

***Superfluid LDA (SLDA)***  
**Local Density Approximation for  
Systems with Superfluid Correlations**

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Transparencies will be available shortly at  
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# Contents

- Rather lengthy introduction, motivating the LDA approach
- Description of the LDA for systems with pairing correlations.
- Results of application of this new LDA approach to a rather large number of spherical nuclei in a fully self-consistent approach with continuum correctly accounted for.
- Description of the new features of the vortex state in low density neutron matter (neutron stars)
- Application of this new LDA approach in the limit of strong coupling, (when the pairing gap is of the order of the Fermi energy) and the description of the vortex state in a dilute atomic Fermi gas
- The role of pairing correlations on the particle number density profiles in cases when pairing correlations are in the weak and in the strong coupling limits respectively
- Summary

# References

- A. Bulgac and Y. Yu, Phys.Rev.Lett. **88**, 042504 (2002)  
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A. Bulgac and Y. Yu, Phys.Rev.Lett. **91**, 190404 (2003)
- Y. Yu, PhD thesis (2003), almost done
- A. Bulgac, Phys.Rev. C **65**, 051305(R) (2002)  
A. Bulgac and Y. Yu, nucl-th/0109083 (Lectures)  
Y. Yu and A. Bulgac, nucl-th/0302007 (Appendix to PRL)  
A. Bulgac and Y. Yu, nucl-th/0310066  
A. Bulgac and Y. Yu in preparation

# Superconductivity and superfluidity in Fermi systems

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

*units (1 eV > 10<sup>4</sup> K)*

## A rather incomplete list of major questions still left unanswered in nuclear physics concerning pairing correlations:

- ✓ **Do nuclear pairing correlations have a volume or/and surface character?**  
Phenomenological approaches give no clear answer as anything fits equally well.
- **The density dependence of the pairing gap (partially related to the previous topic), the role of higher partial waves (p-wave etc.) especially in neutron matter.**
- ✓ **The role of the isospin symmetry in nuclear pairing.**  
Routinely the isospin symmetry is broken in phenomenological approaches with really very lame excuses.
- **Role of collective modes, especially surface modes in finite nuclei, role of “screening effects.”**
- ✓ **Is pairing interaction momentum or/and energy dependent at any noticeable level?**
- **Pairing in  $T = 0$  channel?**
- ✓ **Does the presence or absence of neutron superfluidity have any influence on the presence and/or character of proton superfluidity and *vice versa*.**  
New question raised recently: are neutron stars type I or II superconductors?
- **We should try to get away from the heavily phenomenological approach which dominated nuclear pairing studies most of last 40 years and put more effort in an *ab initio* and many-body theory of pairing and be able to make reliable predictions, especially for neutron stars. The studies of dilute atomic gases with tunable interactions could serve as an extraordinary testing ground of theories.**



To tell me how to describe pairing correlations in nuclei and nuclear/neutron matter?

Most likely you will come up with one of the standard doctrines, namely:

- BCS within a limited single-particle energy shell (the size of which is chosen essentially arbitrarily) and with a coupling strength chosen to fit some data. Theoretically it makes no sense to limit pairing correlations to a single shell only. This is a pragmatic limitation.
- HFB theory with some kind of “effective” interaction, e.g. Gogny interaction.

Many would (or used to) argue that the Gogny interaction in particular is realistic, as, in particular, its matrix elements are essentially identical to those of the Bonn potential or some Other realistic bare NN-interaction

- In neutron stars often the Landau-Ginzburg theory was used (for the lack of a more practical theory mostly).

**How does one decide if one or another theoretical approach is meaningful?**

**Really, this is a very simple question. One has to check a few things.**

**☹ Is the theoretical approach based on a sound approximation scheme?**

**Well,..., maybe!**

**☺ Does the particular approach chosen describe known key experimental results, and moreover, does this approach predict new qualitative features, which are later on confirmed experimentally?**

**☹ Are the theoretical corrections to the leading order result under control, understood and hopefully not too big?**

Let us check a simple example, homogeneous dilute Fermi gas with a weak attractive interaction, when pairing correlations occur in the ground state.

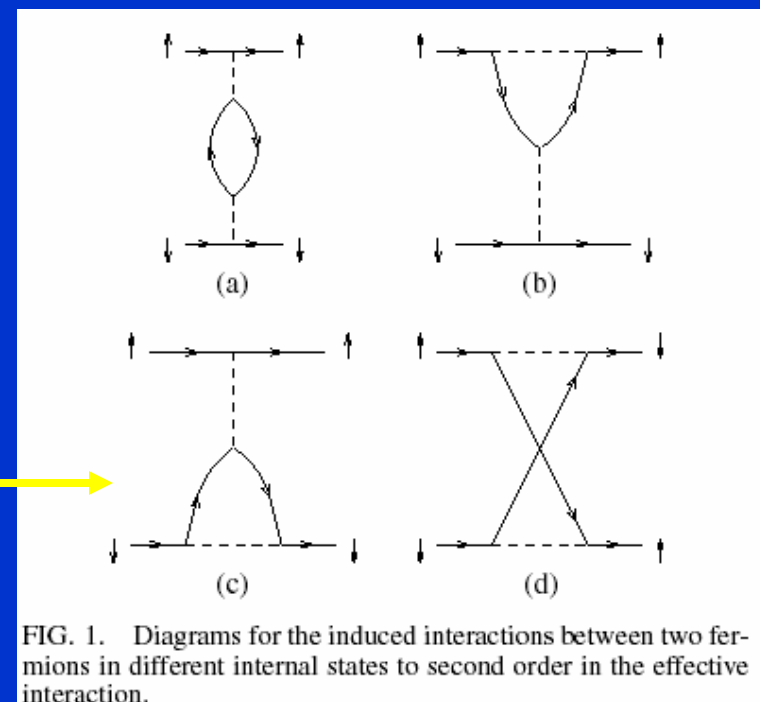
$$\Delta = \frac{8}{e^2} \frac{\hbar^2 k_F^2}{2m} \exp\left(\frac{\pi}{2k_F a}\right)$$

↑  
BCS result

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

An additional factor of  $1/(4e)^{1/3} \approx 0.45$  is due to induced interactions  
Gorkov and Melik-Barkhudarov in 1961.

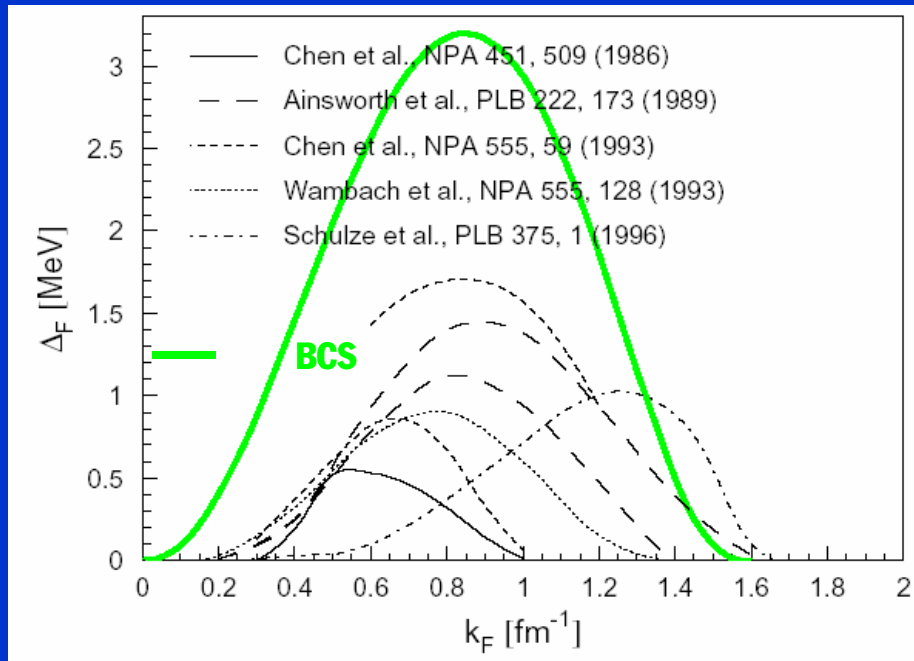
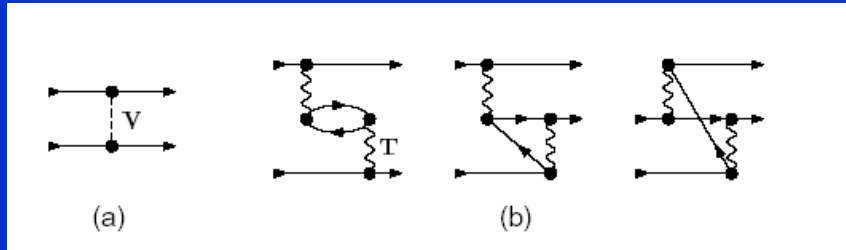
BCS/HFB in error even when the interaction is very weak, unlike HF!



from Heiselberg et al  
Phys. Rev. Lett. 85, 2418, (2000)



# “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.

# Density Functional Theory (DFT)

Hohenberg and Kohn, 1964

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

**particle density**



# Local Density Approximation (LDA)

Kohn and Sham, 1965

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

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

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

**Normal Fermi systems only!**

$$\Psi_A(\vec{r}_1, \dots, \vec{r}_N) \Rightarrow \rho(\vec{r})$$

$$\Psi_B(\vec{r}_1, \dots, \vec{r}_N) \Rightarrow \rho(\vec{r})$$

$$\Psi_A(\vec{r}_1, \dots, \vec{r}_N) \neq \Psi_B(\vec{r}_1, \dots, \vec{r}_N)$$

$$H = \sum_i T_i + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$

$$E_A = \left\langle \Psi_A \left| H + \sum_i V_i \right| \Psi_A \right\rangle = \langle \Psi_A | H | \Psi_A \rangle + \text{Tr}(V\rho)$$

$$E_B = \left\langle \Psi_B \left| H + \sum_i U_i \right| \Psi_B \right\rangle = \langle \Psi_B | H | \Psi_B \rangle + \text{Tr}(U\rho)$$

$$E_A < \langle \Psi_B | H | \Psi_B \rangle + \text{Tr}(V\rho)$$

$$E_B < \langle \Psi_A | H | \Psi_A \rangle + \text{Tr}(U\rho)$$

$$E_A + E_B < E_A + E_B$$

Assume that there are two different many-body wave functions, corresponding to the same number particle density!

**Nonsense!**

# LDA (Kohn-Sham) for superfluid fermi systems (Bogoliubov-de Gennes equations)

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

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

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

$$\begin{pmatrix} T + U(\vec{r}) - \lambda & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \lambda) \end{pmatrix} \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix}$$

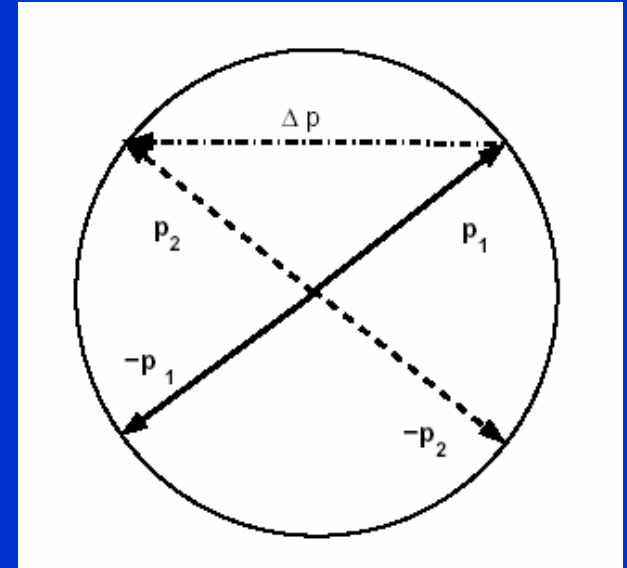
**Mean-field and pairing field are both local fields!**

(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.



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

radius of interaction      inter-particle separation

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

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

coherence length  
size of the Cooper pair

## Nature of the problem

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

← at small separations

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

It is easier to show how this singularity appears in infinite homogeneous matter (BCS model)

$$v_k(\vec{r}) = v_k \exp(i\vec{k} \cdot \vec{r}), \quad u_k(\vec{r}) = u_k \exp(i\vec{k} \cdot \vec{r})$$

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

$$v(r) = \frac{\Delta m}{2\pi^2 \hbar^2} \int_0^\infty dk \frac{\sin(kr)}{kr} \frac{k^2}{\sqrt{(k^2 - k_F^2)^2 + \delta^2}}$$

## A (too) simple case

$$k_F \rightarrow 0, \delta \rightarrow 0$$

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

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

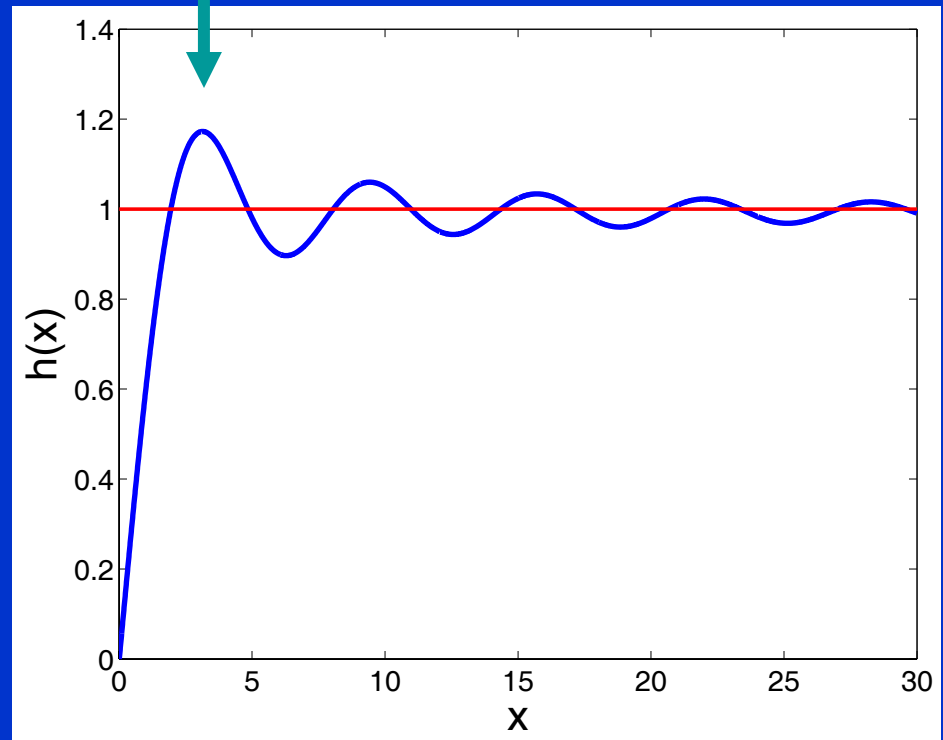
The divergence is due to high momenta and thus its nature is independent of whether the system is finite or infinite

If one introduces an explicit momentum cut-off one has deal with this integral **iff**  $r > 0$ .

$$h(x) = \frac{2}{\pi} \int_0^x dy \frac{\sin y}{y}$$

If  $r=0$  then the integral is simply:

$$h(x) = \frac{2}{\pi} \int_0^x dy = \frac{2x}{\pi}$$



In the final analysis all is an issue of the order of taking various limits:  
 $r \rightarrow 0$  versus cut-off  $x \rightarrow \infty$



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

Gap equation

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

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

Lippmann-Schwinger equation  
(zero energy collision)

$$T = V + VGT$$



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

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

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

# How 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  $E_c = \hbar^2/mr_0^2$

- 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.

## 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)

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

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

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

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

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

How to deal with an inhomogeneous/finite system?

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

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

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

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

**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  $G$ .

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

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

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

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

↑  
Regularized anomalous density

↑  
Regular part of  $G$

New renormalization scheme

Vacuum renormalization

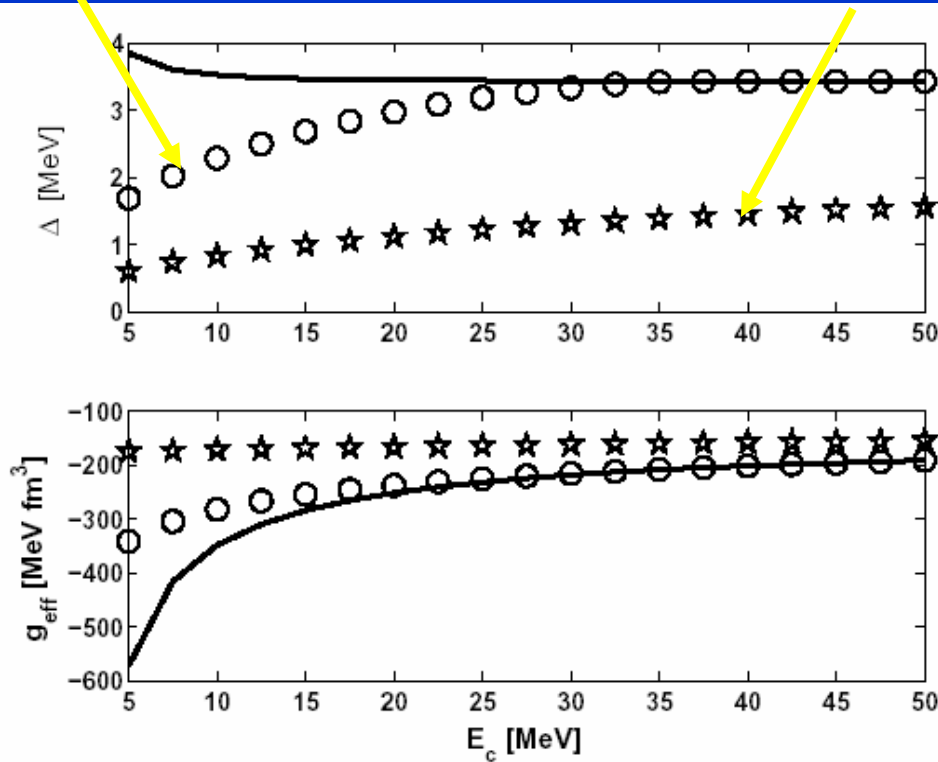


FIG. 2. The gap  $\Delta$  and the effective coupling constant  $g_{\text{eff}}$  as a function of the cut-off energy  $E_c$  for three regularization schemes. The full lines correspond to calculations using Eqs. (15) – (17). Circles correspond to the regularization scheme presented in Ref. [5] (when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

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

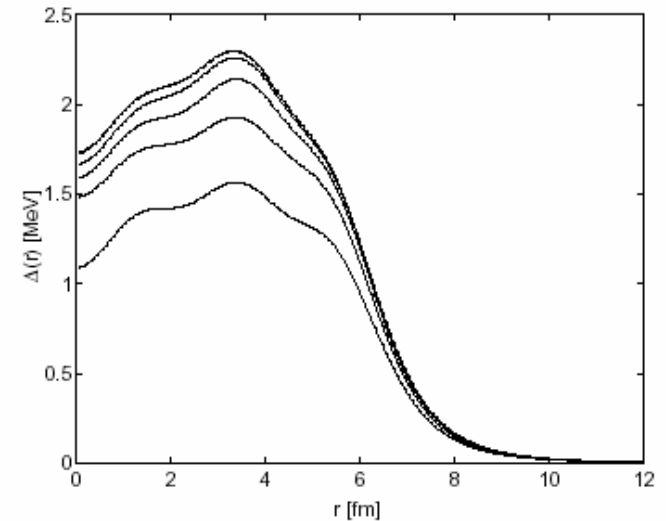


FIG. 1. The neutron pairing field (17) as a function of the radial coordinate and of the cut-off energy  $E_c$ . Upward various curves correspond to  $E_c = 20, 30, 35, 40, 45$  and  $50$  MeV respectively. On the scale of the figure the last two curves are indistinguishable.

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

## The renormalized equations:

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

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

$$\begin{cases} [h(\mathbf{r}) - \mu]u_i(\mathbf{r}) + \Delta(\mathbf{r})v_i(\mathbf{r}) = E_i u_i(\mathbf{r}), \\ \Delta^*(\mathbf{r})u_i(\mathbf{r}) - [h(\mathbf{r}) - \mu]v_i(\mathbf{r}) = E_i v_i(\mathbf{r}), \end{cases}$$

$$h(\mathbf{r}) = -\nabla \frac{\hbar^2}{2m(\mathbf{r})} \nabla + U(\mathbf{r}), \quad \Delta(\mathbf{r}) := -g_{eff}(\mathbf{r})\nu_c(\mathbf{r}),$$

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

$$\rho_c(\mathbf{r}) = \sum_{E_i \geq 0}^{E_c} 2|v_i(\mathbf{r})|^2, \quad \nu_c(\mathbf{r}) = \sum_{E_i \geq 0}^{E_c} v_i^*(\mathbf{r})u_i(\mathbf{r}),$$

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

Typo: replace m by m(r)

## 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 D'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.

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

Still diverges!

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

Isospin symmetry  $\longrightarrow$

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

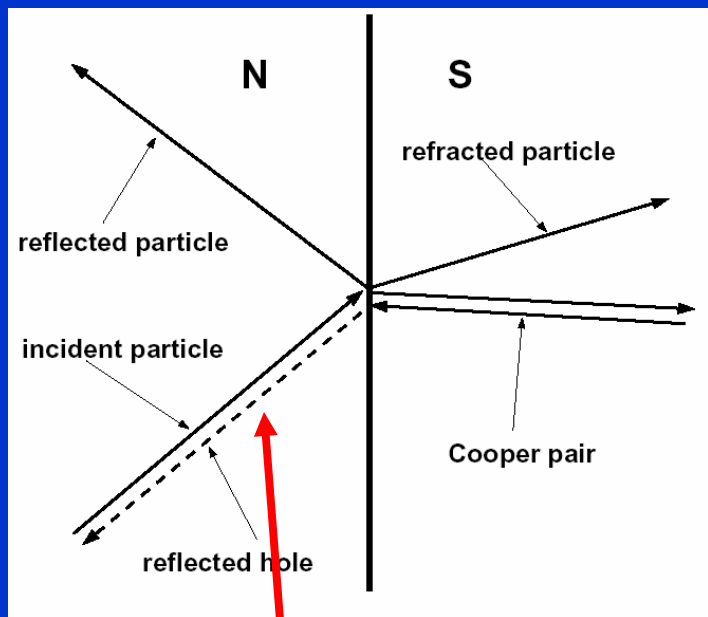
We considered so far only the case  $g_0=g_1$ .



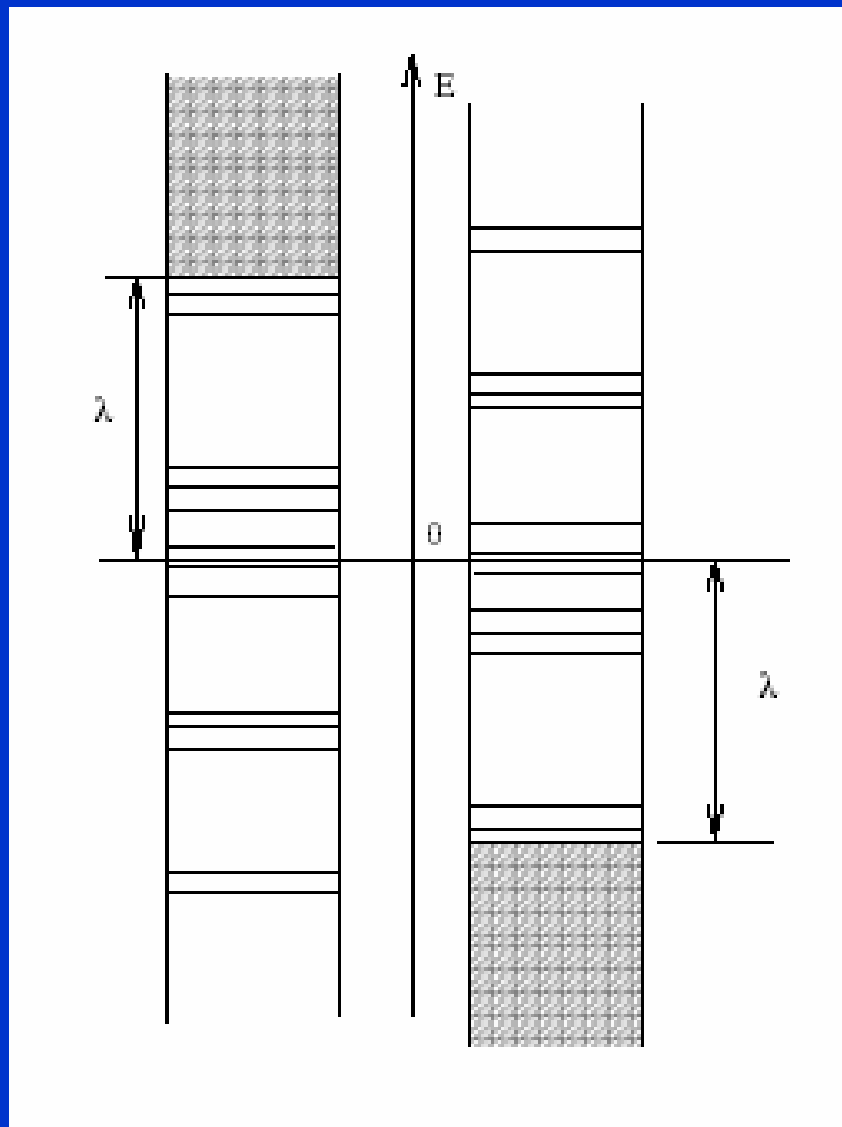
# Peculiarity of the finite systems: deep hole states are continuum states.

$$\begin{pmatrix} \hbar - \lambda & \Delta \\ \Delta^+ & -(\hbar^* - \lambda) \end{pmatrix} \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix} = E_k \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix}$$

outside      inside

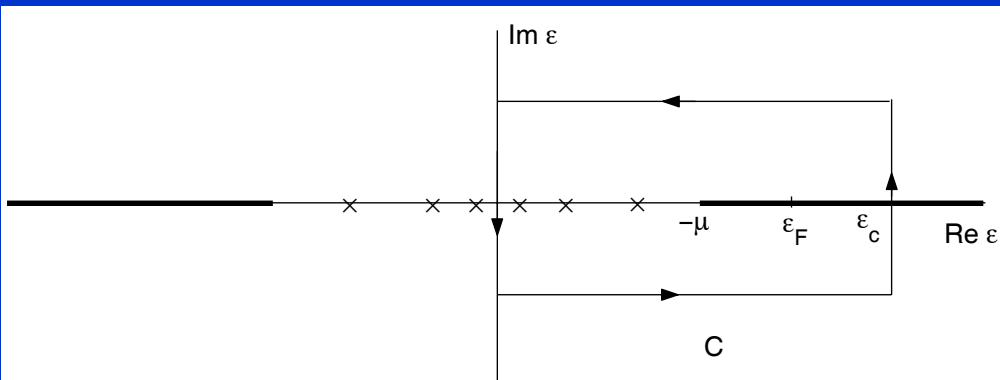


Andreev reflection

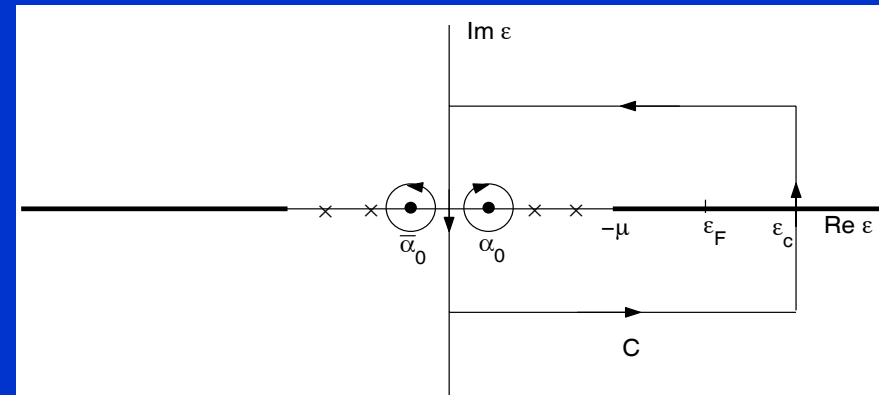


Integration contours used to construct the normal and anomalous densities from the Gorkov Green functions  
 Belyaev *et al*, Sov. J. Nucl. Phys. 45, 783 (1987).

$$\begin{pmatrix} E - (h - \lambda) & -\Delta \\ -\Delta^* & E + (h^* - \lambda) \end{pmatrix} \begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

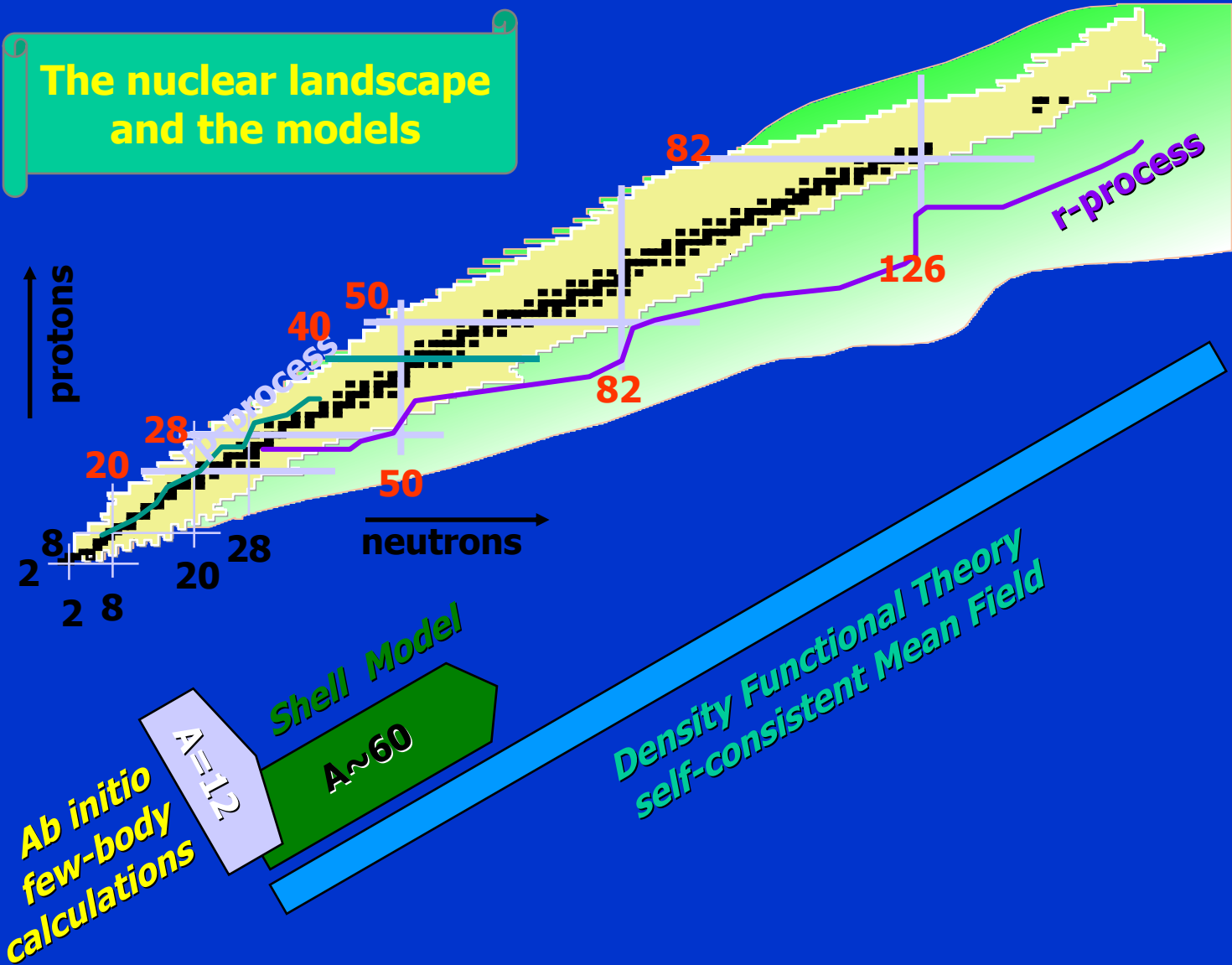


Even systems



Odd systems

# The nuclear landscape and the models



Courtesy of Mario Stoitsov

The isotope and isotone chains treated by us are indicated with red numbers.

# 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.

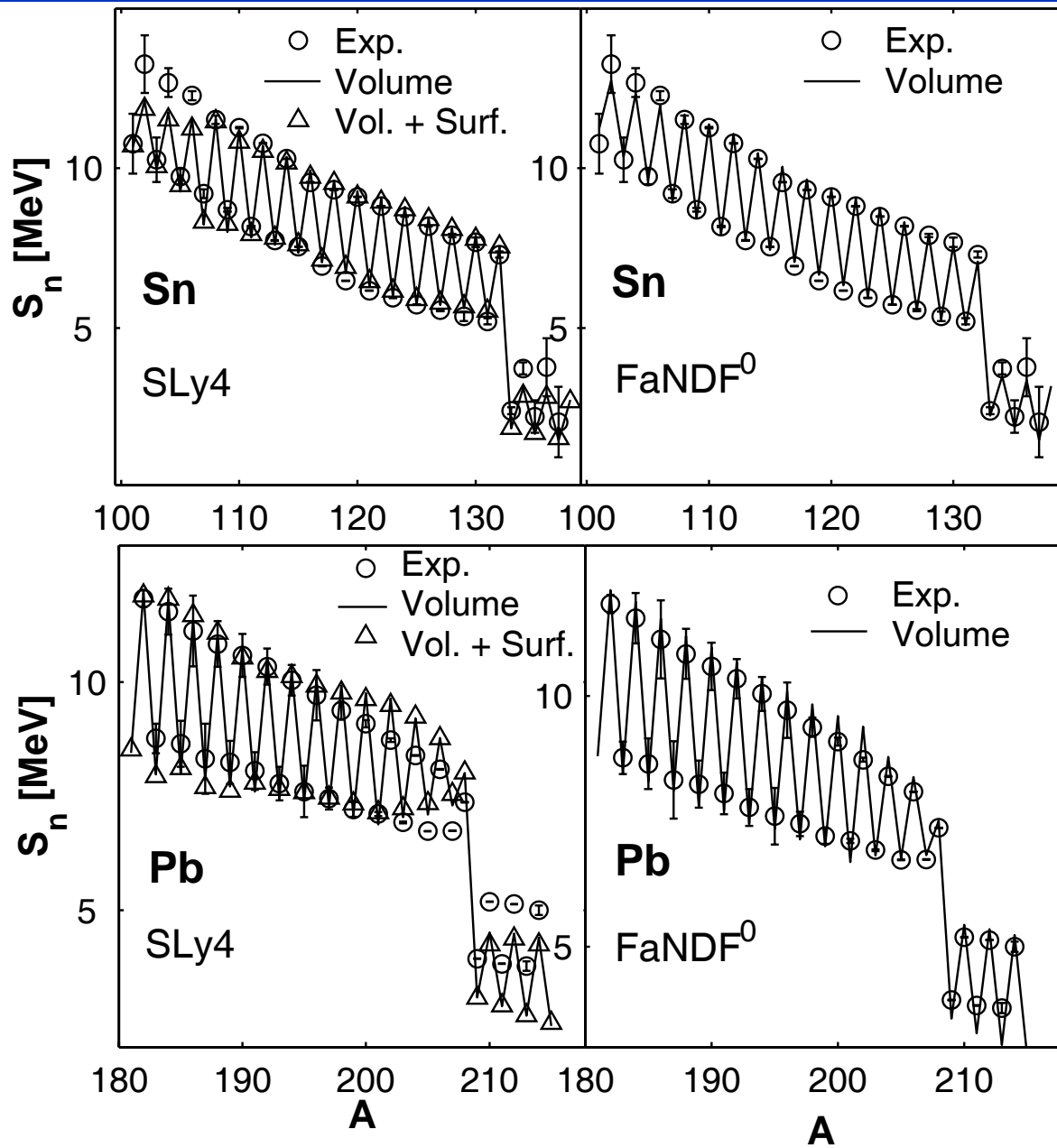
$Z$ or $N$ chain	$S_{2N}/S_N$ present	$S_{2N}/S_N$ Ref. [11]	$S_{2N}$ Ref. [23]
$Z = 20$	0.82/0.76	1.02/0.92	0.96
$Z = 28$	0.67/0.50	0.66/0.55	1.30
$Z = 40$	0.93/0.63	0.66/0.63	2.21
$Z = 50$	0.29/0.21	0.43/0.35	0.95
$Z = 82$	0.23/0.37	0.58/0.53	0.74
$N = 50$	0.37/0.26	0.41/0.23	NA
$N = 82$	0.43/0.31	0.50/0.56	NA
$N = 126$	0.42/0.23	0.88/0.52	NA

Ref. 21, Audi and Wapstra, Nucl. Phys. **A595**, 409 (1995).

Ref. 11, S. Goriely *et al.* Phys. Rev. C **66**, 024326 (2002) - HFB

Ref. 23, S.Q. Zhang *et al.* nucl-th/0302032. - RMF

# One-neutron separation energies



Volume pairing

$$g(\vec{r}) = g$$

Volume + Surface pairing

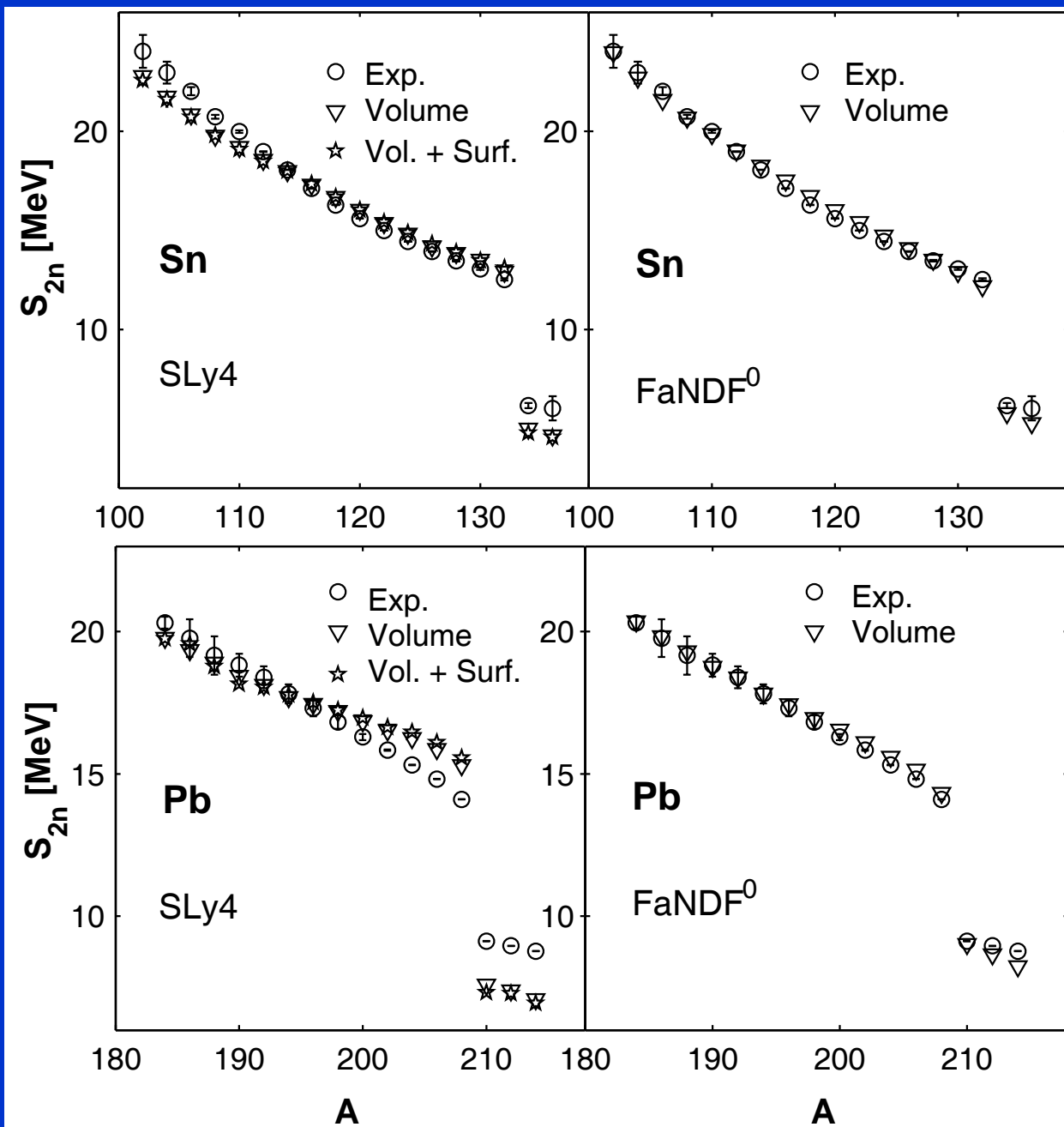
$$g(\vec{r}) = V_0 \left( 1 - \frac{\rho(\vec{r})}{\rho_c} \right)$$

Normal EDF:

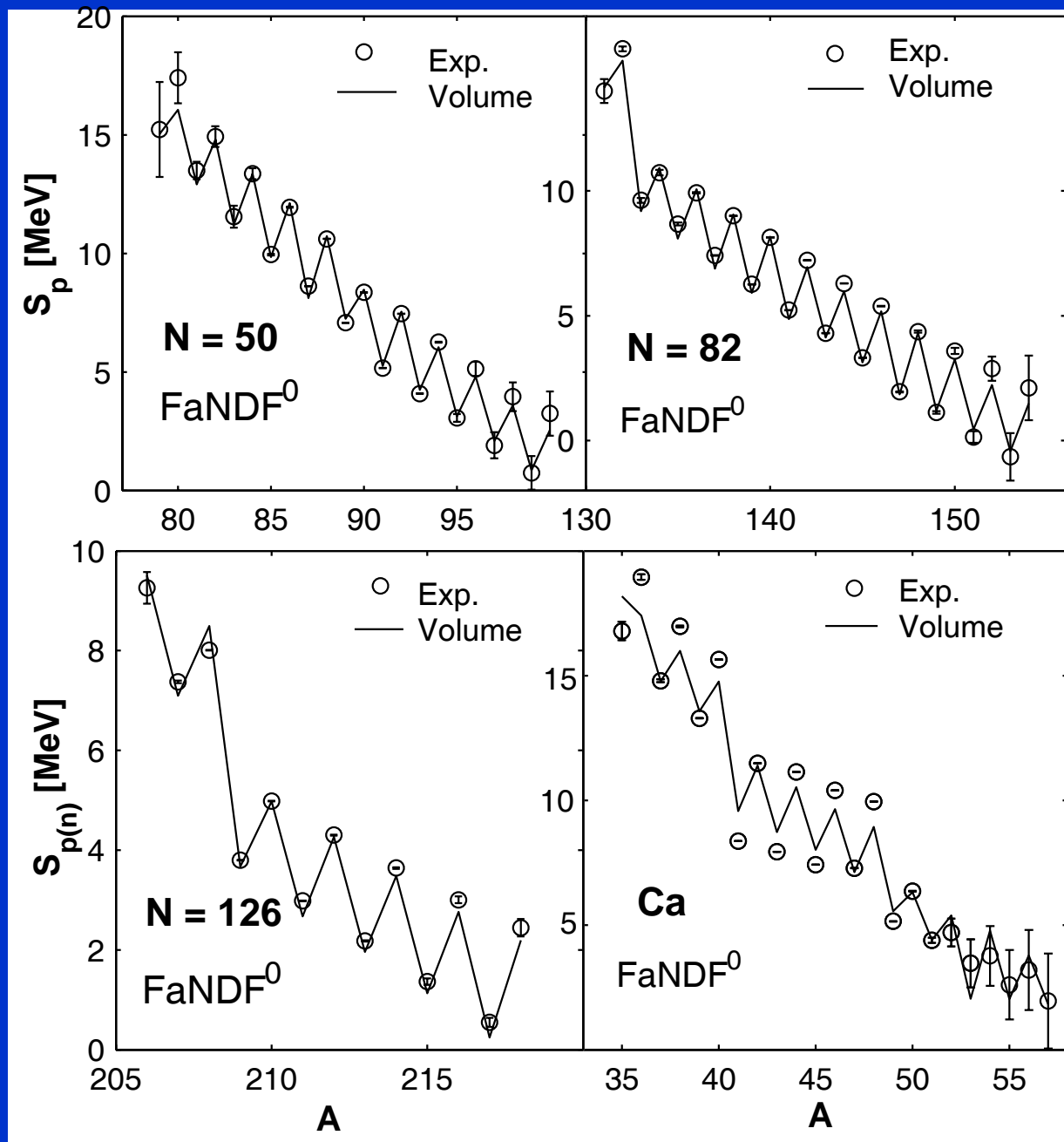
- SLy4 - Chabanat et al.  
Nucl. Phys. A627, 710 (1997)  
Nucl. Phys. A635, 231 (1998)  
Nucl. Phys. A643, 441(E)(1998)

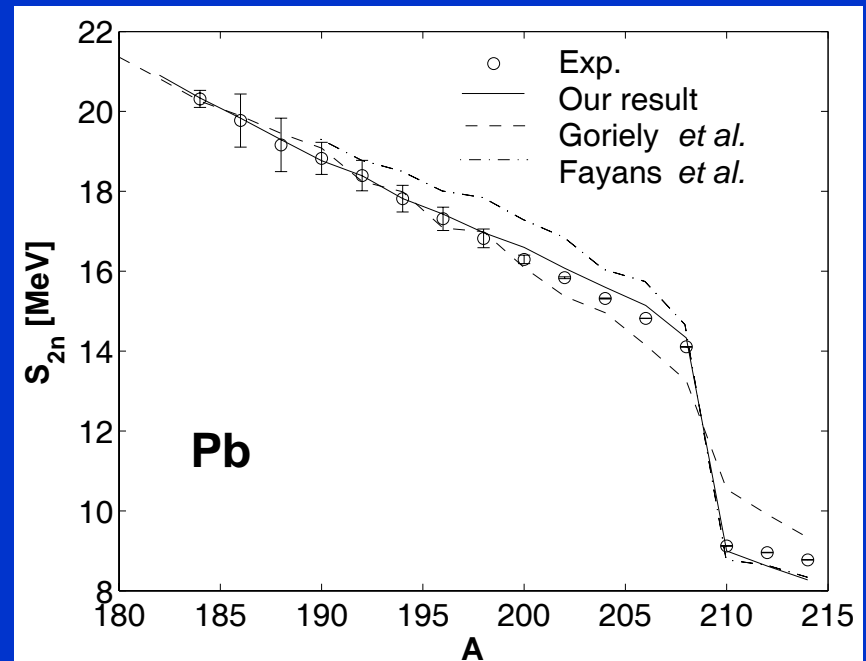
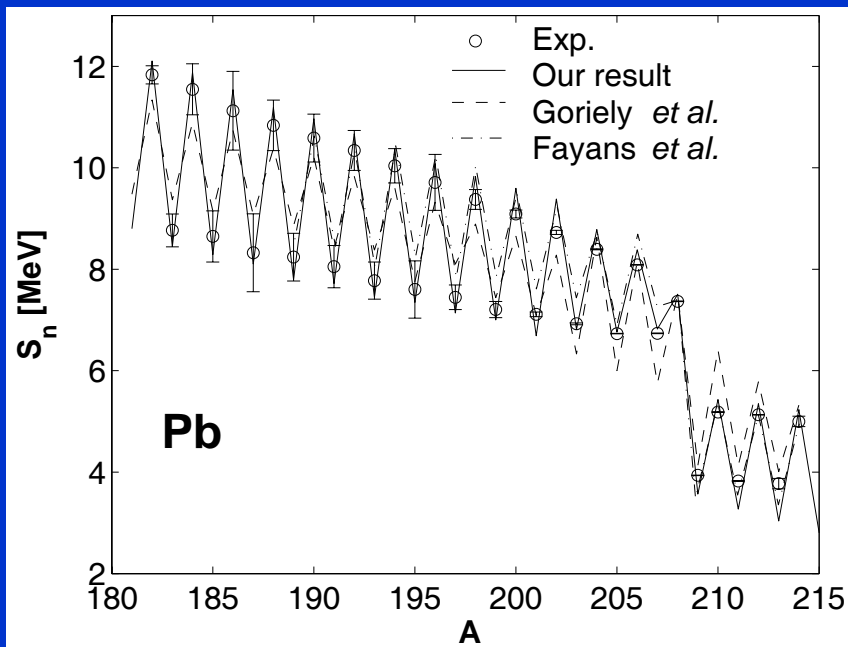
- FaNDF<sup>0</sup> – Fayans  
JETP Lett. 68, 169 (1998)

# Two-neutron separation energies



# One-nucleon separation energies

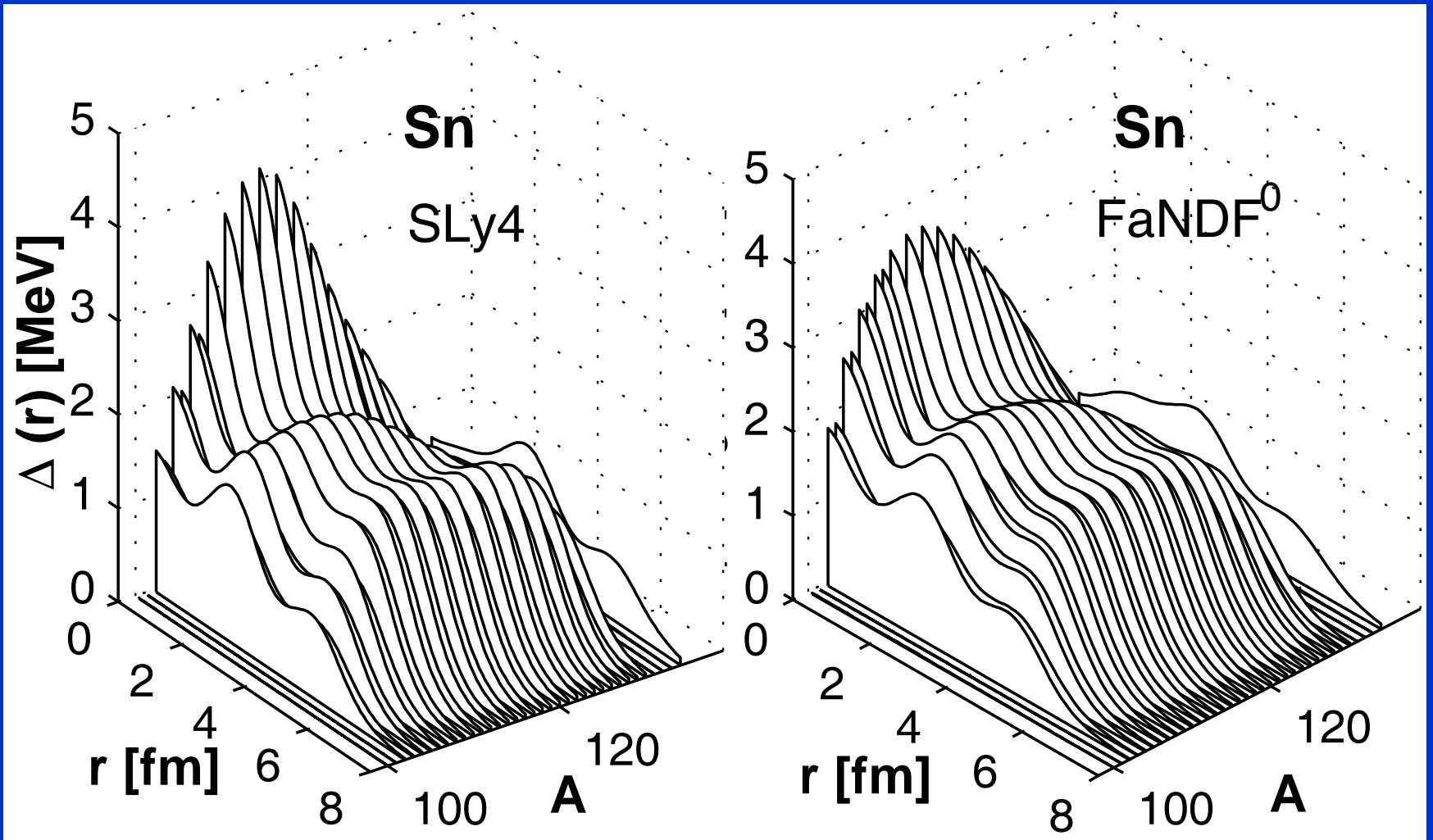




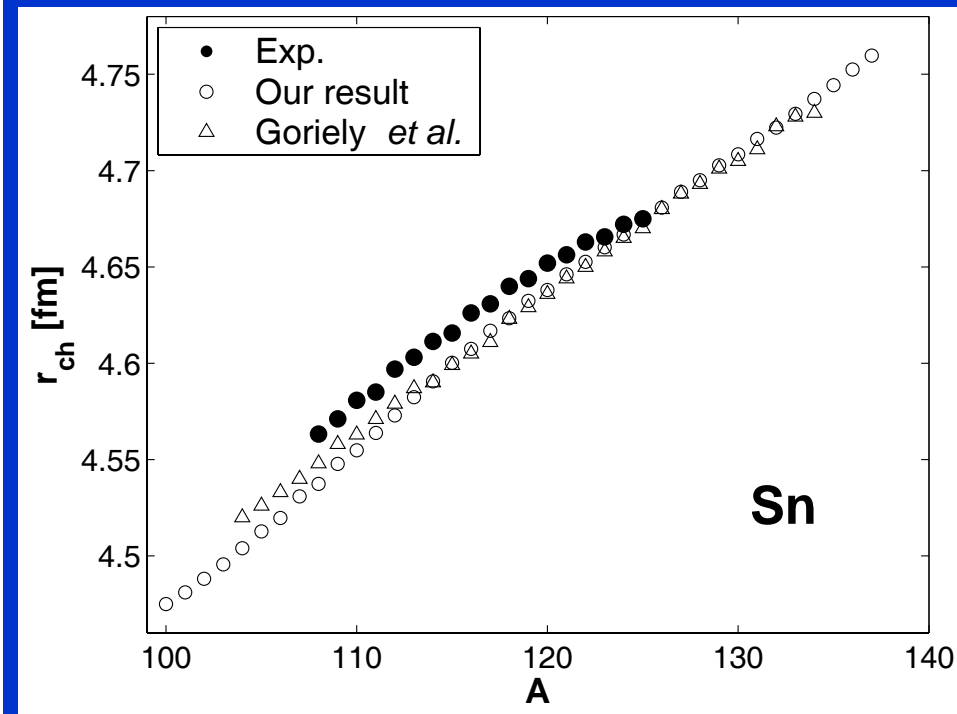
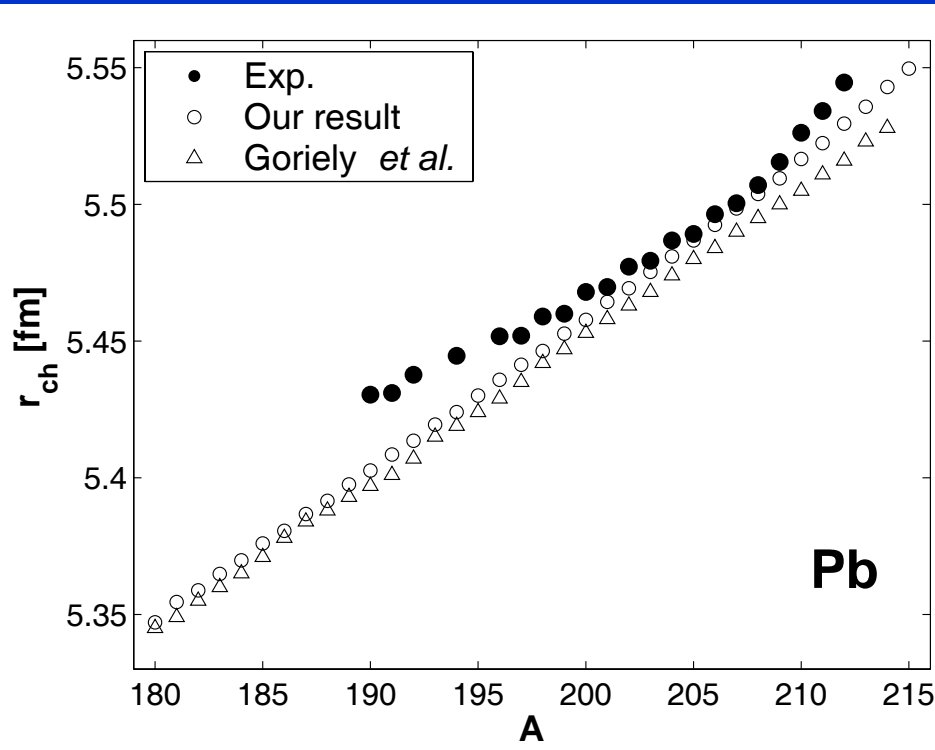
- We use the same normal EDF as Fayans *et al.* volume pairing only with one universal constant
- Fayans *et al.* Nucl. Phys. A676, 49 (2000) *5 parameters for pairing (density dependence with gradient terms (neutrons only)).*
- Goriely *et al.* Phys. Rev. C 66, 024326 (2002) *volume pairing, 5 parameters for pairing, isospin symmetry broken*
- Exp. - Audi and Wapstra, Nucl. Phys. A595, 409 (1995)



# Spatial profiles of the pairing field for tin isotopes and two different (normal) energy density functionals



# 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

ED contribution due to superfluid correlations

$$E_{gs} = \int d^3r \left\{ \varepsilon_N[\rho_n(\vec{r}), \rho_p(\vec{r})] + \varepsilon_S[\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] \right\}$$

$$\left\{ \begin{array}{l} \varepsilon_N[\rho_n(\vec{r}), \rho_p(\vec{r})] = \varepsilon_N[\rho_p(\vec{r}), \rho_n(\vec{r})] \\ \varepsilon_S[\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] = \varepsilon_S[\rho_p(\vec{r}), \rho_n(\vec{r}), \nu_p(\vec{r}), \nu_n(\vec{r})] \end{array} \right.$$

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.

$$\varepsilon_S[\rho_p, \rho_n, \nu_p, \nu_n] = g_0 \underbrace{|\nu_p + \nu_n|^2}_{\text{like } \rho_p + \rho_n} + g_1 \underbrace{|\nu_p - \nu_n|^2}_{\text{like } \rho_p - \rho_n}$$

$g_0$  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

$$\begin{aligned}\mathcal{E}_S[\mathbf{v}_p, \mathbf{v}_n] &= g_0 |\mathbf{v}_p + \mathbf{v}_n|^2 + g_1 |\mathbf{v}_p - \mathbf{v}_n|^2 \\ &= g [|\mathbf{v}_p|^2 + |\mathbf{v}_n|^2] + g' [\mathbf{v}_p^* \mathbf{v}_n + \mathbf{v}_n^* \mathbf{v}_p] \\ g &= g_0 + g_1 \quad g' = g_0 - g_1\end{aligned}$$

?

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.

- Zavischa, Regge and Stapel, Phys. Lett. B 185, 299 (1987)
- Apostol, Bulboaca, Carstoiu, Dumitrescu and Horoi, Europhys. Lett. 4, 197 (1987) and Nucl. Phys. A 470, 64 (1987)
- Dumitrescu and Horoi, Nuovo Cimento A 103, 635 (1990)
- Horoi, Phys. Rev. C 50, 2834 (1994)

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  $\propto |v_n|^2 |v_p|^2$

- 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

$$\mathcal{E}_S[\mathbf{v}_p, \mathbf{v}_n] = g(\rho_p, \rho_n)[|\mathbf{v}_p|^2 + |\mathbf{v}_n|^2] + f(\rho_p, \rho_n)[|\mathbf{v}_p|^2 - |\mathbf{v}_n|^2] \frac{\rho_p - \rho_n}{\rho_p + \rho_n}$$

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

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

Charge symmetric

Goriely *et al*, Phys. Rev. C 66, 024326 (2002) in the most extensive and by far the most accurate fully self-consistent description of all known nuclear masses (2135 nuclei with  $A \geq 8$ ) with an rms better than 0.7 MeV use for pairing couplings:

$$\left. \begin{aligned} V_{pp}^+ &= -265.3 \text{ MeV} \\ V_{nn}^+ &= -237.6 \text{ MeV} \end{aligned} \right\} \text{for even systems}$$
$$\left. \begin{aligned} V_{pp}^- &= -277.8 \text{ MeV} \\ V_{nn}^- &= -246.9 \text{ MeV} \end{aligned} \right\} \text{for odd systems}$$
$$E_c = 15 \text{ MeV} \quad \text{cutoff energy}$$

While no other part of their nuclear EDF violates isospin symmetry, and moreover, while they were unable to incorporate any contribution from CSB-like forces, this fact remains as one of the major drawbacks of their results and it is an embarrassment and needs to be resolved. Without that the entire approach is in the end a mere interpolation, with limited physical significance.

Let us now remember that there are more neutron rich nuclei and let me estimate the following quantity from all measured nuclear masses:

$$\overline{\frac{N-Z}{A}} = 0.1473$$

Conjecturing now that Goriely *et al*, Phys. Rev. C 66, 024326 (2002) have as a matter of fact replaced in the “true” pairing EDF the isospin density dependence simply by its average over all masses, one can easily extract from their pairing parameters the following relation:

$$\mathcal{E}_S [v_p, v_n] = g [ |v_p|^2 + |v_n|^2 ] + f [ |v_p|^2 - |v_n|^2 ] \frac{\rho_p - \rho_n}{\rho_p + \rho_n}$$

where  $f \approx -0.39$   $g > 0$  and  $g < 0$

↑  
repulsion

↑  
attraction



The most general form of the superfluid contribution (s-wave only) to the LDA energy density functional, compatible with known nuclear symmetries.

$$\mathcal{E}_S[v_p, v_n] = g(\rho_p, \rho_n) |v_p|^2 + g(\rho_n, \rho_p) |v_n|^2$$

- ✓ In principle one can consider as well higher powers terms in the anomalous densities, but so far I am not aware of any need to do so, if one considers binding energies alone.
- ✓ There is so far no clear evidence for gradient corrections terms in the anomalous density or energy dependent effective pairing couplings.

How can one determine the density dependence of the coupling constant  $g$ ? I know two methods.

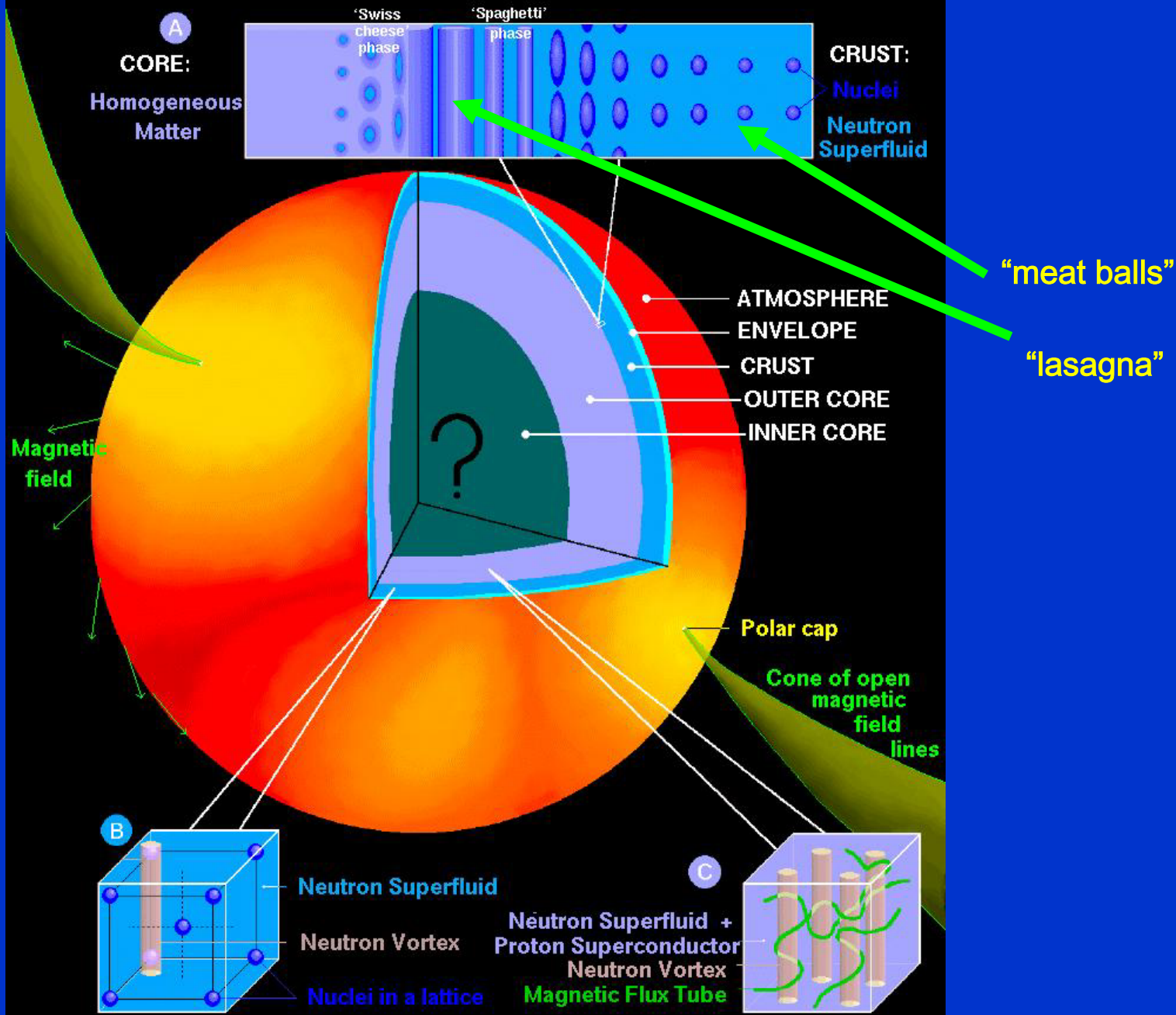
✓ In homogeneous low density matter one can compute the pairing gap as a function of the density. **NB this is not a BCS or HFB result!**

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

✓ One compute also 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.

# A NEUTRON STAR: SURFACE and INTERIOR



# Landau criterion for superflow stability

(flow without dissipation)

Consider a superfluid flowing in a pipe with velocity  $v_s$ :

$$E_0 + \frac{Nm v_s^2}{2} < E_0 + \varepsilon_{\vec{p}} + \vec{v}_s \cdot \vec{p} + \frac{Nm v_s^2}{2} \Rightarrow v_s < \frac{\varepsilon_{\vec{p}}}{p}$$

no internal excitations

One single quasi-particle excitation with momentum  $p$

In the case of a Fermi superfluid this condition becomes

$$v_s < \frac{\Delta}{\hbar k_F}$$

# Vortex in neutron matter

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

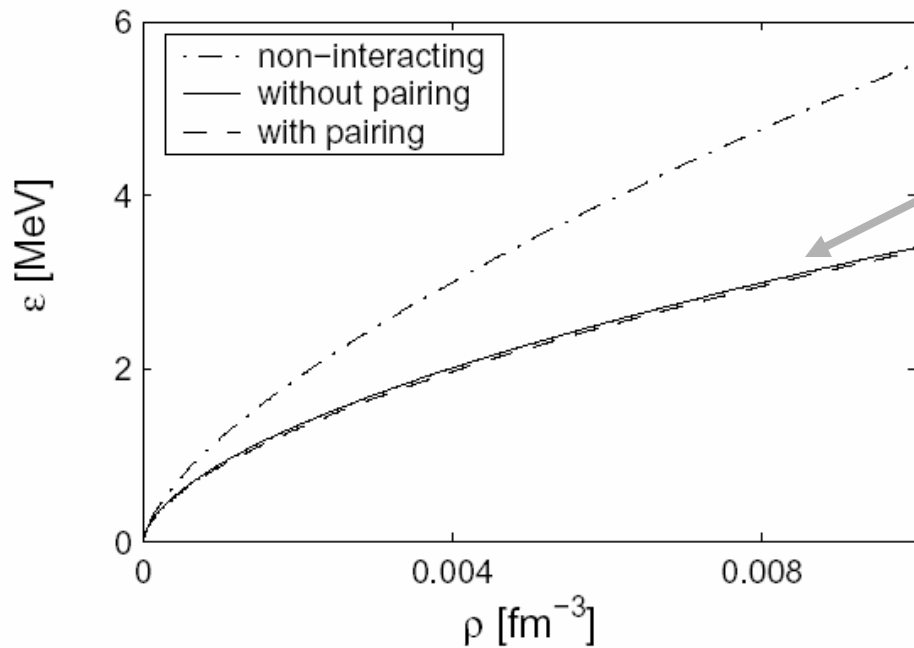
$$\Delta(\vec{r}) = \Delta(r) \exp(i\phi), \quad \vec{r} = (r, \phi, z) \text{ [cylindrical coordinates]}$$

Oz - vortex symmetry axis

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

$$\vec{V}_v(\vec{r}) = \frac{\hbar}{2mr^2} (y, -x, 0) \quad \Leftarrow \quad \frac{1}{2\pi} \oint_C \vec{V}_v(\vec{r}) \cdot d\vec{r} = \frac{\hbar}{2m}$$

# Fayans's FaNDF<sup>0</sup>



$$\Delta = \left(\frac{2}{e}\right)^{7/3} \frac{\hbar^2 k_F^2}{2m} \exp\left(-\frac{\pi}{2 \tan \delta(k_F)}\right)$$

An additional factor of  $1/(4e)^{1/3}$  is due to induced interactions  
 Again, HFB not valid.

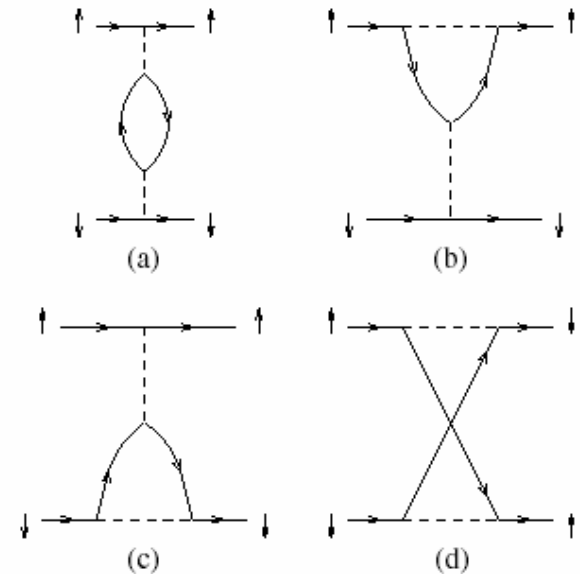
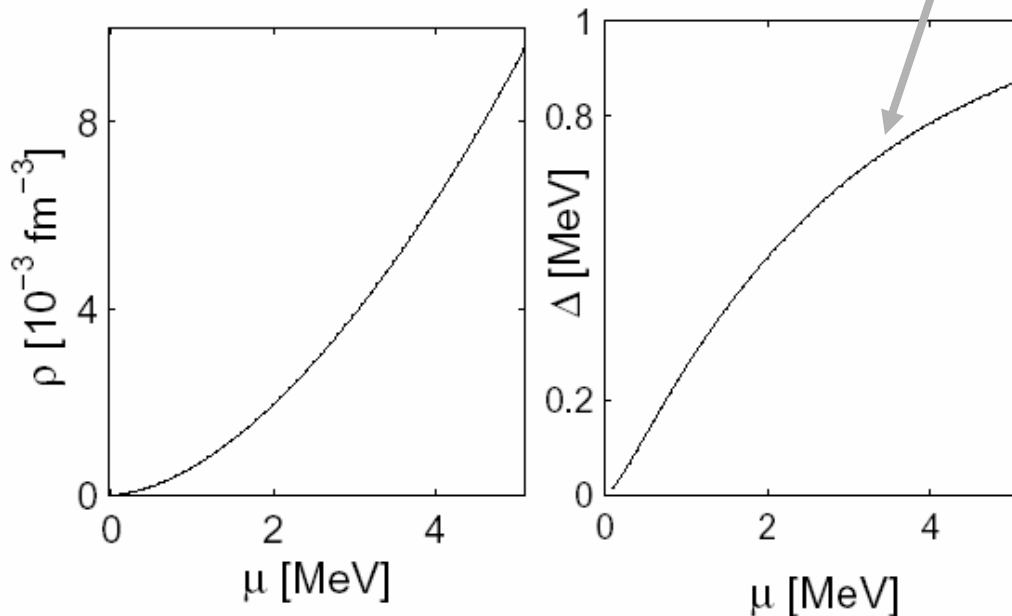
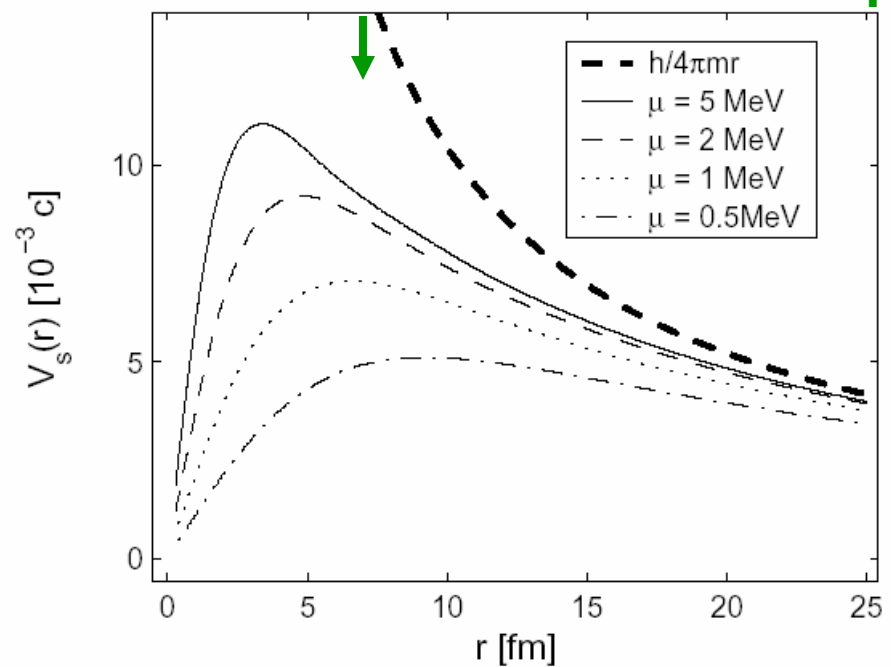
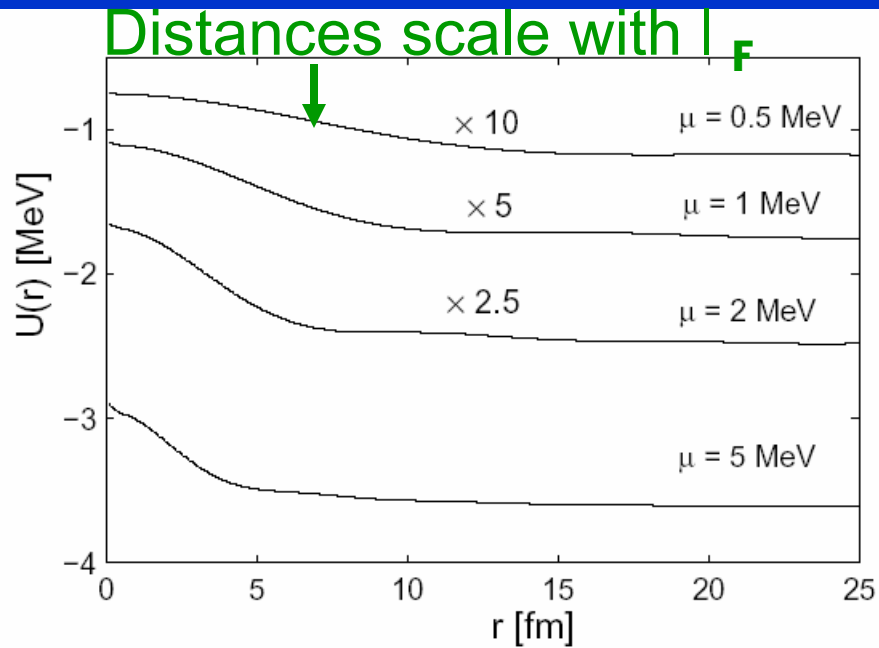
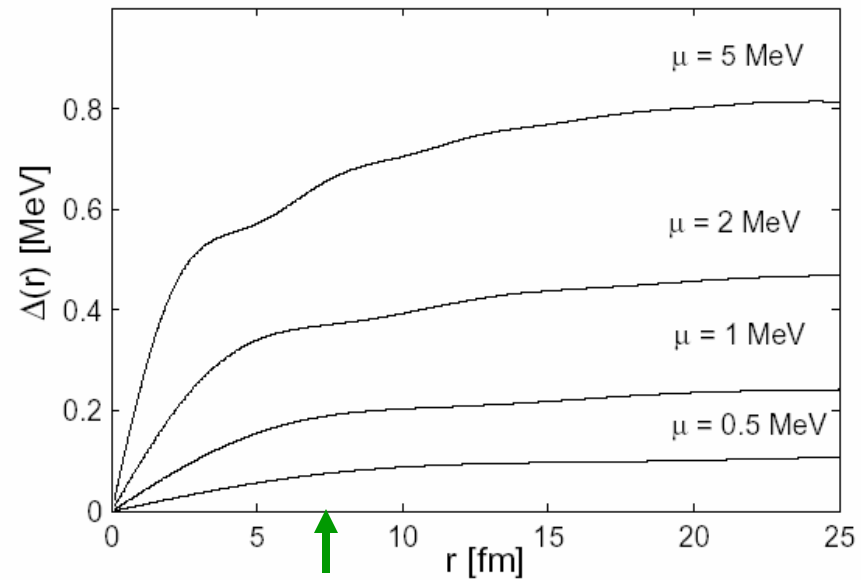
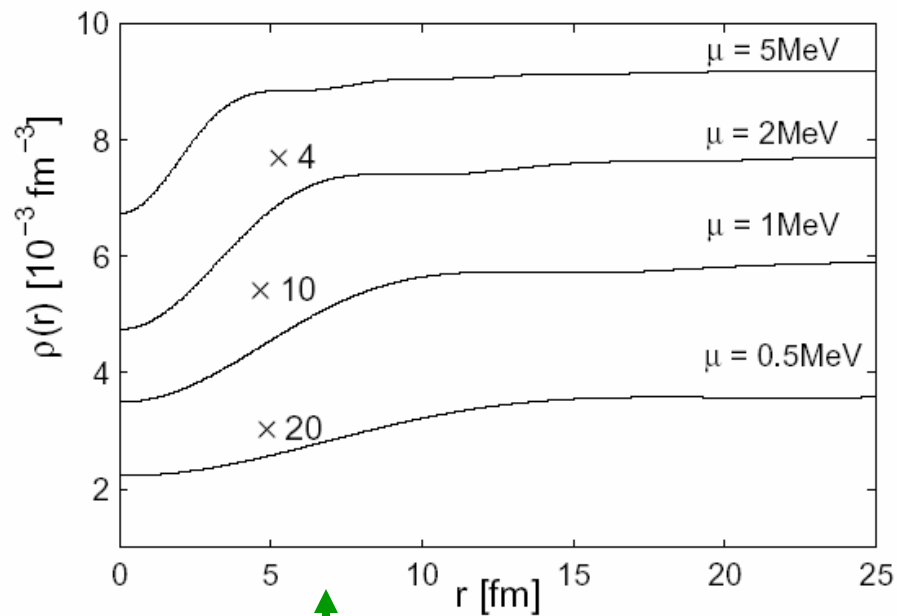


FIG. 1. Diagrams for the induced interactions between two fermions in different internal states to second order in the effective interaction.

from Heiselberg et al  
 Phys. Rev. Lett. 85, 2418, (2000)



# Dramatic structural changes of the vortex state naturally lead to significant changes in the energy balance of a neutron star

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

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

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

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

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



# Vortices in dilute atomic Fermi systems in traps

- ✓ 1995 BEC was observed.
- ✓ 2000 vortices in BEC were created, thus BEC confirmed un-ambiguously.
- ✓ In 1999 DeMarco and Jin created a degenerate atomic Fermi gas.
- ✓ 2002 O'Hara, Hammer, Gehm, Granada and Thomas observed expansion of a Fermi cloud compatible with the existence of a superfluid fermionic phase.

Observation of stable/quantized vortices in Fermi systems would provide the ultimate and most spectacular proof for the existence of a Fermionic superfluid phase.

*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.

What we learned from the structure of a vortex in low density neutron matter can help 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.

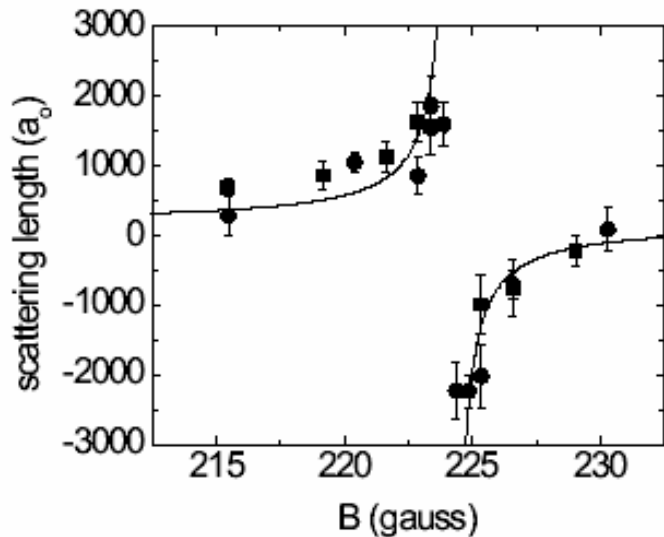
One can change the magnitude of the gap by altering the scattering length between two atoms with magnetic fields by means of a Feshbach resonance.

# Feshbach resonance

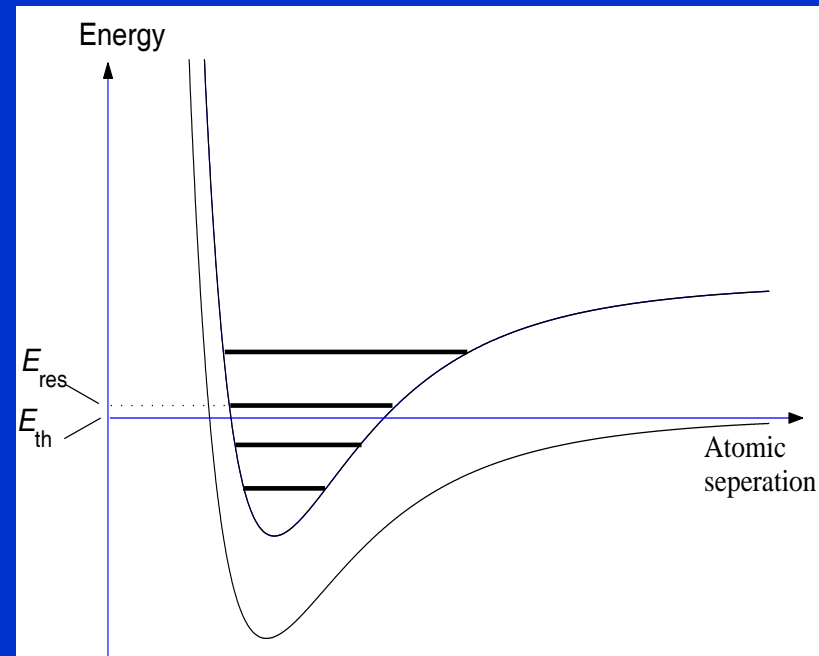
$$H = \frac{\vec{p}^2}{2\mu_r} + \sum_{i=1}^2 (V_i^{hf} + V_i^Z) + V_0(\vec{r})P_0 + V_1(\vec{r})P_1 + V^d$$

$$V^{hf} = \frac{a_{hf}}{\hbar^2} \vec{S}^e \cdot \vec{S}^n, \quad V^Z = (\gamma_e S_z^e - \gamma_n S_z^n) B$$

Tiesinga, Verhaar, Stoof  
 Phys. Rev. A 47, 4114 (1993)



Regal and Jin  
 Phys. Rev. Lett. 90, 230404 (2003)



Consider Bertsch's MBX challenge (1999): "Find the ground state of infinite homogeneous neutron matter interacting with an infinite scattering length."

➤ Carlson, Morales, Pandharipande and Ravenhall, nucl-th/0302041, 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.

Now one can construct an LDA functional to describe this new state of Fermionic matter

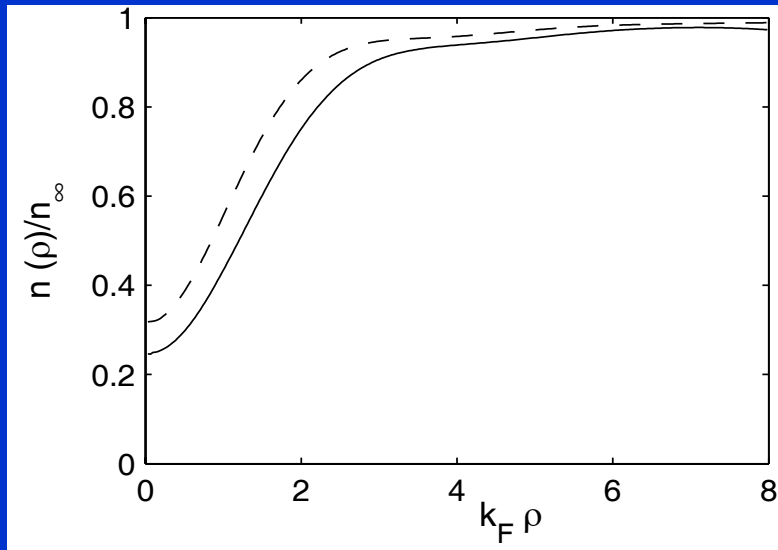
$$\mathcal{E}(\mathbf{r})n(\mathbf{r}) = \frac{\hbar^2}{m} \left[ \frac{m}{2m^*} \tau(\mathbf{r}) + \beta n(\mathbf{r})^{5/3} + \gamma \frac{|\nu(\mathbf{r})|^2}{n(\mathbf{r})^{1/3}} \right],$$

$$n(\mathbf{r}) = \sum_{\alpha} |v_{\alpha}(\mathbf{r})|^2, \quad \tau(\mathbf{r}) = \sum_{\alpha} |\nabla v_{\alpha}(\mathbf{r})|^2,$$

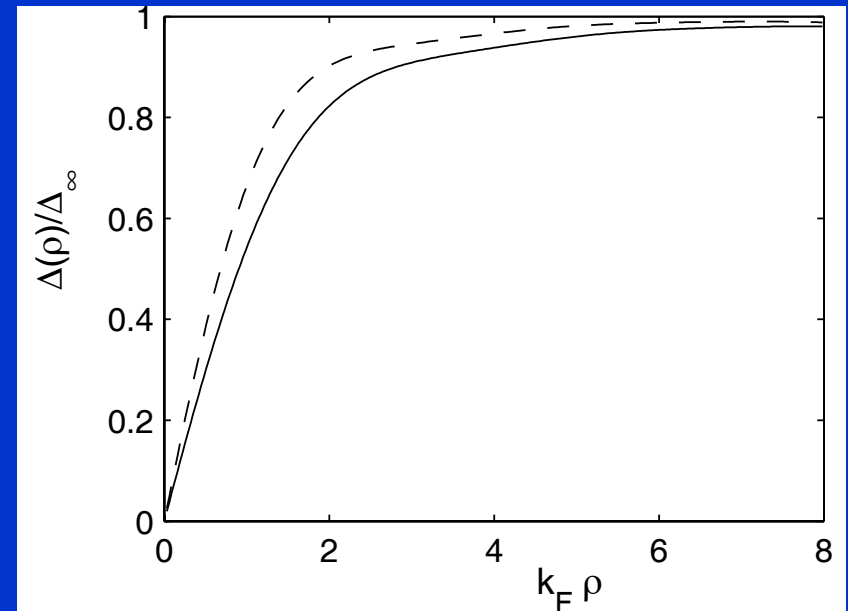
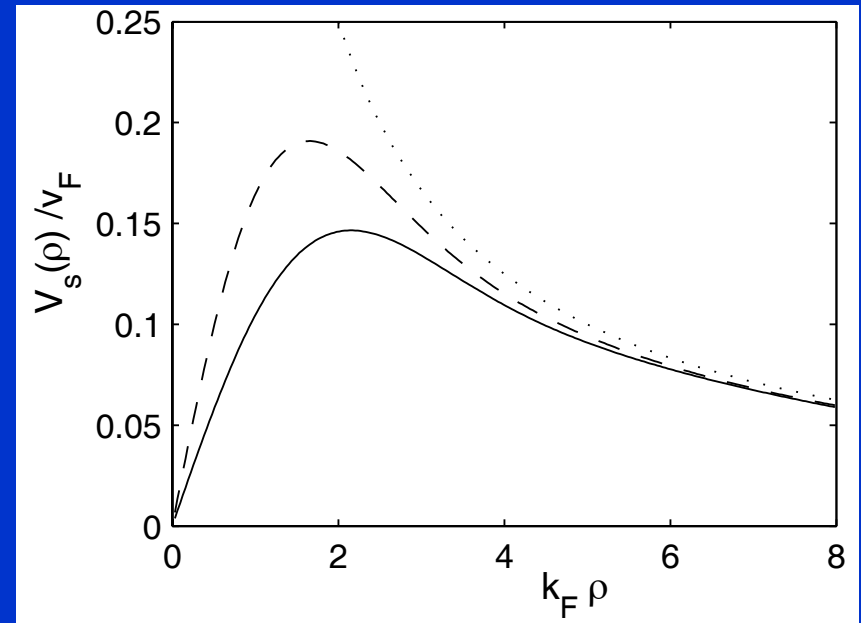
$$\nu(\mathbf{r}) = \sum_{\alpha} v_{\alpha}^*(\mathbf{r}) u_{\alpha}(\mathbf{r}).$$

- This form is not unique, as one can have either:  
b=0 (set I) or b≠0 and m\*=m (set II).
- Gradient terms not determined yet (expected minor role).

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.

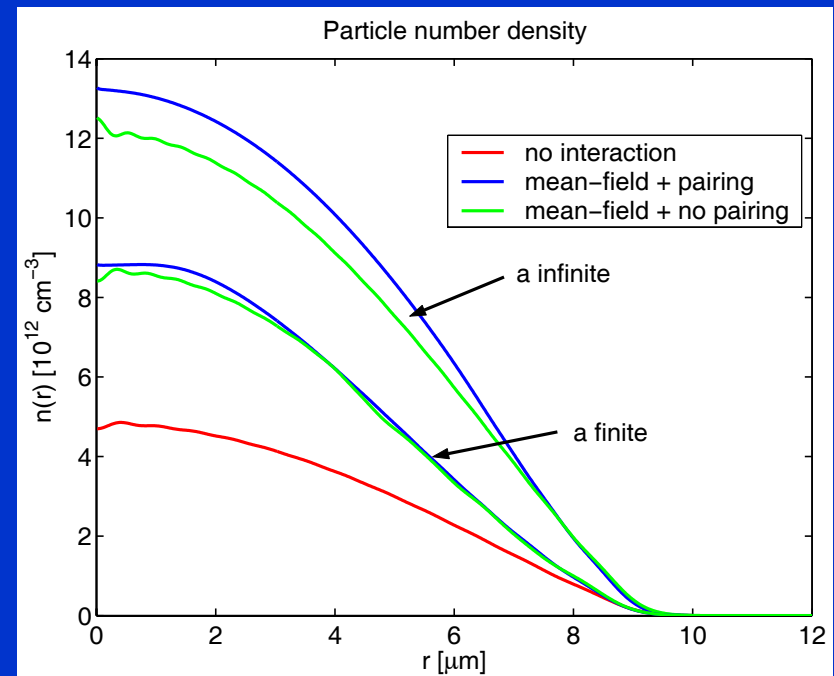
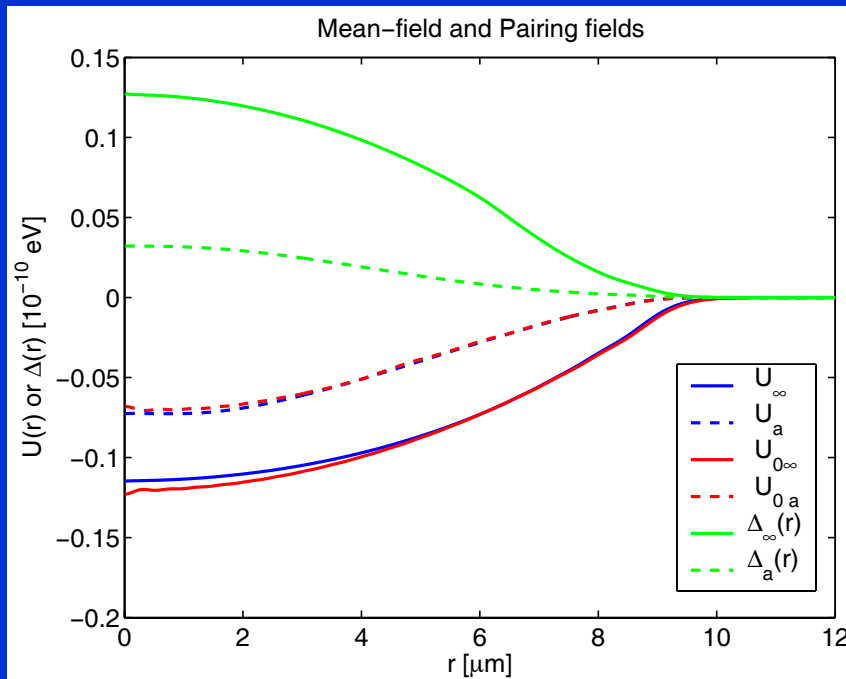


Solid lines are results for parameter set I, dashed lines for parameter set II (dots – velocity profile for ideal vortex)



# 40K (Fermi) atoms in a spherical harmonic trap

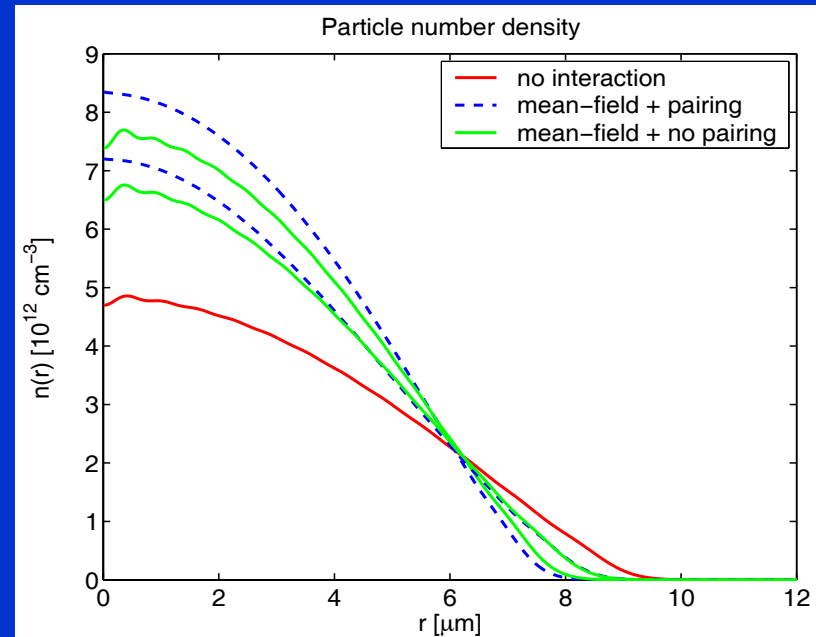
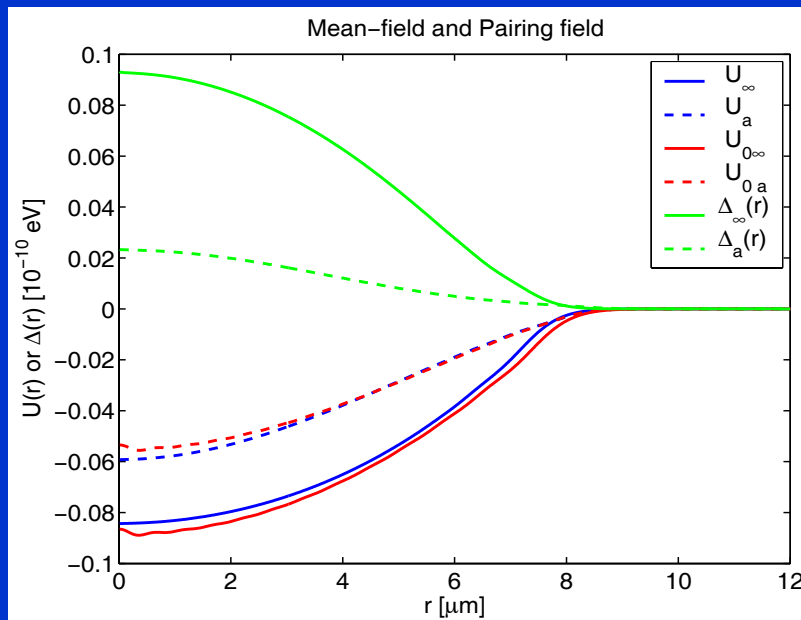
Effect of interaction, with and without weak and strong pairing correlations with fixed chemical potential.



$m \approx 0.14 \mu 10^{-10} \text{ eV}$ ,  $\hbar \omega = 0.568 \mu 10^{-12} \text{ eV}$ ,  
 $a = -12.63 \text{ nm}$  (when finite)

# 40K (Fermi) atoms in a spherical harmonic trap

Effect of interaction, with and without weak and strong pairing correlations with fixed particle number,  $N = 5200$ .



$\hbar\omega = 0.568 \mu\text{eV}$ ,  $a = -12.63\text{nm}$  (when finite)



# 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**
- ✓ Nuclear symmetries lead to a relatively simple form of the superfluid contributions to the energy density functional.
- ✓ Phenomenological analysis of a relatively large number of nuclei (more than 200) indicates that with a single coupling constant one can describe very accurately proton and neutron pairing correlations in both odd and even nuclei. However, there seem to be a need to introduce a consistent isospin dependence of the pairing EDF.
- ✓ There is a need to understand the behavior of the pairing as a function of density, from very low to densities several times nuclear density, in particular pairing in higher partial waves, in order to understand neutron stars.
- ✓ It is not clear so far whether proton and neutron superfluids do influence each other in a direct manner, if one considers binding energies alone.
- ✓ The formalism has been applied as well to vortices in neutron stars and to describe various properties of dilute atomic Fermi gases and there is also an extension to 2-dim quantum dots due to Yu, Aberg and Reinman.