Density Functional Theory
for Dilute Fermions at Unitarity

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Density Functional Theory

The quantum many-body problem: Solve

\[ H\psi(r_1, r_2, \ldots, r_N) = E\psi(r_1, r_2, \ldots, r_N) \]

Difficulty grows very quickly with \( N \)

Energy Density Functional \( E[\rho(r)] \): Solve

\[ \frac{\delta E[\rho(r)]}{\delta \rho(r)} = 0 \quad \int d^3 r \rho(r) = N \]

Effective 1-body problem

Hohenberg-Kohn showed that \( E[\rho(r)] \) exists, but they did not provide a practical way to construct it.
DFT and the nuclear landscape
Traditional Approach

\[ H \Psi = E \Psi \]

\[ V_{NN}, V_{NNN}, \ldots \]
Modern Approach: From EFT to DFT
Consider a non-relativistic field theory

\[ S = \int \psi^\dagger(x) \left( i\partial_0 + \frac{\nabla^2}{2M} \right) \psi(x) + \int \int (\psi^\dagger \psi)(x_1)V(x_1 - x_2)(\psi^\dagger \psi)(x_2) \]

Generating functional \( W[j] = \log Z[j] \)

\[ Z[j(x)] = \int D\psi D\psi^\dagger \exp \left( iS + i \int \psi^\dagger \psi(x)j(x) \right) \]

\[ \rho(x) = \langle \psi^\dagger \psi(x) \rangle = \frac{\delta W[j(x)]}{\delta j(x)} \]

Consider Legendre transform

\[ \Gamma[\rho(x)] = W[j(x)] - \int j(x)\rho(x) \quad j(x) = \frac{\delta \Gamma[\rho(x)]}{\delta \rho(x)} \]

Groundstate: Current vanishes and \( \mathcal{E}[\rho(x)] = T \Gamma[\rho(x)] \)
DFT and perturbative QFT

Consider a perturbative interaction

\[ V(x - y) = \lambda \delta(x - y) \]

Zeroth order: Free field theory in the presence of a source

\[ W[j(x)] = \log \det \left( i\partial_0 + \frac{\nabla^2}{2M} + j(x) + v_{\text{ext}}(x) \right) \]

Determinant can be computed in terms of Fermion orbitals

\[ \left( \frac{\nabla^2}{2M} + v_{\text{ext}}(x) \right) \psi_i = \epsilon_i \psi_i \]

\[ \mathcal{E} = \sum_{\epsilon_i < \epsilon_F} \epsilon_i \quad \rho(x) = \sum_{\epsilon_i < \epsilon_F} \psi_i^\dagger \psi_i(x) \]

DFT with auxiliary Fermion orbitals: Kohn-Sham theory
DFT and perturbative QFT

First order correction

\[ \Gamma_1[\rho] = \frac{C_0}{4} \int d^3 x |\rho(x)|^2 \]

Second order correction

Non-local
Density matrix expansion
DFT in Nuclear Physics: Problems

Interactions are non-perturbative

- **Scattering length large, strong tensor force**

Interactions are not local

- **Pion exchanges**

Broken Symmetries

- **Translations, rotations, particle number**

Nuclei are self-bound

- **No external potential, intrinsic density needed**

Here: Study role of large scattering length
Designer Fluids

Atomic gas with two spin states: “↑” and “↓”

Feshbach resonance

\[ a(B) = a_0 \left( 1 + \frac{\Delta}{B - B_0} \right) \]

“Unitarity” limit \( a \to \infty \)

\[ \sigma = \frac{4\pi}{k^2} \]
Universality

What does this system have in common with nuclear matter?

dilute: \( r \rho^{1/3} \ll 1 \)

strongly correlated: \( a \rho^{1/3} \gg 1 \)

Feshbach Resonance in \(^6\text{Li}\)

Neutron Matter
Effective Field Theory

Effective field theory for pointlike, non-relativistic neutrons

\[ \mathcal{L}_{\text{eff}} = \psi^\dagger \left( i\partial_0 + \frac{\nabla^2}{2M} \right) \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 + \frac{C_2}{16} \left[ (\psi \psi)^\dagger (\psi \nabla^2 \psi) + \text{h.c.} \right] + \ldots \]

Match to effective range expansion

\[ C_0 = \frac{4\pi a}{M} \quad a = -18 \text{ fm} \]

\[ C_2 = \frac{4\pi a^2}{M} \frac{r}{2} \quad r = 2.8 \text{ fm} \]

Unitarity limit: \( C_0 \to \infty, \ C_2 \to 0 \)
Effective Low Energy Lagrangian

Superfluid phase: Response governed by Goldstone boson

\[ \psi \bar{\psi} = e^{2i\varphi} \langle \psi \bar{\psi} \rangle \]

Effective Lagrangian

\[ \mathcal{L} = f^2 \left( (\partial_0 \varphi)^2 - c_s^2 (\nabla \varphi)^2 \right) + \ldots \]

Higher orders? Need to incorporate symmetry constraints:

- \( U(1) \) symmetry
- Galilean invariance
- Conformal symmetry

Strategy: Promote \( U(1) \) and Galilean invariance to local symmetries
Effective Lagrangian

Leading order

\[ L_1 = c_0 m^{3/2} X^{5/2} \]

\[ X = \mu - A_0 - \dot{\phi} - \frac{(\vec{\nabla} \phi)^2}{2m} \]

Check: \[ L_1 = \frac{15c_0 m^{3/2} \mu^{1/2}}{8} \left( \text{const} + (\partial_0 \phi)^2 - \frac{2\mu}{3m} (\nabla \phi)^2 + \ldots \right) \]

Next-to-leading order

\[ L_2 = c_1 m^{1/2} \frac{(\vec{\nabla} X)^2}{\sqrt{X}} + c_2 \frac{(\nabla^2 \phi)^2 - 9m \nabla^2 A_0}{\sqrt{m}} \sqrt{X} \]
Density Functional

Construct energy functional $\mathcal{E}[n(x)] = \mu n(x) - P[\mu - A_0(x)]$

$$\mathcal{E}(x) = n(x)A_0(x) + \frac{3 \cdot 2^{2/3}}{5^{5/3}mc_0^{2/3}} n(x)^{5/3}$$

$$- \frac{4}{45} \frac{2c_1 + 9c_2}{mc_0} (\nabla n(x))^2 - \frac{12}{5} \frac{c_2}{mc_0} \nabla^2 n(x) + \ldots$$

Non-perturbative physics in $c_0, c_1, c_2, \ldots$

$c_0$ Equation of state, $c_{1,2}$ phonon dispersion relation

Many body physics: Use epsilon ($\epsilon = d - 4$) expansion
Upper and lower critical dimension

Zero energy bound state for arbitrary $d$

$$\psi''(r) + \frac{d-1}{r}\psi'(r) = 0 \quad (r > r_0)$$

$d=2$: Arbitrarily weak attractive potential has a bound state

$$\xi = \frac{\mu}{E_F^0} = 1$$

$d=4$: Bound state wave function

$$\psi \sim 1/r^{d-2}.$$ Pairs do not overlap

$$\xi = \frac{\mu}{E_F^0} = 0$$

Conclude $\xi(d=3) \sim 1/2$?

Try expansion around $d = 4$ or $d = 2$?

Epsilon Expansion

EFT version: Compute scattering amplitude \((d = 4 - \epsilon)\)

\[
T = \frac{1}{\Gamma (1 - \frac{d}{2})} \left( \frac{m}{4\pi} \right)^{-d/2} \left( -p_0 + \frac{\epsilon p}{2} \right)^{1-d/2} \approx \frac{8\pi^2 \epsilon}{m^2} \frac{i}{p_0 + \frac{\epsilon p}{2} + i\delta}
\]

\[
g^2 \equiv \frac{8\pi^2 \epsilon}{m^2} \quad D(p_0, p) = \frac{i}{p_0 + \frac{\epsilon p}{2} + i\delta}
\]

Weakly interacting bosons and fermions
Epsilon Expansion

Effective lagrangian for atoms $\Psi = (\psi_\uparrow, \psi_\downarrow^\dagger)$ and dimers $\phi$

$$\mathcal{L} = \Psi^\dagger \left( i\partial_0 + \frac{\sigma_3 \nabla^2}{2m} \right) \Psi + \mu \Psi^\dagger \sigma_3 \Psi + \Psi^\dagger \sigma_+ \Psi \phi + h.c.$$ 

Perturbative expansion: $\phi = \phi_0 + g\varphi$. Free part

$$\mathcal{L}_0 = \Psi^\dagger \left[ i\partial_0 + \sigma_3 \frac{\vec{\nabla}^2}{2m} + \phi_0 (\sigma_+ + \sigma_-) \right] \Psi + \varphi^\dagger \left( i\partial_0 + \frac{\vec{\nabla}^2}{4m} \right) \varphi.$$ 

Interacting part ($g^2, \mu = O(\epsilon)$)

$$\mathcal{L}_I = g (\Psi^\dagger \sigma_+ \Psi \varphi + h.c) + \mu \Psi^\dagger \sigma_3 \Psi - \varphi^\dagger \left( i\partial_0 + \frac{\vec{\nabla}^2}{4m} \right) \varphi.$$ 

Nishida & Son (2006)
Matching Calculations

Effective potential

\[ P = \#(2m)^{d/2} \mu^{d/2+1} \]

Phonon Propagator

\[ \begin{pmatrix} \cdots \end{pmatrix}^{-1} = \begin{pmatrix} \cdots \end{pmatrix}^{-1} - \Pi \]

\[ -\Pi = \begin{pmatrix} \cdots \end{pmatrix} \]

\[ \omega = c_s p \left\{ 1 + \# \left( \frac{p^2}{m \mu} \right) + \ldots \right\} \]
Matching (continued)

Static susceptibility

\[ \chi(q) = \int d^3x \, e^{iqx} \langle \psi^\dagger \psi(x) \psi^\dagger \psi(0) \rangle \]

\[ \chi(q) = \chi(0) \left\{ 1 - \# \left( \frac{q^2}{m\mu} \right) + \ldots \right\} \]

Nishida, Son (2007)

Rupak, Schaefer (2008)
Density Functional

Unitarity Limit

\[ E(x) = n(x)A_0(x) + 1.364 \frac{n(x)^{5/3}}{m} + 0.032 \frac{(\nabla n(x))^2}{mn(x)} + O(\nabla^4 n) \]

\[ E_{\text{trap}} = \frac{\sqrt{0.475}}{4} \omega(3N)^{4/3} \left( 1 + \frac{2.4}{(3N)^{2/3}} + \ldots \right) \]

Free Fermions

\[ E(x) = n(x)A_0(x) + 2.871 \frac{n(x)^{5/3}}{m} + 0.014 \frac{(\nabla n(x))^2}{mn(x)} + 0.167 \frac{\nabla^2 n(x)}{m} \]

\[ E_{\text{trap}} = \frac{1}{4} \omega(3N)^{4/3} \left( 1 + \frac{0.5}{(3N)^{2/3}} + \ldots \right) \]
Comparison to Data

\[ \frac{E_N}{E^0_\infty} \]

[Graph showing \( \frac{E_N}{E^0_\infty} \) vs. \( N \) with points and curves labeled \( O(\nabla n)^2 \) and \( N^{-1/3} \) fit.]

ETFT
Outlook

Kohn Sham theory at unitarity?

Asymptotic behavior ($N^{-1/3}$ ?)

Superfluid density functional?

Perturbative pions, range corrections?