Superfluid LDA (SLDA)

Local Density Approximation / Kohn-Sham for Systems with Superfluid Correlations

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Slides will be posted shortly at http://www.phys.washington.edu/~bulgac/
What I would like to cover

✓ Brief review of DFT and LDA
✓ Introduce SLDA (+ some technical details)
✓ Apply SLDA to nuclei and neutron stars (vortices)
✓ Apply SLDA to dilute atomic Fermi gases (vortices)
✓ Conclusions
Superconductivity and superfluidity in Fermi systems

- Dilute atomic Fermi gases
  \[ T_c \approx 10^{-12} \text{ – } 10^{-9} \text{ eV} \]

- Liquid $^3\text{He}$
  \[ T_c \approx 10^{-7} \text{ eV} \]

- Metals, composite materials
  \[ T_c \approx 10^{-3} \text{ – } 10^{-2} \text{ eV} \]

- Nuclei, neutron stars
  \[ T_c \approx 10^5 \text{ – } 10^6 \text{ eV} \]

- QCD color superconductivity
  \[ T_c \approx 10^7 \text{ – } 10^8 \text{ eV} \]

units (1 eV $\approx 10^4$ K)
Density Functional Theory (DFT)  
Hohenberg and Kohn, 1964

Local Density Approximation (LDA)  
Kohn and Sham, 1965

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

The energy density is typically determined in \textit{ab initio} calculations of infinite homogeneous matter.

The Kohn-Sham equations

\[
\rho(\mathbf{r}) = \sum_{i=1}^{N} |\psi_i(\mathbf{r})|^2 \\
\tau(\mathbf{r}) = \sum_{i=1}^{N} |\nabla \psi_i(\mathbf{r})|^2 \\
-\frac{\hbar^2 \Delta}{2m} \psi_i(\mathbf{r}) + U(\mathbf{r})\psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})
\]
Extended Kohn-Sham equations

Position dependent mass

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

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

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

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

\[ \mathcal{E}_{SK}(x) = \frac{1}{2M} \tau(x) + \frac{3}{8} t_0 [\rho(x)]^2 + \frac{1}{16} t_3 [\rho(x)]^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho(x) \tau(x) \\
+ \frac{1}{64} (9t_1 - 5t_2) |\nabla \rho(x)|^2 - \frac{3}{4} W_0 \rho(x) \nabla \cdot J(x) + \frac{1}{32} (t_1 - t_2) [J(x)]^2 . \]

One can try to derive it, however, from an *ab initio* (?!) lagrangian

\[ \mathcal{L} = \psi^\dagger \left[ i \partial_t + \frac{\nabla^2}{2M} \right] \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 + \frac{C_2}{16} \left[ (\psi \psi)^\dagger (\psi \nabla^2 \psi) + \text{h.c.} \right] \\
+ \frac{C_2'}{8} (\psi \nabla \psi)^\dagger \cdot (\psi \nabla \psi) + \cdots , \]

Bhattacharyya and Furnstahl, nucl-phys/0408014
\[
\frac{E}{N} = \frac{k_F^2}{2M} \left[ \frac{3}{5} + (g - 1) \left\{ \frac{2}{3\pi} (k_F a_s) + \frac{4}{35\pi^2} (11 - 2 \ln 2) (k_F a_s)^2 + \frac{1}{10\pi} (k_F r_s) (k_F a_s)^2 \right\} + (g + 1) \frac{1}{5\pi} (k_F a_p)^3 \right] + (g - 1) (g - 2) \frac{16}{27\pi^3} (4\pi - 3\sqrt{3}) (k_F a_s)^4 \ln(k_f a_s) + \cdots \,.
\]
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

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

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.

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<th>$\bar{N}_F$</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>
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<td>$\tau$–NNLO (LDA)</td>
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Local Density Approximation (LDA)  
Kohn and Sham, 1965

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

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

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

Normal Fermi systems only!
However, not everyone is normal!
SLDA - Extension of Kohn-Sham approach to superfluid Fermi systems

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

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

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

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

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 inter-particle separation

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

coherence length size of the Cooper pair

\[
 \xi \approx \frac{1}{k_F} \frac{\varepsilon_F}{\Delta} \gg r_0
\]
Nature of the problem

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

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

\[ v(\vec{r}) = \frac{\Delta m}{2\pi^2 \hbar^2} \int_0^\infty dk \frac{\sin(kr)}{kr} \frac{k^2}{\sqrt{(k^2 - k_F^2)^2 + \delta^2}}, \quad r = |\vec{r}_1 - \vec{r}_2| \]

It is easier to show how this singularity appears in infinite homogeneous matter.
A (too) simple case

\[ k_F \to 0, \delta \to 0 \]

\[ \nu(\left|\vec{r}_1 - \vec{r}_2\right|) \to \frac{\Delta m}{2\pi^2 \hbar^2} \int_0^{\infty} dk \frac{\sin kr}{kr} = \frac{\Delta m}{2\pi^2 \hbar^2} \frac{\pi}{2\left|\vec{r}_1 - \vec{r}_2\right|} \]

The integral converges (conditionally) at \( k > 1/r \) (iff \( r > 0 \))

The divergence is due to high momenta and thus its nature is independent of whether the system is finite or infinite
If one introduces an explicit momentum cut-off one has to deal with this integral if \( r > 0 \).

If \( r = 0 \) then the integral is simply:

\[
h(x) = \frac{2}{\pi} \int_{0}^{x} dy \frac{\sin y}{y}
\]

In the final analysis all is an issue of the order of taking various limits: \( r \to 0 \) versus cut-off \( x \to \infty \).
Solution of the problem in the case of the homogeneous matter
(Lee, Huang and Yang and others)

Gap equation

\[ V(\vec{r}_1 - \vec{r}_2) = g \delta(\vec{r}_1 - \vec{r}_2) \]

Lippmann-Schwinger equation
(zero energy collision)

\[ T = V + VGT \]

Now combine the two equations and the divergence is (magically) removed!

\[
\frac{m}{4\pi\hbar^2a} = -\frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \begin{bmatrix}
\frac{1}{\sqrt{(\varepsilon_k - \lambda)^2 + \Delta^2}} - \frac{1}{\varepsilon_k}
\end{bmatrix}
\]

\[
1 = -\frac{g}{2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{(\varepsilon_k - \lambda)^2 + \Delta^2}}
\]

\[
-\frac{mg}{4\pi\hbar^2a} + 1 = -\frac{g}{2} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\varepsilon_k}
\]
How people deal with this problem in finite systems?

- Introduce an explicit energy cut-off, which can vary from 5 MeV to 100 MeV (sometimes significantly higher) from the Fermi energy.
- Use a particle-particle interaction with a finite range, the most popular one being Gogny’s interaction.

Both approaches are in the final analysis equivalent in principle, as a potential with a finite range $r_0$ provides a (smooth) cut-off at an energy $E_c = \frac{\hbar^2}{m r_0^2}$.

- The argument that nuclear forces have a finite range is superfluous, because nuclear pairing is manifest at small energies and distances of the order of the coherence length, which is much smaller than nuclear radii.
- Moreover, LDA works pretty well for the regular mean-field.
- A similar argument fails as well in case of electrons, where the radius of the interaction is infinite and LDA is fine.
How pairing emerges?

Cooper’s argument (1956)

Gap $= 2\Delta$
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)

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

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

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

if \( k r_0 \ll 1 \) then \( V (\vec{r}) \psi (\vec{r}) \Rightarrow g \delta (\vec{r}) \frac{\partial}{\partial r} [r \psi (\vec{r})] \]

Example: \( \psi (\vec{r}) = \frac{A}{r} + B + \ldots \Rightarrow \delta (\vec{r}) \frac{\partial}{\partial r} [r \psi (\vec{r})] = \delta (\vec{r}) B \)
How to deal with an inhomogeneous/finite system?

\[ v_{\text{reg}}(\vec{r}) \stackrel{\text{def}}{=} \sum_i \left[ v_i^*(\vec{r}) u_i(\vec{r}) + \frac{\Delta(\vec{r}) \psi_i^*(\vec{r}) \psi_i(\vec{r})}{2(\lambda - \varepsilon_i)} \right] - \frac{\Delta(\vec{r})}{2} G_{\text{reg}}(\lambda, \vec{r}) \]

\[ G_{\text{reg}}(\lambda, \vec{r}) \stackrel{\text{def}}{=} \lim_{\vec{r}' \to \vec{r}} \left[ G(\vec{r}, \vec{r}', \lambda) + \frac{m}{2\pi \hbar^2 |\vec{r} - \vec{r}'|} \right] \]

\[ [h(\vec{r}) - \varepsilon_i] \psi_i(\vec{r}) = 0 \]

\[ [\lambda - h(\vec{r})] G(\vec{r}, \vec{r}', \lambda) = \delta(\vec{r} - \vec{r}') \]

There is complete freedom in choosing the Hamiltonian \( h \) and we are going to take advantage of this!
We shall use a “Thomas-Fermi” approximation for the propagator $G$.

\[
G(\vec{r}, \vec{r}', \lambda) = -\frac{m \exp(ik_F(\vec{r})|\vec{r} - \vec{r}'|)}{2\pi\hbar^2 |\vec{r} - \vec{r}'|} 
\approx -\frac{m}{2\pi\hbar^2 |\vec{r} - \vec{r}'|} - \frac{ik_F(\vec{r})m}{2\pi\hbar^2} + O(|\vec{r} - \vec{r}'|)
\]

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

\[
\nu_{\text{reg}}(\vec{r}) \overset{\text{def}}{=} \delta_{E_i \leq E_c} \sum_{E_i \leq E_c} v_i^*(\vec{r})u_i(\vec{r}) + \frac{\Delta(\vec{r})}{4\pi^2} \int_0^{k_c(\vec{r})} \frac{k^2 dk}{\lambda - \frac{\hbar^2 k^2}{2m} - U(\vec{r}) + i\gamma} + \frac{i\Delta(\vec{r})k_F(\vec{r})m}{4\pi\hbar^2}
\]

Regularized anomalous density

Regular part of $G$

Vacuum renormalization

FIG. 2. The gap $\Delta$ and the effective coupling constant $g_{\text{eff}}$ as a function of the cut-off energy $E_c$ for three regularization schemes. The full lines correspond to calculations using Eqs. (15–17). Circles correspond to the regularization scheme presented in Ref. [5] (when only terms with $k_c$ are present). The pentagrams correspond to the vacuum regularization scheme [16]. The calculation was performed for homogeneous neutron matter with $\rho = 0.08$ fm$^{-3}$ and $g = -250$ MeV $\cdot$ fm$^3$.


FIG. 1. The neutron pairing field $\Delta(r)$ as a function of the radial coordinate and of the cut-off energy $E_c$. Upward various curves correspond to $E_c = 20, 30, 35, 40, 45$ and $50$ MeV respectively. On the scale of the figure the last two curves are indistinguishable.
The SLDA (renormalized) equations

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

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

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

\[ \left\{ \begin{aligned}
&h(\vec{r}) = -\nabla^2 + \frac{\hbar^2}{2m(\vec{r})} \nabla + U(\vec{r}) \\
&\Delta(\vec{r}) = -g_{\text{eff}} (\vec{r}) \nu_c (\vec{r})
\end{aligned} \]

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

\[ \rho_c (\vec{r}) = 2 \sum_{E_i \geq 0} \left| v_i (\vec{r}) \right|^2, \quad v_c (\vec{r}) = \sum_{E_i \geq 0} v_i^* (\vec{r}) u_i (\vec{r}) \]

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

Position and momentum dependent running coupling constant
Observables are (obviously) independent of cut-off energy (when chosen properly).
A few notes:

- The cut-off energy $E_c$ should be larger than the Fermi energy.
- It is possible to introduce an even faster converging scheme for the pairing field with $E_c$ of a few $\Delta$’s only.
- Even though the pairing field was renormalized, the total energy should be computed with care, as the “pairing” and “kinetic” energies separately diverge.

\[ E_{gs} = \int d^3r [\mathcal{E}_N(r) + \mathcal{E}_S(r)], \]
\[ \mathcal{E}_S(r) := -\Delta(r)\nu_c(r) = g_{eff}(r)|\nu_c(r)|^2 \]

Still diverges!

- One should now introduce the normal and the superfluid contributions to the bare/unrenormalized Energy Density Functional (EDF).

\[
\mathcal{E}_S(r) = g_0(r)|\nu_p(r) + \nu_n(r)|^2 + g_1(r)|\nu_p(r) - \nu_n(r)|^2
\]

"Isospin symmetry"  →  We considered so far only the case $g_0=g_1$. 
The isotope and isotone chains treated by us are indicated with red numbers.
How to describe nuclei?

Fayans parameterization of the infinite matter calculations

This defines the normal part of the EDF.
Pairing correlations show prominently in the staggering of the binding energies. 

*Systems with odd particle number are less bound than systems with even particle number.*
How well does the new approach work?

TABLE I. The rms of $S_{2N}$ and $S_N$ deviations, respectively, from experiment [21] (in MeV's) for several isotope and isotone chains.

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<td>N = 126</td>
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</tbody>
</table>

Ref. 23, S.Q. Zhang et al. nucl-th/0302032. - RMF
One-neutron separation energies

Volume pairing
\[ g(\vec{r}) = g \]

Volume + Surface pairing
\[ g(\vec{r}) = V_0 \left( 1 - \frac{\rho(\vec{r})}{\rho_c} \right) \]

Normal EDF:

- **SLy4** - Chabanat et al.

- **FaNDF0** – Fayans
Two-neutron separation energies

- **Sn**: 
  - SLy4
  - FaNDF
- **Pb**: 
  - SLy4
  - FaNDF

Two-neutron separation energies are shown for Sn and Pb isotopes. The plots compare experimental (Exp.) data with calculated values using the SLy4 and FaNDF nuclear force models. The graphs demonstrate the agreement between experimental and calculated values, with additional data points highlighting the volume and surface contributions.
One-nucleon separation energies

\( S_{p} \) [MeV]

- \( N = 50 \)
- \( N = 82 \)
- \( N = 126 \)
- \( Ca \)

Exp. Volume

FaNDF\(^0\)
• We use the same normal EDF as Fayans et al.
  volume pairing only with one universal constant
  5 parameters for pairing (density dependence with
  gradient terms (neutrons only).
  volume pairing, 5 parameters for pairing,
  isospin symmetry broken
Spatial profiles of the pairing field for tin isotopes and two different (normal) energy density functionals

\[ \Delta(r) \ [\text{MeV}] \]

\[ r \ [\text{fm}] \]

\[ A \]

Sn
SLy4

Sn
FaNDF\(^0\)
Charge radii

Exp. - Nadjakov et al. At. Data and Nucl. Data Tables, **56**, 133 (1994)
Let me backtrack a bit and summarize some of the ingredients of the LDA to superfluid nuclear correlations.

Energy Density (ED) describing the normal system

\[
E_{gs} = \int d^3 r \left\{ \mathcal{E}_N[\rho_n(\vec{r}), \rho_p(\vec{r})] + \mathcal{E}_S[\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] \right\}
\]

ED contribution due to superfluid correlations

\[
\mathcal{E}_N[\rho_n(\vec{r}), \rho_p(\vec{r})] = \mathcal{E}_N[\rho_p(\vec{r}), \rho_n(\vec{r})]
\]

\[
\mathcal{E}_S[\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] = \mathcal{E}_S[\rho_p(\vec{r}), \rho_n(\vec{r}), \nu_p(\vec{r}), \nu_n(\vec{r})]
\]

Isospin symmetry
(Coulomb energy and other relatively small terms not shown here.)

Let us consider the simplest possible ED compatible with nuclear symmetries and with the fact that nuclear pairing correlations are relatively weak.

\[
\mathcal{E}_S[\rho_p, \rho_n, \nu_p, \nu_n] = g_0 \left| \nu_p + \nu_n \right|^2 + g_1 \left| \nu_p - \nu_n \right|^2
\]

\(g_0\) and \(g_1\) could depend as well on \(\rho_p\) and \(\rho_n\).
Let us stare at this part of the ED for a moment, ... or two.

SU(2) invariant

\[ \varepsilon_S[V_p, V_n] = g_0 |V_p + V_n|^2 + g_1 |V_p - V_n|^2 \]

\[ = g \left( |V_p|^2 + |V_n|^2 \right) + g' \left[V_p^* V_n + V_n^* V_p \right] \]

\[ g = g_0 + g_1 \quad g' = g_0 - g_1 \]

NB I am dealing here with s-wave pairing only (S=0 and T=1)!

The last term could not arise from a two-body bare interaction.
considered various mechanisms to couple the proton and neutron superfluids in nuclei, in particular a zero range four-body interaction which could lead to terms like

\[
\alpha |\nu_n|^2 |\nu_p|^2
\]

• Buckley, Metlitski and Zhitnitsky, astro-ph/0308148 considered an SU(2) – invariant Landau-Ginsburg description of neutron stars in order to settle the question of whether neutrons and protons superfluids form a type I or type II superconductor. However, I have doubts about the physical correctness of the approach.
In the end one finds that a suitable superfluid nuclear EDF has the following structure:

Isospin symmetric

\[ \varepsilon_S[\nu_p, \nu_n] = g(\rho_p, \rho_n)[|\nu_p|^2 + |\nu_n|^2] + f(\rho_p, \rho_n)[|\nu_p|^2 - |\nu_n|^2] \]

where \( g(\rho_p, \rho_n) = g(\rho_n, \rho_p) \)

and \( f(\rho_p, \rho_n) = f(\rho_n, \rho_p) \)

Charge symmetric
How can one determine the density dependence of the coupling constant \( g \)? I know two methods.

- In homogeneous low density matter one can compute the pairing gap as a function of the density. **NB this is not a BCS or HFB result!**

\[
\Delta = \left( \frac{2}{e} \right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp \left( \frac{\pi}{2k_F a} \right)
\]

- One can also compute the energy of the normal and superfluid phases as a function of density, as was recently done by Carlson et al, Phys. Rev. Lett. 91, 050401 (2003) for a Fermi system interacting with an infinite scattering length (Bertsch’s MBX 1999 challenge)

In both cases one can extract from these results the superfluid contribution to the LDA energy density functional in a straight forward manner.
Anderson and Itoh, Nature, 1975
“Pulsar glitches and restlessness as a hard superfluidity phenomenon”

The crust of neutron stars is the only other place in the entire Universe where one can find solid matter, except planets.

- A neutron star will cover the map at the bottom
- The mass is about 1.5 solar masses
- Density $10^{14}$ g/cm³
“Screening effects” are significant!

s-wave pairing gap in infinite neutron matter with realistic NN-interactions from Lombardo and Schulze astro-ph/0012209

These are major effects beyond the naïve HFB when it comes to describing pairing correlations.
\[ \Delta = \left( \frac{2}{e} \right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp \left[ -\frac{\pi}{2 \tan \delta(k_F)} \right] \]

**NB! Extremely high relative \( T_c \)**

Corrected Emery formula (1960)

NN-phase shift

**RG- renormalization group calculation**

Vortex in neutron matter

\[
\begin{pmatrix}
    u_{\alpha kn}(\vec{r}) \\
    v_{\alpha kn}(\vec{r})
\end{pmatrix} = \begin{pmatrix}
    u_{\alpha}(r) \exp[i(n + 1/2)\phi - ikz] \\
    v_{\alpha}(r) \exp[i(n - 1/2)\phi - ikz]
\end{pmatrix}, \quad n \text{ - half - integer}
\]

\[\Delta(\vec{r}) = \Delta(r) \exp(i\phi), \quad \vec{r} = (r, \phi, z) \text{ [cylindrical coordinates]}\]

Oz - vortex symmetry axis

Ideal vortex, Onsager's quantization (one $\hbar$ per Cooper pair)

\[
\vec{V}_{v}(\vec{r}) = \frac{\hbar}{2mr^2} (y, -x, 0) \quad \Leftrightarrow \quad \frac{1}{2\pi} \oint_{C} \vec{V}_{v}(\vec{r}) \cdot d\vec{r} = \frac{\hbar}{2m}
\]
Distances scale with $\lambda_F$ and $\xi_F$.
Dramatic structural changes of the vortex state naturally lead to significant changes in the energy balance of a neutron star.

- \( \frac{v_S}{v_F} \leq \frac{\Delta}{2\varepsilon_F} \approx 0.12 \), extremely fast vortical motion,
- \( \frac{\lambda_F}{\xi} \propto \frac{\Delta}{\varepsilon_F} \)

In low density region \( \varepsilon(\rho_{\text{out}})\rho_{\text{out}} > \varepsilon(\rho_{\text{in}})\rho_{\text{in}} \)
which thus leads to a large anti-pinning energy \( E_{\text{pin}}^V > 0 \):

\[
E_{\text{pin}}^V = [\varepsilon(\rho_{\text{out}})\rho_{\text{out}} - \varepsilon(\rho_{\text{in}})\rho_{\text{in}}]V
\]

- The energy per unit length is going to be changed dramatically when compared to previous estimates, by

\[
\frac{\Delta E_{\text{vortex}}}{L} \approx [\varepsilon(\rho_{\text{out}})\rho_{\text{out}} - \varepsilon(\rho_{\text{in}})\rho_{\text{in}}]\pi R^2
\]

- Specific heat, transport properties are expected to significantly affected as well.

Some similar conclusions have been reached recently also by Donati and Pizzochero, Phys. Rev. Lett. 90, 211101 (2003).
What are the ground state properties of the many-body system composed of spin ½ 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)

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

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

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

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
\[ \Delta(2n + 1) = E(2n + 1) - \frac{1}{2}(E(2n) + E(2n + 2)) \]

Pairing gap ($\Delta$) = 0.9 $E_{\text{FG}}$

\[ E = 0.44 N E_{\text{FG}} \]

Result for $\alpha k_F = -\infty$

\[ E_{\text{FG}} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} \]
\[ \Delta_{Gorkov} = \left( \frac{2}{e} \right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp \left( \frac{\pi}{2k_F a} \right) \]

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

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)

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

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

\[
\varepsilon_2 = -\frac{\hbar^2}{ma^2} \quad \text{and} \quad n_b a^3 \ll 1, \quad \text{where} \quad n_b = \frac{n_f}{2} \quad \text{and} \quad a_{bb} = 0.6a > 0
\]
SLDA for dilute atomic Fermi gases

Parameters determined from GFMC results of Chang, Carlson, Pandharipande and Schmidt, physics/0404115

\[ r_0 \ll \frac{1}{n^{1/3}} \ll |a| \]

\[ \frac{E}{N}_{GFMC} = \varepsilon[n] \approx \frac{3}{5} \varepsilon_F \left[ \xi - \frac{\zeta}{k_F a} - \frac{5i}{3(k_F a)^2} \right] \]

\[ \Delta_{GFMC} \approx \varepsilon_F \left( \frac{2}{e} \right)^{7/3} \exp \left( \frac{\pi}{2k_F a} \right) \]

\[ \varepsilon_{SLDA}[n] n = \varepsilon_{kin} + \frac{\hbar^2}{m} \beta[x] n^{5/3} + \frac{\hbar^2}{m} \gamma[x] \frac{|\nu|^2}{n^{1/3}} \]

\[ \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}, \quad n = \frac{k_F^3}{3\pi^2}, \quad x = \frac{1}{k_F a} \]

Dimensionless coupling constants
Now we are going to look at vortices in dilute atomic gases in the vicinity of the Feshbach resonance.

Why would one study vortices in neutral Fermi superfluids?

They are perhaps just about the only phenomenon in which one can have a true stable superflow!
How can one put in evidence a vortex in a Fermi superfluid?

Hard to see, since density changes are not expected, unlike the case of a Bose superfluid.

However, if the gap is not small one can expect a noticeable density depletion along the vortex core, and the bigger the gap the bigger the depletion!

One can change the magnitude of the gap by altering the scattering length between two atoms with magnetic fields by means of a Feshbach resonance.
The depletion along the vortex core is reminiscent of the corresponding density depletion in the case of a vortex in a Bose superfluid, when the density vanishes exactly along the axis for 100% BEC.

Fermions with $1/k_F a = 0.3, 0.1, 0, -0.1, -0.5$

Bosons with $n a^3 = 10^{-3}$ and $10^{-5}$

Extremely fast quantum vortical motion!

Local vortical speed as fraction of Fermi speed
Conclusions:

- An LDA-DFT formalism for describing pairing correlations in Fermi systems has been developed. This represents the first genuinely local extension of the Kohn-Sham LDA from normal to superfluid systems - SLDA.
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✓ An LDA-DFT formalism for describing pairing correlations in Fermi systems has been developed. This represents the first genuinely local extension of the Kohn-Sham LDA from normal to superfluid systems - SLDA