Local Density Functional Theory for Superfluid Fermionic Systems

The Unitary Fermi Gas
Outline:

• What is a unitary Fermi gas

• Very brief/skewed summary of DFT

• Bogoliubov-de Gennes equations, renormalization

• Superfluid Local Density Approximation (SLDA) for a unitary Fermi gas

• Fermions at unitarity in a harmonic trap
What is a unitary Fermi gas
What are the ground state properties of the many-body system composed of spin $\frac{1}{2}$ fermions interacting via a zero-range, infinite scattering-length contact interaction.

In 1999 it was not yet clear, either theoretically or experimentally, whether such fermion matter is stable or not.

- systems of bosons are unstable (Efimov effect)
- systems of three or more fermion species are unstable (Efimov effect)

• Baker (winner of the MBX challenge) concluded that the system is stable. See also Heiselberg (entry to the same competition)

• Chang et al (2003) Fixed-Node Green Function Monte Carlo and Astrakharchik et al. (2004) FN-DMC provided best the theoretical estimates for the ground state energy of such systems.

• Thomas’ Duke group (2002) demonstrated experimentally that such systems are (meta)stable.
Consider Bertsch’s MBX challenge (1999): “Find the ground state of infinite homogeneous neutron matter interacting with an infinite scattering length.”

\[ r_0 \to 0 \ll \lambda_F \ll |a| \to \infty \]

- Carlson, Morales, Pandharipande and Ravenhall, PRC 68, 025802 (2003), with Green Function Monte Carlo (GFMC)

\[
\frac{E_N}{N} = \alpha_N \frac{3}{5} \varepsilon_F, \quad \alpha_N = 0.54
\]

normal state

- Carlson, Chang, Pandharipande and Schmidt, PRL 91, 050401 (2003), with GFMC

\[
\frac{E_S}{N} = \alpha_S \frac{3}{5} \varepsilon_F, \quad \alpha_S = 0.44
\]

superfluid state

This state is half the way from BCS→BEC crossover, the pairing correlations are in the strong coupling limit and HFB invalid again.
Solid line with open circles – Chang et al. physics/0404115
Dashed line with squares - Astrakharchik et al. cond-mat/0406113
Green Function Monte Carlo with Fixed Nodes
S.-Y. Chang, J. Carlson, V. Pandharipande and K. Schmidt
physics/0403041
\[ \Delta_{Gorkov} = \left( \frac{2}{e} \right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp \left( \frac{\pi}{2k_F a} \right) \]

\[ \Delta_{BCS} = \frac{8}{e^2} \frac{\hbar^2 k_F^2}{2m} \exp \left( \frac{\pi}{2k_F a} \right) \]

Fixed node GFMC results, S.-Y. Chang et al. (2003)
If $a<0$ at $T=0$ a Fermi system is a BCS superfluid

$$
\Delta \approx \left(\frac{2}{e}\right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp\left(\frac{\pi}{2k_F a}\right) \ll \varepsilon_F, \quad \text{iff} \quad k_F |a| \ll 1 \quad \text{and} \quad \xi = \frac{1}{k_F} \frac{\varepsilon_F}{\Delta} \gg \frac{1}{k_F}
$$

If $|a| = \infty$ and $nr_0^3 \ll 1$ a Fermi system is strongly coupled and its properties are universal. Carlson et al. PRL 91, 050401 (2003)

$$
\frac{E_{\text{normal}}}{N} \approx 0.54 \frac{3}{5} \varepsilon_F, \quad \frac{E_{\text{superfluid}}}{N} \approx 0.44 \frac{3}{5} \varepsilon_F \quad \text{and} \quad \xi = O(\lambda_F), \ \Delta = O(\varepsilon_F)
$$

If $a>0$ ($a \gg r_0$) and $na^3 \ll 1$ the system is a dilute BEC of tightly bound dimers

$$
\varepsilon_2 = -\frac{\hbar^2}{ma^2} \quad \text{and} \quad n_b a^3 \ll 1, \quad \text{where} \quad n_b = \frac{n_f}{2} \quad \text{and} \quad a_{bb} = 0.6a > 0
$$
Very brief/skewed summary of DFT
Density Functional Theory (DFT)
Hohenberg and Kohn, 1964

$$E_{gs} = E[\rho(\vec{r})]$$

Local Density Approximation (LDA)
Kohn and Sham, 1965

The energy density is typically determined in *ab initio* calculations of infinite homogeneous matter.

$$E_{gs} = \int d^3r \left\{ \frac{\hbar^2}{2m} \tau(\vec{r}) + \varepsilon[\rho(\vec{r})] \rho(\vec{r}) \right\}$$

$$\rho(\vec{r}) = \sum_{i=1}^{N} |\psi_i(\vec{r})|^2 \quad \tau(\vec{r}) = \sum_{i=1}^{N} |\nabla \psi_i(\vec{r})|^2$$

$$-\frac{\hbar^2 \Delta}{2m} \psi_i(\vec{r}) + U(\vec{r}) \psi_i(\vec{r}) = \varepsilon_i \psi_i(\vec{r})$$

Kohn-Sham equations
One can construct however an EDF which depends both on particle density and kinetic energy density and use it in a extended Kohn-Sham approach (perturbative result)

\[
E[\rho(x), \tau(x)] = \int d^3x \left\{ \frac{1}{2M} \tau(x) + v(x) \rho(x) + \frac{1}{2} \left( \frac{\nu - 1}{\nu} \right) \frac{4\pi a_s}{M} [\rho(x)]^2 \\
+ (B_2 a_s^2 r_s + B_3 a_p^3) \frac{1}{2M} \rho(x) \tau(x) + (3B_2 a_s^2 r_s - B_3 a_p^3) \frac{1}{8M} [\nabla \rho(x)]^2 \\
+ b_1 \frac{a_s^2}{2M} [\rho(x)]^{7/3} + b_4 \frac{a_s^3}{2M} [\rho(x)]^{8/3} \right\}.
\]

Notice that dependence on kinetic energy density and on the gradient of the particle density emerges because of finite range effects.

Bhattacharyya and Furnstahl, nucl-phys/0408014
The single-particle spectrum of usual Kohn-Sham approach is unphysical, with the exception of the Fermi level. The single-particle spectrum of extended Kohn-Sham approach has physical meaning.

<table>
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<th>$\nu$</th>
<th>$N_F$</th>
<th>$A$</th>
<th>$a_p$</th>
<th>$E/A$</th>
<th>$\langle k_F \rangle$</th>
<th>$\sqrt{\langle r^2 \rangle}$</th>
<th>approximation</th>
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<td>$\tau$–NNLO (LDA)</td>
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<td>2.77</td>
<td>3.09</td>
<td>$\tau$–NNLO (LDA)</td>
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TABLE I: Energies per particle, averages of the local Fermi momentum $k_F$, and rms radii for sample parameters and particle numbers for a dilute Fermi gas in a harmonic trap. See the text for a description of units. The scattering length is fixed at $a_s = 0.16$ and the effective range is set to $r_s = 2a_s/3$ when $a_p \neq 0$. Results with the DFT functional including $\tau$ are marked “$\tau$–NNLO.”
Extended Kohn-Sham equations

Position dependent mass

\[ E_{gs} = \int d^3r \left\{ \frac{\hbar^2}{2m^*[\rho(\vec{r})]} \tau(\vec{r}) + \varepsilon[\rho(\vec{r})] \rho(\vec{r}) \right\} \]

\[ \rho(\vec{r}) = \sum_{i=1}^{N} |\psi_i(\vec{r})|^2 \quad \tau(\vec{r}) = \sum_{i=1}^{N} |\nabla \psi_i(\vec{r})|^2 \]

\[ -\nabla \frac{\hbar^2}{2m^*[\rho(\vec{r})]} \nabla \psi_i(\vec{r}) + U(\vec{r})\psi_i(\vec{r}) = \varepsilon_i \psi_i(\vec{r}) \]

Normal Fermi systems only!
However, not everyone is normal!
Superconductivity and superfluidity in Fermi systems

- Dilute atomic Fermi gases \( T_c \approx 10^{-12} - 10^{-9} \text{ eV} \)
- Liquid \(^3\text{He}\) \( T_c \approx 10^{-7} \text{ eV} \)
- Metals, composite materials \( T_c \approx 10^{-3} - 10^{-2} \text{ eV} \)
- Nuclei, neutron stars \( T_c \approx 10^5 - 10^6 \text{ eV} \)
- QCD color superconductivity \( T_c \approx 10^7 - 10^8 \text{ eV} \)

*units (1 eV \( \approx 10^4 \text{ K}\))*
Bogoliubov-de Gennes equations and renormalization
SLDA - Extension of Kohn-Sham approach to superfluid Fermi systems

\[ E_{gs} = \int d^3 r \varepsilon(\rho(\vec{r}), \tau(\vec{r}), \nu(\vec{r})) \]

\[ \rho(\vec{r}) = 2 \sum_k |v_k(\vec{r})|^2, \quad \tau(\vec{r}) = 2 \sum_k |\vec{\nabla}v_k(\vec{r})|^2 \]

\[ \nu(\vec{r}) = \sum_k u_k(\vec{r}) v_k^*(\vec{r}) \]

\[
\begin{pmatrix}
T + U(\vec{r}) - \mu \\
\Delta^*(\vec{r})
\end{pmatrix}
\begin{pmatrix}
\Delta(\vec{r}) \\
-(T + U(\vec{r}) - \mu)
\end{pmatrix}
= \begin{pmatrix}
u_k(\vec{r}) \\
v_k(\vec{r})
\end{pmatrix}
\begin{pmatrix}
u_k(\vec{r}) \\
v_k(\vec{r})
\end{pmatrix}
= E_k
\]

Mean-field and pairing field are both local fields!
(for sake of simplicity spin degrees of freedom are not shown)

There is a little problem! The pairing field \( \Delta \) diverges.
Why would one consider a local pairing field?

✓ Because it makes sense physically!
✓ The treatment is so much simpler!
✓ Our intuition is so much better also.

\[ r_0 \approx \frac{\hbar}{p_F} = k_F^{-1} \]

radius of interaction \hspace{1cm} inter-particle separation

\[ \Delta = \omega_D \exp\left(-\frac{1}{|V|N}\right) \ll \varepsilon_F \]

\[ \xi \approx \frac{1}{k_F} \frac{\varepsilon_F}{\Delta} \gg r_0 \]

coherece length

size of the Cooper pair
Nature of the problem

\[ \nu(\vec{r}_1, \vec{r}_2) = \sum_{E_k > 0} v_k^*(\vec{r}_1) u_k(\vec{r}_2) \propto \frac{1}{|\vec{r}_1 - \vec{r}_2|} \]

\[ \Delta(\vec{r}_1, \vec{r}_2) = -V(\vec{r}_1, \vec{r}_2) \nu(\vec{r}_1, \vec{r}_2) \]

It is easier to show how this singularity appears in infinite homogeneous matter.

\[ v_k(\vec{r}_1) = v_k \exp(ik \cdot \vec{r}_1), \quad u_k(\vec{r}_2) = u_k \exp(ik \cdot \vec{r}_2) \]

\[ v_k^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k - \mu}{\sqrt{(\epsilon_k - \mu)^2 + \Delta^2}} \right), \quad u_k^2 + v_k^2 = 1, \quad \epsilon_k = \frac{\hbar^2 k^2}{2m} + U, \quad \Delta = \frac{\hbar^2 \delta}{2m} \]

\[ \nu(r) = \frac{\Delta m}{2\pi^2 \hbar^2} \int_0^\infty dk \frac{\sin(kr)}{kr} \frac{k^2}{\sqrt{(k^2 - k_F^2)^2 + \delta^2}}, \quad r = |\vec{r}_1 - \vec{r}_2| \]
**Pseudo-potential approach**
(appropriate for very slow particles, very transparent, but somewhat difficult to improve)

Lenz (1927), Fermi (1931), Blatt and Weiskopf (1952)
Lee, Huang and Yang (1957)

\[-\frac{\hbar^2 \Delta \vec{r}}{m} \psi (\vec{r}) + V (\vec{r}) \psi (\vec{r}) = E \psi (\vec{r}), \quad V (\vec{r}) \approx 0 \text{ if } r > R\]

\[\psi (\vec{r}) = \exp (i k \cdot \vec{r}) + \frac{f}{r} \exp (ikr) \approx 1 + \frac{f}{r} + \ldots \approx 1 - \frac{a}{r} + O(kr)\]

\[f^{-1} = -\frac{1}{a} + \frac{1}{2} r_0 k^2 - ik, \quad g = \frac{4\pi \hbar^2 a}{m(1 + ika)} + \ldots\]

if \(kr_0 \ll 1\) then \(V (\vec{r}) \psi (\vec{r}) \Rightarrow g \delta (\vec{r}) \frac{\partial}{\partial r} [r \psi (\vec{r})]\)

Example: \(\psi (\vec{r}) = \frac{A}{r} + B + \ldots \Rightarrow \delta (\vec{r}) \frac{\partial}{\partial r} [r \psi (\vec{r})] = \delta (\vec{r}) B\)
The SLDA (renormalized) equations

\[ E_{gs} = \int d^3 r \left\{ \varepsilon_N \left[ \rho(\vec{r}), \tau(\vec{r}) \right] + \varepsilon_S \left[ \rho(\vec{r}), \nu(\vec{r}) \right] \right\} \]

\[ \varepsilon_S \left[ \rho(\vec{r}), \nu(\vec{r}) \right] = -\Delta(\vec{r}) \nu_c(\vec{r}) = g_{\text{eff}}(\vec{r}) |\nu_c(\vec{r})|^2 \]

\[
\begin{align*}
\left\{
[h(\vec{r}) - \mu]u_i(\vec{r}) + \Delta(\vec{r})\nu_i(\vec{r}) &= E_i u_i(\vec{r}) \\
\Delta^*(\vec{r}) u_i(\vec{r}) - [h(\vec{r}) - \mu]\nu_i(\vec{r}) &= E_i \nu_i(\vec{r})
\end{align*}
\]

\[
\begin{align*}
h(\vec{r}) &= -\tilde{V} \frac{\hbar^2}{2m(\vec{r})} \tilde{V} + U(\vec{r}) \\
\Delta(\vec{r}) &= -g_{\text{eff}}(\vec{r}) \nu_c(\vec{r})
\end{align*}
\]

\[
\frac{1}{g_{\text{eff}}(\vec{r})} = \frac{1}{g[\rho(\vec{r})]} - \frac{m(\vec{r})k_c(\vec{r})}{2\pi^2\hbar^2} \left\{ 1 - \frac{k_F(\vec{r})}{2k_c(\vec{r})} \ln \frac{k_c(\vec{r}) + k_F(\vec{r})}{k_c(\vec{r}) - k_F(\vec{r})} \right\}
\]

\[ \rho_c(\vec{r}) = 2 \sum_{E_i \geq 0} |\nu_i(\vec{r})|^2, \quad \nu_c(\vec{r}) = \sum_{E_i \geq 0} \nu_i^*(\vec{r}) u_i(\vec{r}) \]

\[ E_c + \mu = \frac{\hbar^2 k_c^2(\vec{r})}{2m(\vec{r})} + U(\vec{r}), \quad \mu = \frac{\hbar^2 k_F^2(\vec{r})}{2m(\vec{r})} + U(\vec{r}) \]

Position and momentum dependent running coupling constant
Observables are (obviously) independent of cut-off energy (when chosen properly).
Superfluid Local Density Approximation (SLDA) for a unitary Fermi gas
The naïve SLDA energy density functional suggested by dimensional arguments

\[ \varepsilon(\vec{r}) = \alpha \frac{\tau(\vec{r})}{2} + \beta \frac{3(3\pi^2)^{2/3} n^{5/3}(\vec{r})}{5} + \gamma \frac{|\nu(\vec{r})|^2}{n^{1/3}(\vec{r})} \]

\[ n(\vec{r}) = 2 \sum_k |\nu_k(\vec{r})|^2 \]

\[ \tau(\vec{r}) = 2 \sum_k \left| \nabla \nu_k(\vec{r}) \right|^2 \]

\[ \nu(\vec{r}) = \sum_k u_k(\vec{r}) v_k^*(\vec{r}) \]
The renormalized SLDA energy density functional

\[ \varepsilon(\vec{r}) = \alpha \frac{\tau_c(\vec{r})}{2} + \beta \frac{3(3\pi^2)^{2/3} n^{5/3}(\vec{r})}{5} + g_{\text{eff}}(\vec{r})|\nu_c(\vec{r})|^2 \]

\[ \tau_c(\vec{r}) = 2 \sum_{E<E_c} |\nabla \nu_k(\vec{r})|^2, \quad \nu_c(\vec{r}) = \sum_{E<E_c} u_k(\vec{r})v_k^*(\vec{r}) \]

\[ \frac{1}{g_{\text{eff}}(\vec{r})} = \frac{n^{1/3}(\vec{r})}{\gamma} - \frac{k_c(\vec{r})}{2\pi^2\alpha} \left[ 1 - \frac{k_0(\vec{r})}{2k_c(\vec{r})} \ln \frac{k_c(\vec{r}) + k_0(\vec{r})}{k_c(\vec{r}) - k_0(\vec{r})} \right] \]

\[ E_c + \mu = \alpha \frac{k_c^2(\vec{r})}{2} + U(\vec{r}), \quad \mu = \alpha \frac{k_0^2(\vec{r})}{2} + U(\vec{r}) \]

\[ U(\vec{r}) = \beta \frac{(3\pi^2)^{2/3} n^{2/3}(\vec{r})}{2} - \frac{|\Delta(\vec{r})|^2}{3\gamma n^{2/3}(\vec{r})} + V_{\text{ext}}(\vec{r}) + \text{small correction} \]

\[ \Delta(\vec{r}) = -g_{\text{eff}}(\vec{r})\nu_c(\vec{r}) \]
How to determine the dimensionless parameters $\alpha$, $\beta$ and $\gamma$?

$$n = \frac{k_F^3}{3\pi^2} = \int \frac{d^3k}{(2\pi)^3} \left(1 - \frac{\alpha k^2 / 2 + \bar{\beta} k_F^2 / 2 - \mu}{\sqrt{(\alpha k^2 / 2 + \bar{\beta} k_F^2 / 2 - \mu)^2 + \Delta^2}}\right)$$

$$= \int \frac{d^3k}{(2\pi)^3} \left(1 - \frac{\varepsilon_k}{E_k}\right)$$

$$\frac{3}{5} \varepsilon_F n \xi_S = \frac{3}{5} \varepsilon_F n \beta + \int \frac{d^3k}{(2\pi)^3} \left[ \alpha \frac{k^2}{2} \left(1 - \frac{\varepsilon_k}{E_k}\right) - \frac{\Delta^2}{2E_k} \right]$$

$$n^{1/3} = \int \frac{d^3k}{(2\pi)^3} \left(\frac{1}{\alpha k^2} - \frac{1}{2E_k}\right)$$
One thus obtains:

\[
\begin{align*}
\xi_s &= \frac{5E}{3N\varepsilon_F} = 0.42(2) \\
\eta &= \frac{\Delta}{\varepsilon_F} = 0.504(24) \Rightarrow \quad \alpha = 1.14 \\
\varsigma &= \frac{\mu}{\varepsilon_F} = 0.42(2) \Rightarrow \frac{1}{\gamma} = -0.0906
\end{align*}
\]
**Bonus!**

**Quasiparticle spectrum in homogeneous matter**

- **Solid line** - SLDA
- **Circles** - GFMC due to Carlson and Reddy
Extra Bonus!

The normal state has been also determined in GFMC

\[ \xi_N = \frac{5E}{3N \varepsilon_F} = 0.55(2) \]

SLDA functional predicts

\[ \xi_N = \alpha + \beta = 0.59 \]
Fermions at unitarity in a harmonic trap

GFMC calculations of Chang and Bertsch
GFMC - Chang and Bertsch
TABLE I: Table 1. The energies $E(N)$ calculated within the GFMC [15] and SLDA. When two numbers are present the first was calculated as the expectation value of the Hamiltonian/functional, while the second is the value obtained using the virial theorem [20].

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<tr>
<th>$N$</th>
<th>$E_{GFMC}$</th>
<th>$E_{SLDA}$</th>
<th>$N$</th>
<th>$E_{GFMC}$</th>
<th>$E_{SLDA}$</th>
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<td>22</td>
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$$\delta_2 E(N) = E(N) - \frac{1}{2}[E(N + 1) + E(N - 1)]$$
Densities for $N=8$ (solid), $N=14$ (dashed) and $N=20$ (dot-dashed) 
GFMC (red), SLDA (blue)
• Agreement between GFMC and SLDA very good
  (a few percent accuracy)

Why not better?
* A better agreement would have really signaled big troubles!

• Energy density functional is not unique,
in spite of the strong restrictions imposed by unitarity

• Self-interaction correction neglected
  smallest systems affected the most

• Absence of polarization effects
  spherical symmetry imposed, odd systems mostly affected

• Spin number densities not included
  extension from SLDA to SLSD(A) needed
  *ab initio* results for asymmetric system needed

• Gradient corrections not included