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 dilute atomic Fermi gases (vortices)
- ✓ Conclusions

Superconductivity and superfluidity in Fermi systems

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

units (1 eV $\approx 10^4$ K)

Density Functional Theory (DFT)
Hohenberg and Kohn, 1964

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

particle density only!

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

Local Density Approximation (LDA)
(LDA) Kohn and Sham, 1965

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

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

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

Kohn-Sham equations

Extended Kohn-Sham equations

Position dependent mass

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

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

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

Phenomenological nuclear Skyrme EDF

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

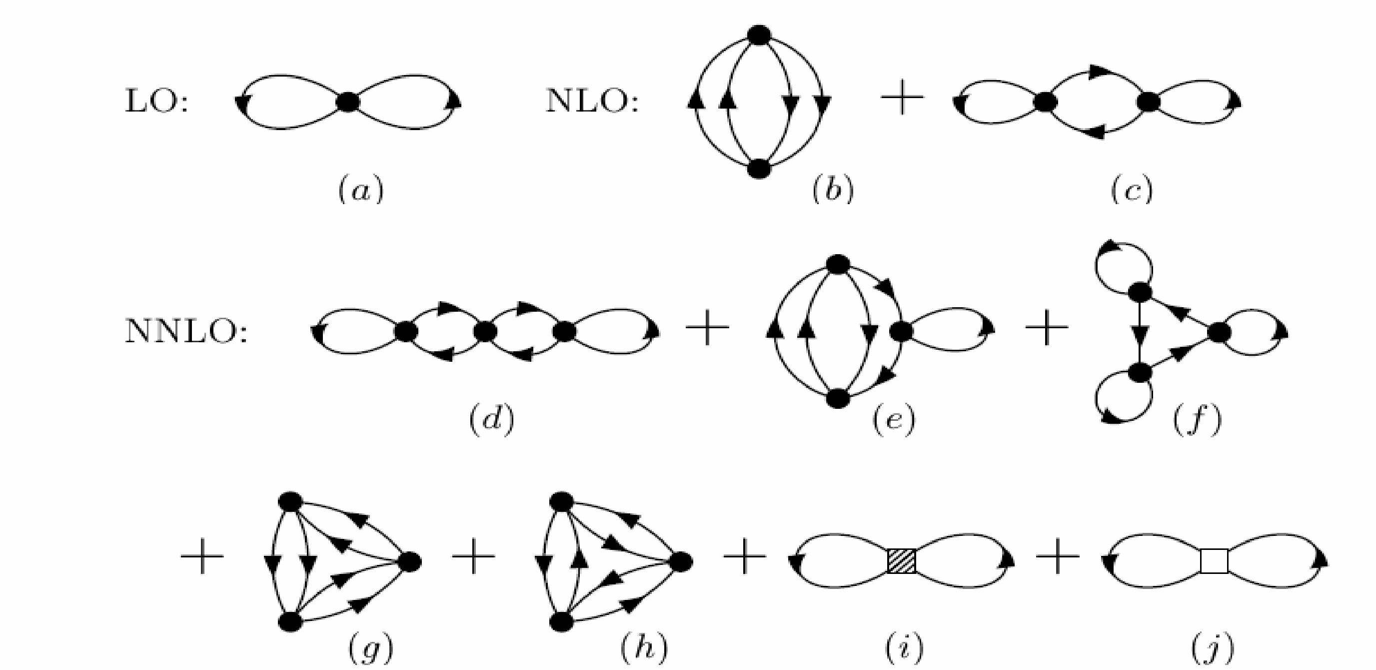
One can try to derive it, however, from an *ab initio (?)* lagrangian

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

$$C_0 = \frac{4\pi a_s}{M}, \qquad C_2 = C_0\frac{a_s r_s}{2}, \qquad \text{and} \qquad C_2' = \frac{4\pi a_p^3}{M}$$

Bhattacharyya and Furnstahl, nucl-phys/0408014

$$
\begin{aligned}
\frac{E}{N} = \frac{k_{\mathrm{F}}^2}{2M}\Big[\frac{3}{5} &+ (g-1)\Big\{\frac{2}{3\pi}(k_{\mathrm{F}}a_s) + \frac{4}{35\pi^2}(11-2\ln 2)(k_{\mathrm{F}}a_s)^2 + \frac{1}{10\pi}(k_{\mathrm{F}}r_s)(k_{\mathrm{F}}a_s)^2 \\
&+ (0.076+0.057(g-3))(k_{\mathrm{F}}a_s)^3\Big\} + (g+1)\frac{1}{5\pi}(k_{\mathrm{F}}a_p)^3 \\
&+ (g-1)(g-2)\frac{16}{27\pi^3}(4\pi-3\sqrt{3})(k_{\mathrm{F}}a_s)^4\ln(k_{\mathrm{F}}a_s) + \cdots\Big] .
\end{aligned}
$$

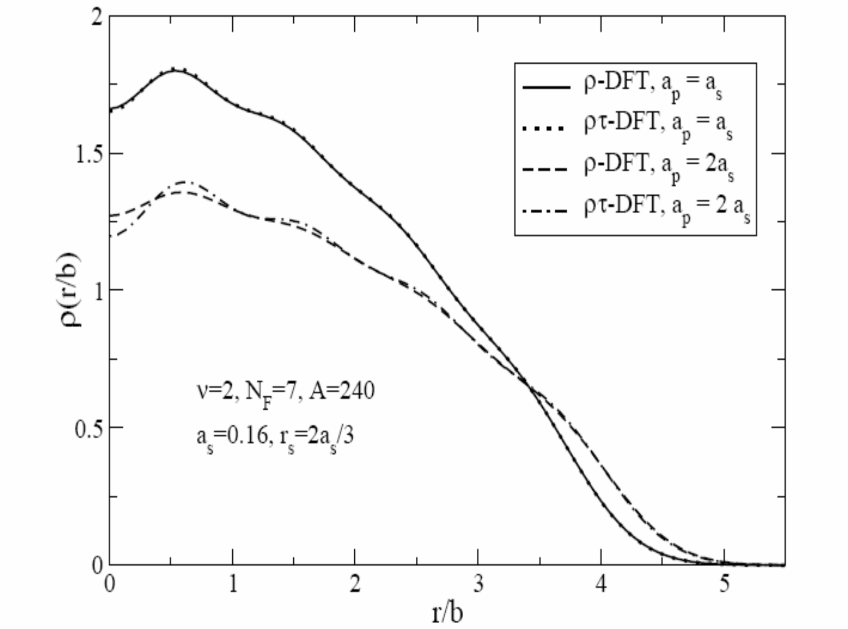


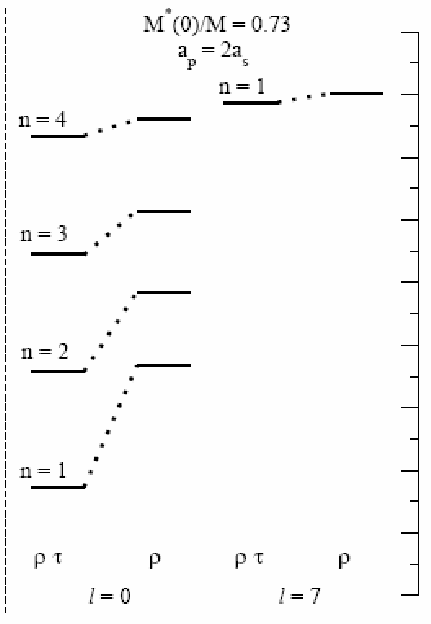
One can construct however an EDF which depends both on particle density and kinetic energy density and use it in a extended Kohn-Sham approach

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

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!

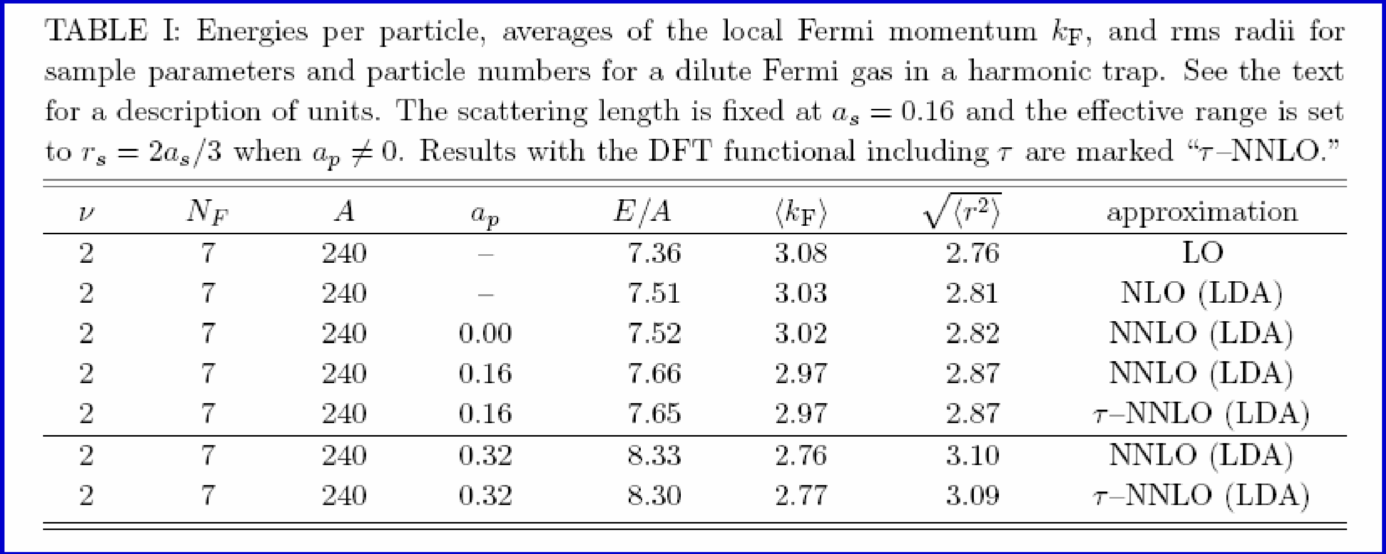


TABLE I: Energies per particle, averages of the local Fermi momentum k_{F}, and rms radii for sample parameters and particle numbers for a dilute Fermi gas in a harmonic trap. See the text for a description of units. The scattering length is fixed at $a_s = 0.16$ and the effective range is set to $r_s = 2a_s/3$ when $a_p \neq 0$. Results with the DFT functional including τ are marked "τ–NNLO."

ν	N_F	A	a_p	E/A	$\langle k_{\mathrm{F}} \rangle$	$\sqrt{\langle r^2 \rangle}$	approximation
2	7	240	–	7.36	3.08	2.76	LO
2	7	240	–	7.51	3.03	2.81	NLO (LDA)
2	7	240	0.00	7.52	3.02	2.82	NNLO (LDA)
2	7	240	0.16	7.66	2.97	2.87	NNLO (LDA)
2	7	240	0.16	7.65	2.97	2.87	τ–NNLO (LDA)
2	7	240	0.32	8.33	2.76	3.10	NNLO (LDA)
2	7	240	0.32	8.30	2.77	3.09	τ–NNLO (LDA)

Local Density Approximation (LDA)

Kohn and Sham, 1965

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

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

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

Normal Fermi systems only!

However, not everyone is normal!

SLDA - Extension of Kohn-Sham approach to superfluid Fermi systems

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

$$\rho(\vec{r}) = 2\sum_k |\mathrm{v}_k(\vec{r})|^2, \quad \tau(\vec{r}) = 2\sum_k |\vec{\nabla}\mathrm{v}_k(\vec{r})|^2$$

$$\nu(\vec{r}) = \sum_k \mathrm{u}_k(\vec{r})\mathrm{v}_k^*(\vec{r})$$

$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix}$$

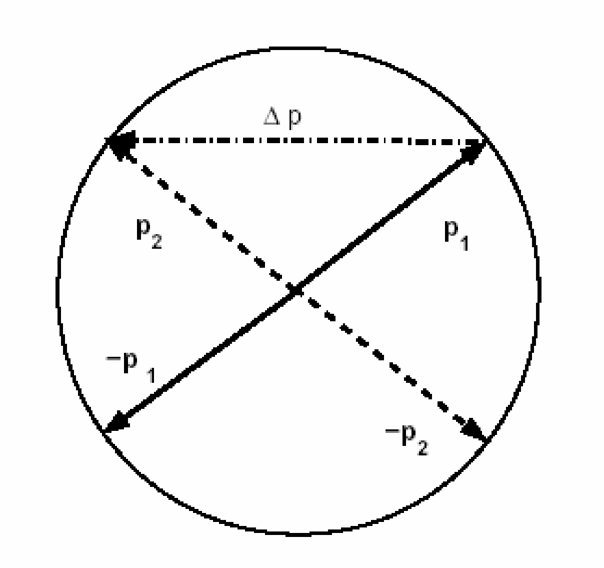
Mean-field and pairing field are both local fields!

(for sake of simplicity spin degrees of freedom are not shown)

There is a little problem! The pairing field Δ 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.



$$r_0 \cong \frac{\hbar}{p_F} = k_F^{-1}$$

radius of interaction inter-particle separation

$$\Delta = \omega_D Exp\left(-\frac{1}{|V|N}\right) << \varepsilon_F$$

$$\xi \approx \frac{1}{k_F}\frac{\varepsilon_F}{\Delta} >> r_0$$

coherence length
size of the Cooper pair

Nature of the problem

$$\nu(\vec{r}_1,\vec{r}_2)=\sum_{E_k>0}\mathrm{v}_{\mathrm{k}}^{*}(\vec{r}_1)\mathrm{u}_{\mathrm{k}}(\vec{r}_2)\propto\frac{1}{|\vec{r}_1-\vec{r}_2|}$$

at small separations

$$\Delta(\vec{r}_1,\vec{r}_2)=\frac{1}{2}V(\vec{r}_1,\vec{r}_2)\nu(\vec{r}_1,\vec{r}_2)$$

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

$$\mathrm{v}_{\mathrm{k}}(\vec{r}_1)=\mathrm{v}_{\mathrm{k}}\exp(i\vec{k}\cdot\vec{r}_1),\qquad \mathrm{u}_{\mathrm{k}}(\vec{r}_2)=\mathrm{u}_{\mathrm{k}}\exp(i\vec{k}\cdot\vec{r}_2)$$

$$\mathrm{v}_{\mathrm{k}}^2=\frac{1}{2}\left(1-\frac{\varepsilon_{\mathrm{k}}-\mu}{\sqrt{(\varepsilon_{\mathrm{k}}-\mu)^2+\Delta^2}}\right),\quad \mathrm{u}_{\mathrm{k}}^2+\mathrm{v}_{\mathrm{k}}^2=1,\quad \varepsilon_{\mathrm{k}}=\frac{\hbar^2\vec{k}^2}{2m}+U,\quad \Delta=\frac{\hbar^2\delta}{2m}$$

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

A (too) simple case

$$k_F \to 0, \delta \to 0$$

$$v(|\vec{r}_1 - \vec{r}_2|) \to \frac{\Delta m}{2\pi^2\hbar^2}\int_0^\infty dk\,\frac{\sin kr}{kr} = \frac{\Delta m}{2\pi^2\hbar^2}\,\frac{\pi}{2|\vec{r}_1 - \vec{r}_2|}$$

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

Solution of the problem in the case of the homogeneous matter
(Lee, Huang and Yang and others)

Gap equation

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

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

Lippmann-Schwinger equation
(zero energy collision)
T = V + VGT →

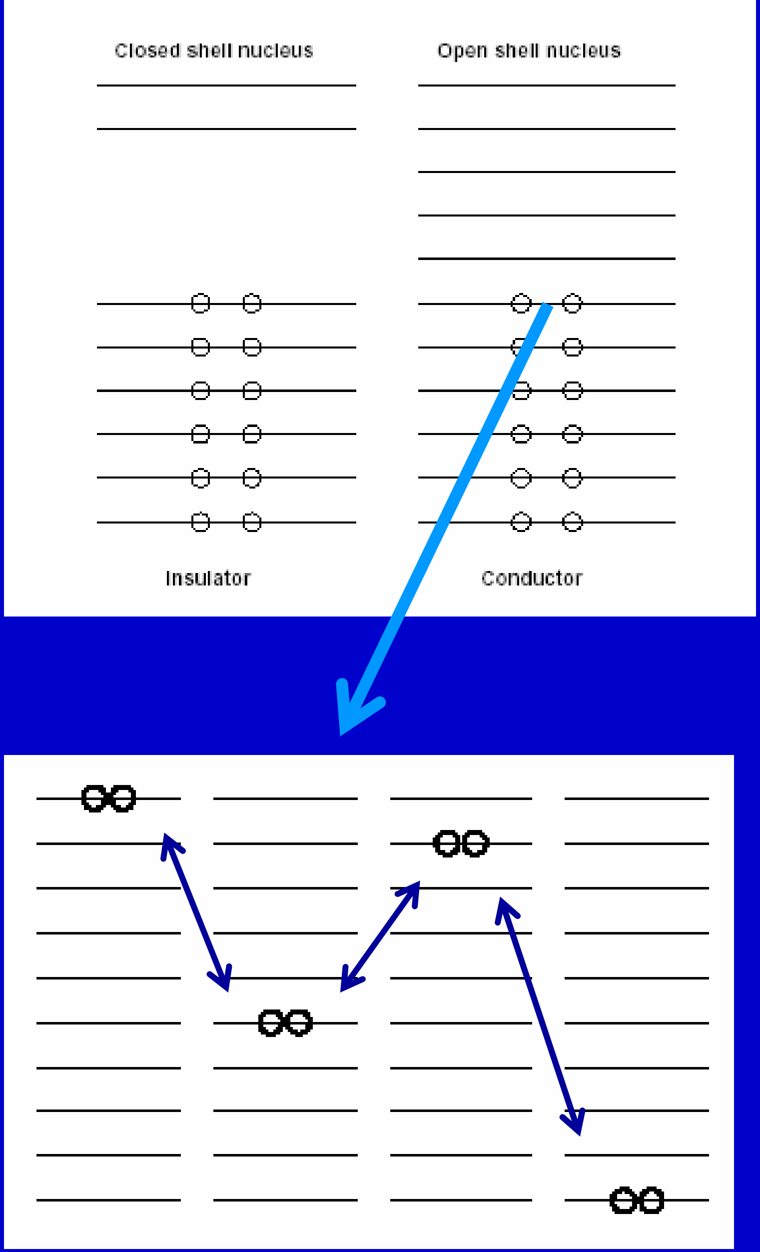
$$-\frac{mg}{4\pi\hbar^2a}+1=-\frac{g}{2}\int\frac{d^3k}{(2\pi)^3}\frac{1}{\varepsilon_k}$$

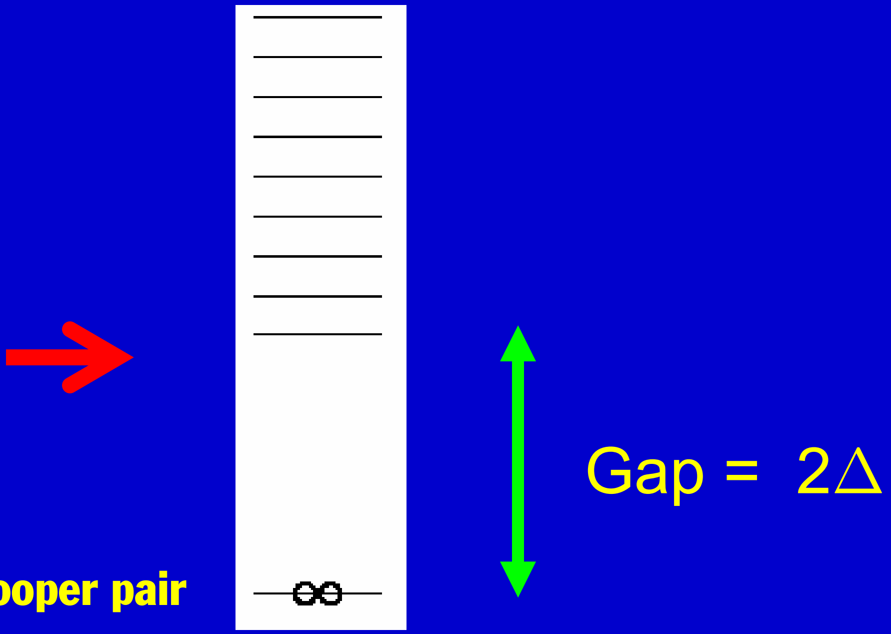
Now combine the two equations and
the divergence is (magically) removed!

$$\frac{m}{4\pi\hbar^2a}=-\frac{1}{2}\int\frac{d^3k}{(2\pi)^3}\left\{\frac{1}{\sqrt{(\varepsilon_k-\lambda)^2+\Delta^2}}-\frac{1}{\varepsilon_k}\right\}$$

How pairing emerges?

Cooper's argument (1956)





Cooper pair

Gap = 2Δ

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)

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

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

$$f^{-1}=-\frac{1}{a}+\frac{1}{2}r_0k^2-ik,\qquad g=\frac{4\pi\hbar^2 a}{m(1+ika)}+\ldots$$

$$\text{if } kr_0<<1 \quad \text{then} \quad V(\vec{r})\psi(\vec{r})\Rightarrow g\delta(\vec{r})\frac{\partial}{\partial r}\left[r\psi(\vec{r})\right]$$

$$\text{Example}:\ \psi(\vec{r})=\frac{A}{r}+B+\ldots\Rightarrow\delta(\vec{r})\frac{\partial}{\partial r}\left[r\psi(\vec{r})\right]=\delta(\vec{r})B$$

How to deal with an inhomogeneous/finite system?

$$v_{reg}(\vec{r}) \overset{def}{=} \sum_i \left[\mathrm{v}_i^*(\vec{r})\mathrm{u}_i(\vec{r}) + \frac{\Delta(\vec{r})\psi_i^*(\vec{r})\psi_i(\vec{r})}{2(\lambda-\varepsilon_i)} \right] - \frac{\Delta(\vec{r})}{2} G_{reg}(\lambda,\vec{r})$$

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

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

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

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.

$$G(\vec r,\vec r\,',\lambda) = -\frac{m\exp(ik_F(\vec r)|\vec r-\vec r\,'|)}{2\pi\hbar^2|\vec r-\vec r\,'|}$$

$$\approx -\frac{m}{2\pi\hbar^2|\vec r-\vec r\,'|} - \frac{ik_F(\vec r)m}{2\pi\hbar^2} + \mathrm{O}(|\vec r-\vec r\,'|)$$

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

$$\nu_{\mathrm{reg}}(\vec r) \overset{def}{=} \left\{ \sum_{E_i\le E_c} \mathrm{v}_i^*(\vec r)\mathrm{u}_i(\vec r) + \frac{\Delta(\vec r)}{4\pi^2}\int_0^{k_c(\vec r)} \frac{1}{\lambda - \frac{\hbar^2k^2}{2m} - U(\vec r) + i\gamma}k^2dk \right\} + \frac{i\Delta(\vec r)k_F(\vec r)m}{4\pi\hbar^2}$$

Regularized anomalous density

Regular part of G

New renormalization scheme

Vacuum renormalization

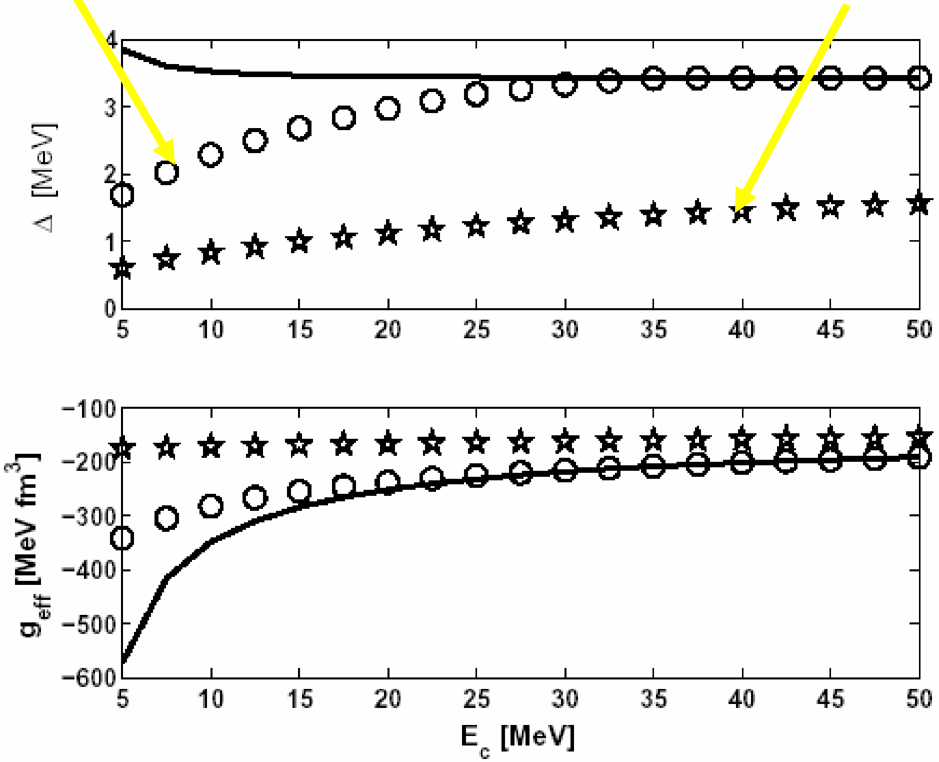


FIG. 2. The gap Δ and the effective coupling constant g_{eff} as a function of the cut-off energy E_c for three regularization schemes. The full lines correspond to calculations using Eqs. (15 – 17). Circles correspond to the regularization scheme presented in Ref. [5] (when only terms with k_c are present).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

A. Bulgac, Phys. Rev. C **65**, 051305 (2002)

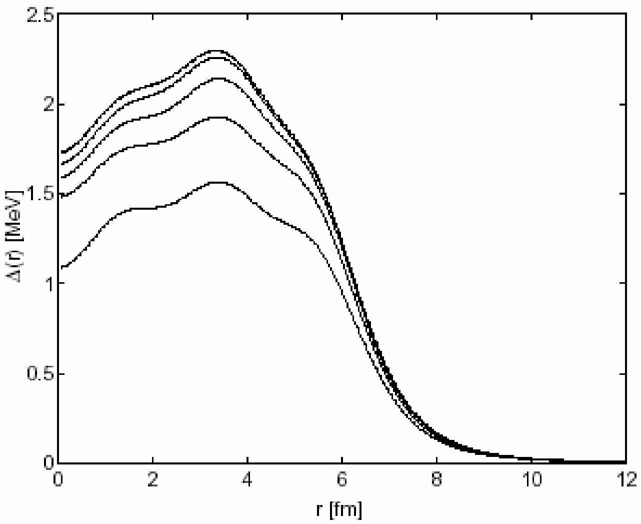


FIG. 1. The neutron pairing field (17) as a function of the radial coordinate and of the cut–off energy E_c. Upward various curves correspond to E_c = 20, 30, 35, 40, 45 and 50 MeV respectively. On the scale of the figure the last two curves are indistinguishable.

A. Bulgac and Y. Yu,
Phys. Rev. Lett. **88**, 042504 (2002)

The SLDA (renormalized) equations

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

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

$$\begin{cases}[h(\vec r)-\mu]\mathrm{u}_i(\vec r)+\Delta(\vec r)\mathrm{v}_i(\vec r)=E_i\mathrm{u}_i(\vec r)\\ \Delta^*(\vec r)\mathrm{u}_i(\vec r)-[h(\vec r)-\mu]\mathrm{v}_i(\vec r)=E_i\mathrm{v}_i(\vec r)\end{cases}\qquad \begin{cases}h(\vec r)=-\vec\nabla\dfrac{\hbar^2}{2m(\vec r)}\vec\nabla+U(\vec r)\\ \Delta(\vec r)=-g_{\text{eff}}(\vec r)\nu_c(\vec r)\end{cases}$$

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

$$\rho_c(\vec r)=2\sum_{E_i\ge 0}^{E_c}\left|\mathrm{v}_i(\vec r)\right|^2,\qquad \nu_c(\vec r)=\sum_{E_i\ge 0}^{E_c}\mathrm{v}_i^*(\vec r)\mathrm{u}_i(\vec r)$$

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

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 Δ'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.

$$E_{gs} = \int d^3r[\mathcal{E}_N(\boldsymbol{r}) + \mathcal{E}_S(\boldsymbol{r})],$$

$$\mathcal{E}_S(\boldsymbol{r}) := -\Delta(\boldsymbol{r})\nu_c(\boldsymbol{r}) = g_{\mathrm{eff}}(\boldsymbol{r})|\nu_c(\boldsymbol{r})|^2$$

Still diverges!
However, the gs energy is well defined!

Bertsch Many-Body X challenge, Seattle, 1999

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."

$$r_0 \to 0 \quad << \quad \lambda_F \quad << \quad |a| \to \infty$$

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

$$\frac{E_N}{N} = \alpha_N \frac{3}{5} \varepsilon_F, \qquad \alpha_N = 0.54$$

normal state

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

$$\frac{E_S}{N} = \alpha_S \frac{3}{5} \varepsilon_F, \qquad \alpha_S = 0.44$$

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.

BCS →BEC crossover

Eagles (196?), Leggett (1980), Nozieres and Schmitt-Rink (1985), Randeria *et al.* (1993),…

If $a<0$ at $T=0$ a Fermi system is a BCS superfluid

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

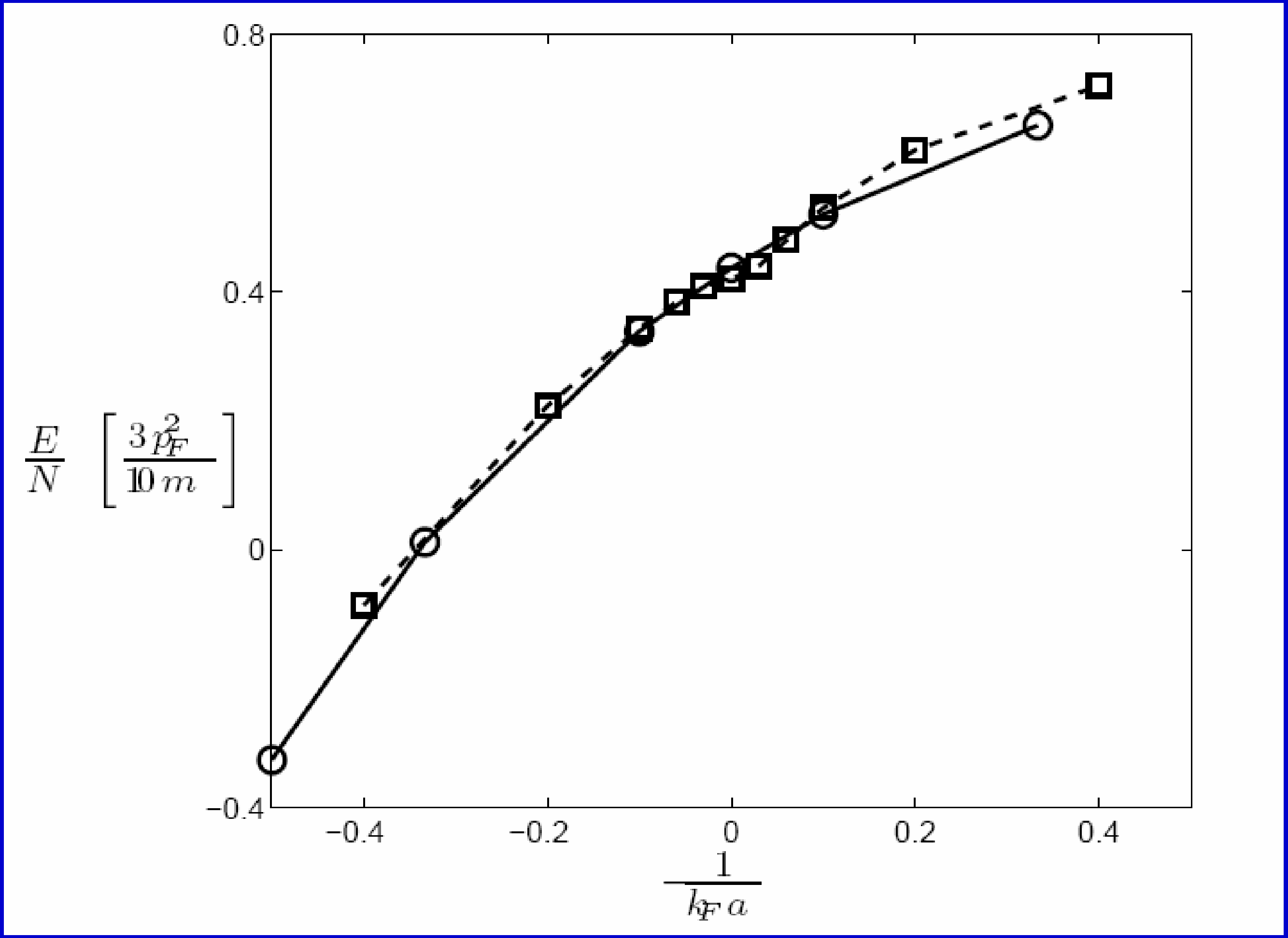
If $|a|=\infty$ and $nr_0^3 \ll 1$ a Fermi system is strongly coupled and its properties are universal. Carlson *et al*. PRL 91, 050401 (2003)

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

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

$$\varepsilon_2 = -\frac{\hbar^2}{ma^2} \quad \text{and} \quad n_b a^3 << 1, \quad \text{where} \quad n_b = \frac{n_f}{2} \ \text{and} \ a_{bb} = 0.6a > 0$$

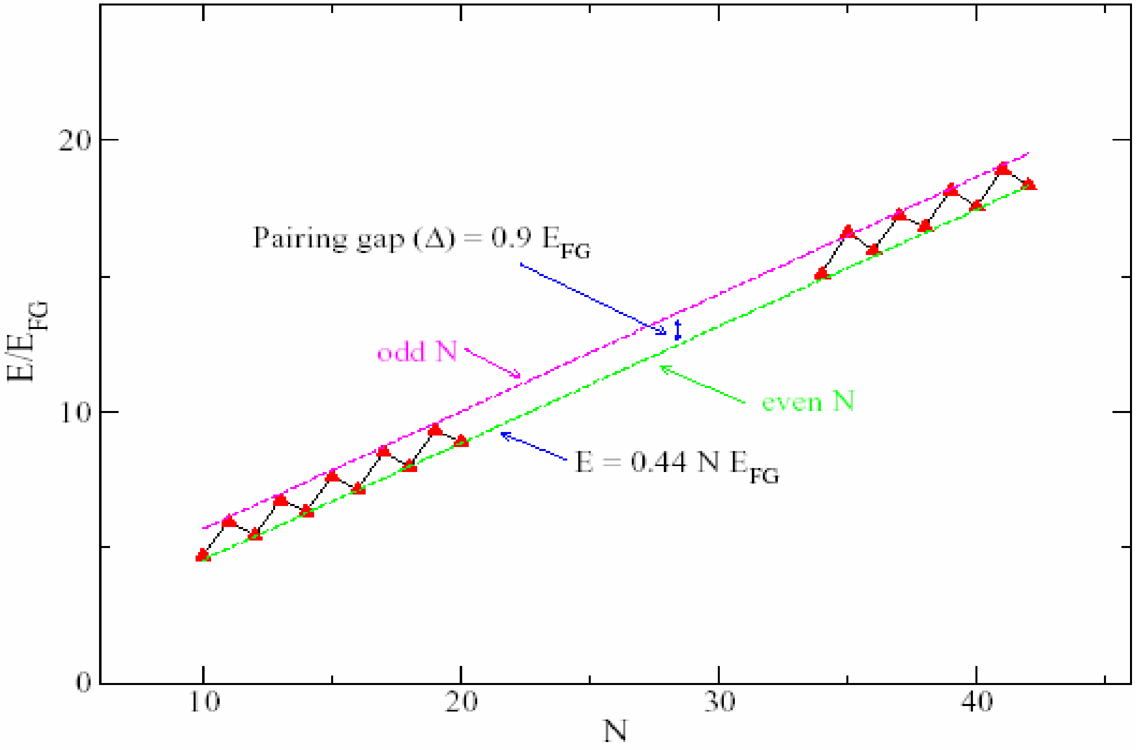
BEC side **BCS side**



Solid line with open circles – Chang *et al.* physics/0404115

Dashed line with squares - Astrakharchik *et al.* cond-mat/0406113

$$\Delta(2n+1) = E(2n+1) - \frac{1}{2}\left(E(2n) + E(2n+2)\right)$$



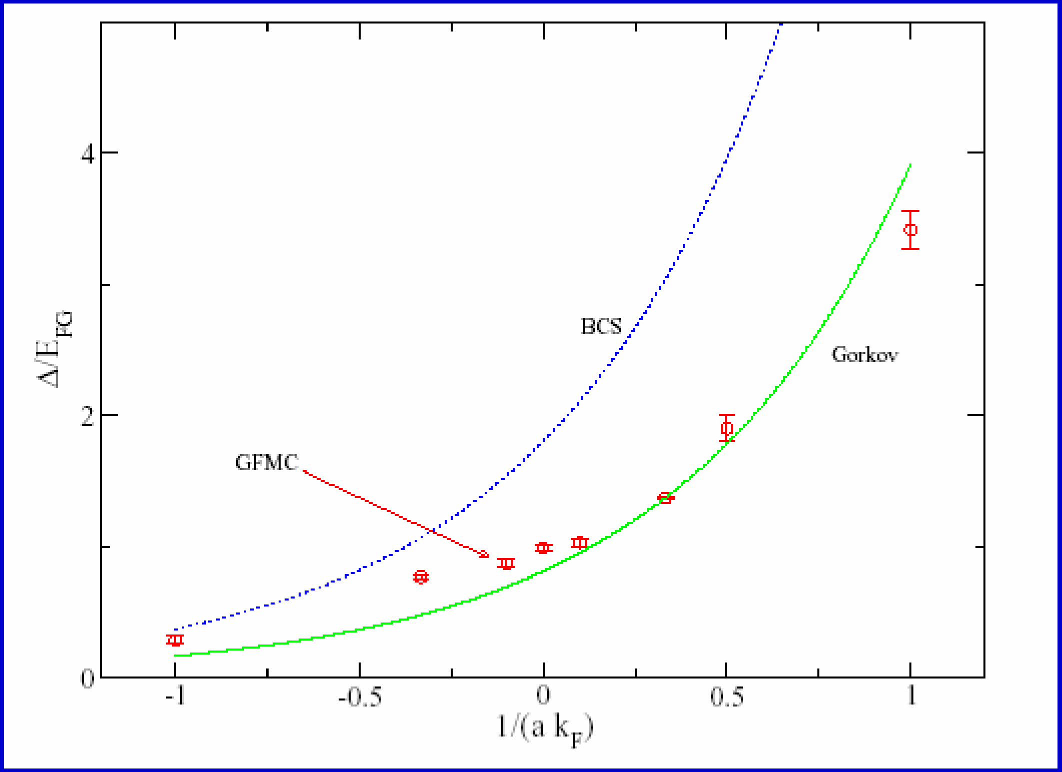
Result for $ak_F = -\infty$

$$E_{FG} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}$$

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)

SLDA for dilute atomic Fermi gases

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

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

$$\left.\frac{E}{N}\right|_{GFMC} = \varepsilon[n] \approx \frac{3}{5}\varepsilon_F\left[\xi - \frac{\varsigma}{k_F a} - \frac{5\iota}{3\left(k_F a\right)^2}\right], \qquad \xi \approx 0.44, \qquad \varsigma \approx 1, \qquad \iota \approx 1$$

$$\Delta_{GFMC} \approx \varepsilon_F \left(\frac{2}{e}\right)^{7/3} \exp\left(\frac{\pi}{2k_F a}\right), \qquad n = \frac{k_F^3}{3\pi^2}, \quad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}, \quad x = \frac{1}{k_F a}$$

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

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!

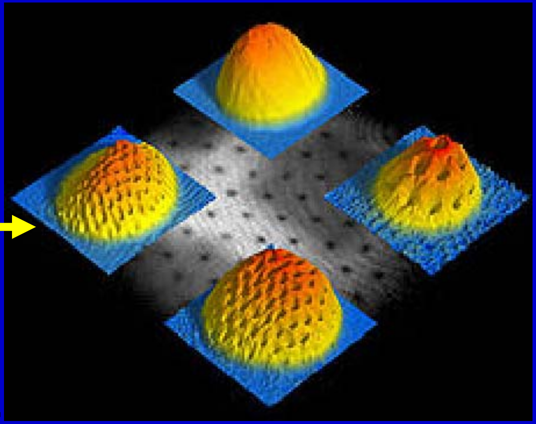
How can one put in evidence a vortex in a Fermi superfluid?

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!

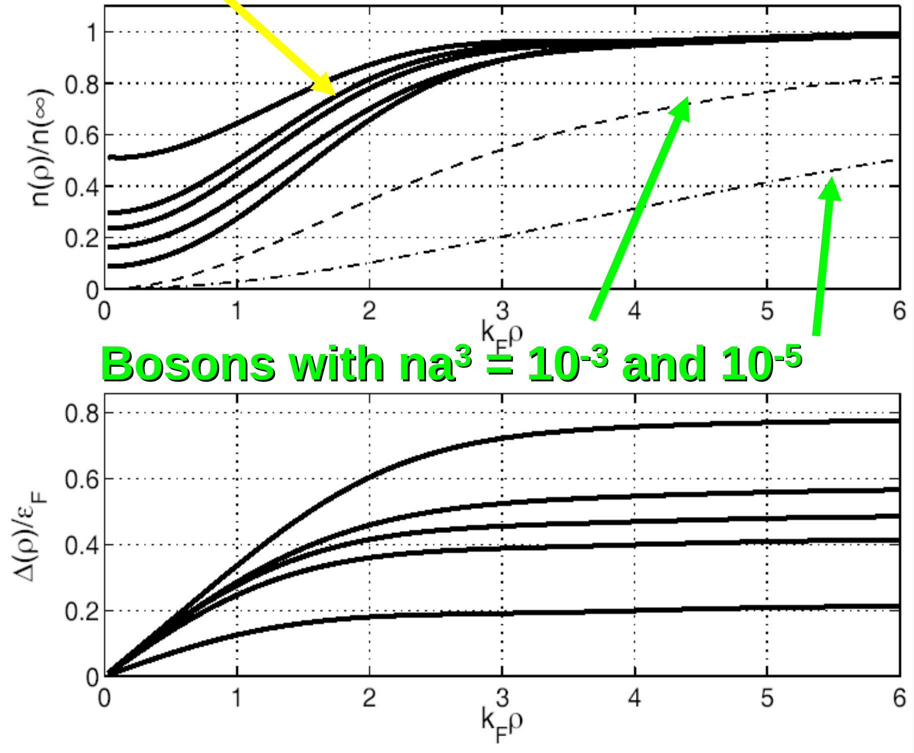
One can change the magnitude of the gap by altering the scattering length between two atoms with magnetic fields by means of a Feshbach resonance.

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.

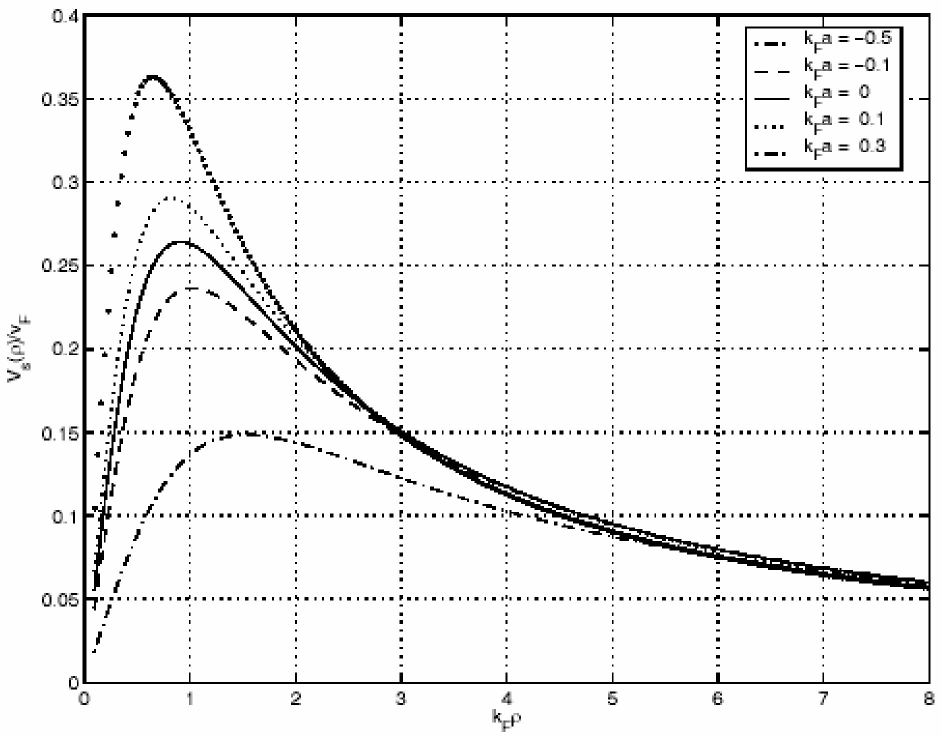


From Ketterle's group

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



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



Extremely fast quantum vortical motion!

Number density and pairing field profiles

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 extention of the Kohn-Sham LDA from normal to superfluid systems - **SLDA**

✓ SLDA has been successfully applied to nuclei

✓ “ has used in order to describe the vortex structure in neutron stars

✓ “ has been used to describe pairing properties of dilute atomic Fermi gases

✓ Stay tuned!