defined with a subtraction

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

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

\[
\phi(x) = 2 \sum_i E_c \frac{M k_c(x)}{2\pi^2} - j_0(x) \frac{M k_c(x)}{2\pi^2} \quad \text{with} \quad E_c = \frac{k_c^2(x)}{2M} + V_{KS}(x) - \mu
\]

- Convergence is very slow as the energy cutoff is increased
  \( \Rightarrow \) Bulgac/Yu: make a different subtraction

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

- Compare convergence in uniform system, in nuclei with LDA
**Even Better!** [Bulgac, PRC 65 (2002) 051305]

- Convergence is rapid above Fermi surface but not below
  \[\Rightarrow\] scale set by Fermi energy rather than gap
- Solution: Energy cutoff *around* $\mu$

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**Diagram:**

- Graph showing $U(r)$ vs. $r$ in $[\text{fm}]$
- Graph showing $\Delta$ vs. $E_c$ in $[\text{MeV}]$
- Graph showing $g_{\text{eff}}$ vs. $E_c$ in $[\text{MeV fm}^3]$
Dominant application: inhomogeneous electron gas
Interacting point electrons in static potential of atomic nuclei
"Ab initio" calculations of atoms, molecules, crystals, surfaces
HF is good starting point, DFT/LDA is better, DFT/GGA is best

Atomization Energies of Hydrocarbon Molecules

% deviation from experiment

Hartree-Fock
DFT Local Spin Density Approximation
DFT Generalized Gradient Approximation

molecule

\[ \begin{array}{cccccccc}
H_2 & C_2 & C_2H_2 & CH_4 & C_2H_4 & C_2H_6 & C_6H_6 \\
-100 & -80 & -60 & -40 & -20 & 0 & 20
\end{array} \]
Scale contributions according to average density or $\langle k_F \rangle$.

Reasonable estimates $\Rightarrow$ truncation errors understood.