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
- ✓ 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 — $T_c \approx 10^{-12} - 10^{-9}$ 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)
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

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

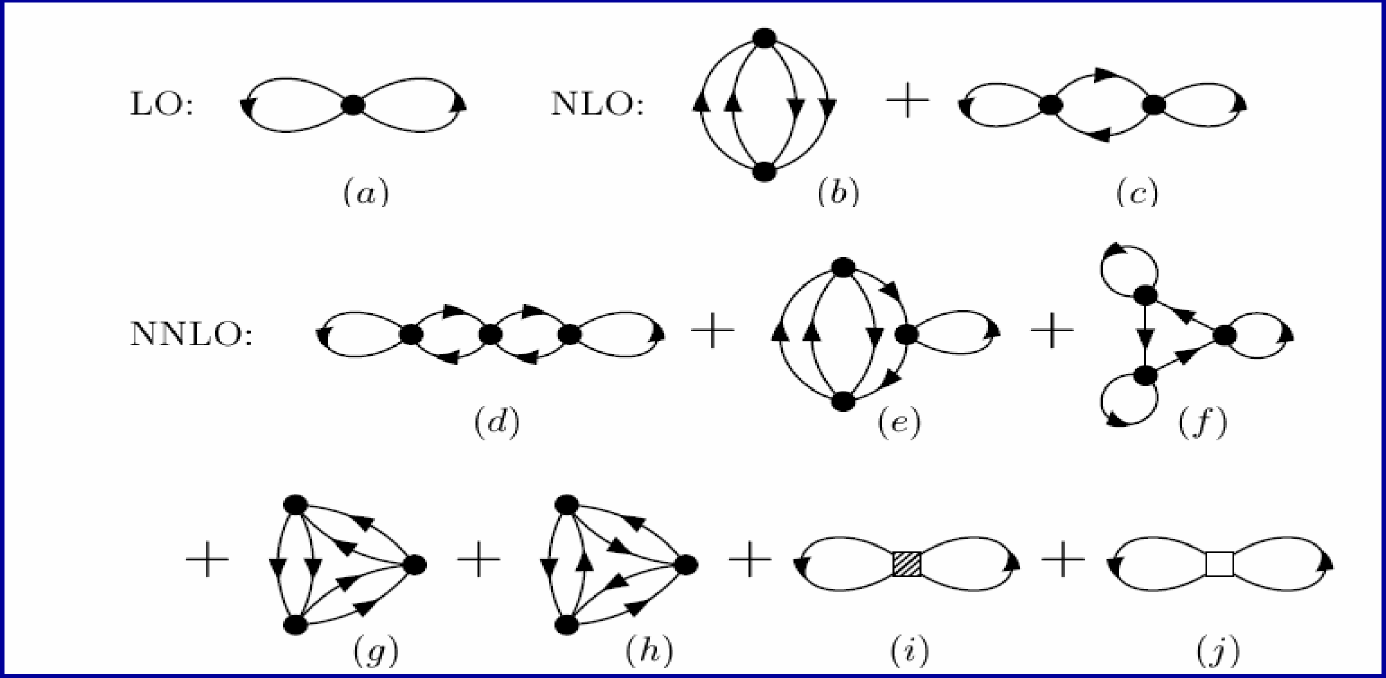
One can try to derive it, however, from an *ab initio (?)* lagrangian

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

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

Bhattacharyya and Furnstahl, nucl-phys/0408014

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

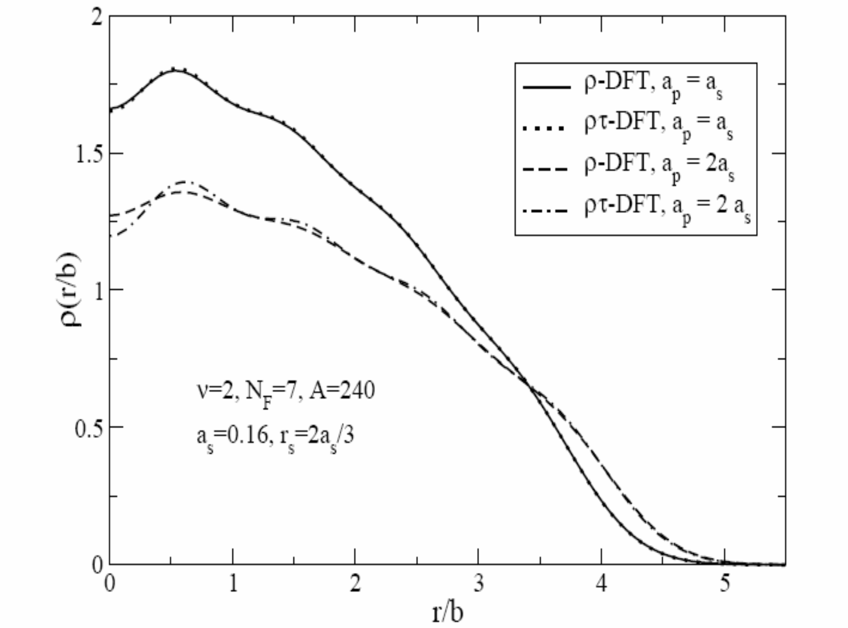


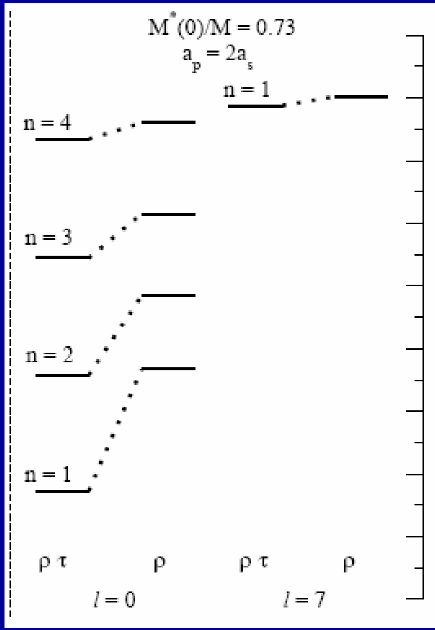
One can construct however an EDF which depends both on particle density and kinetic energy density and use it in a extended Kohn-Sham approach

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

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

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

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

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

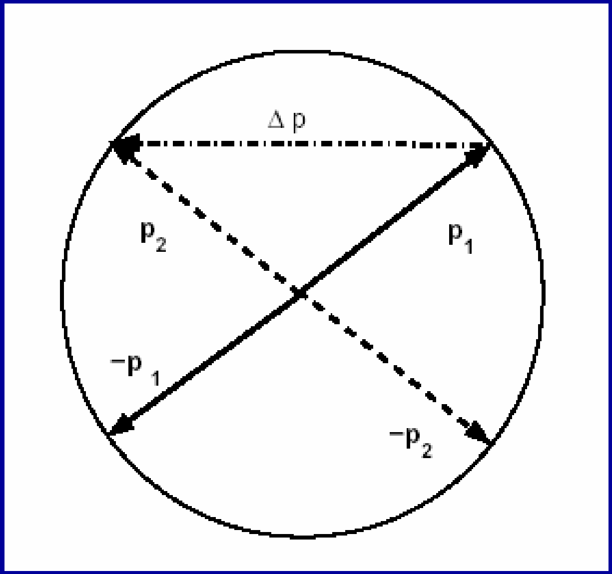
$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix}$$

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.

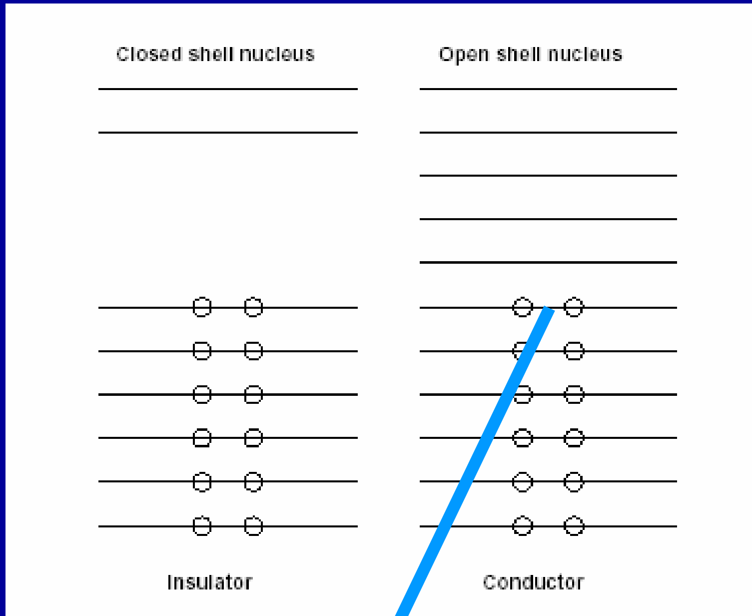
$$\mathrm{v}_\mathrm{k}(\vec{r}_1) = \mathrm{v}_\mathrm{k} \exp(i\vec{k}\cdot\vec{r}_1), \qquad \mathrm{u}_\mathrm{k}(\vec{r}_2) = \mathrm{u}_\mathrm{k} \exp(i\vec{k}\cdot\vec{r}_2)$$

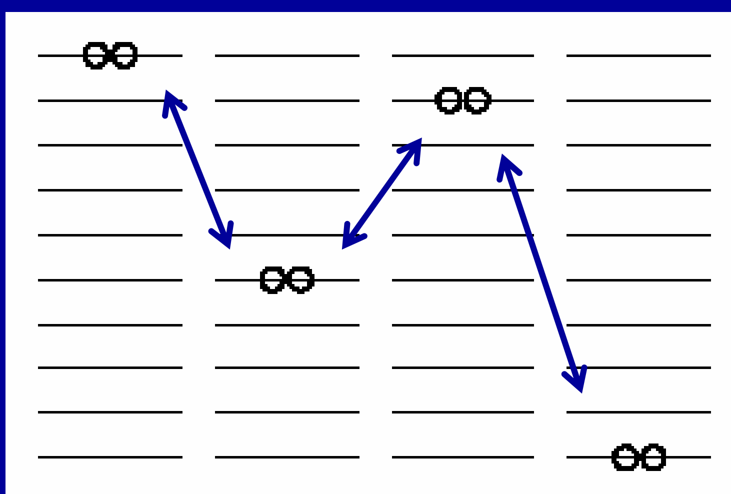
$$\mathrm{v}_\mathrm{k}^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_\mathrm{k} - \mu}{\sqrt{(\varepsilon_\mathrm{k} - \mu)^2 + \Delta^2}}\right), \quad \mathrm{u}_\mathrm{k}^2 + \mathrm{v}_\mathrm{k}^2 = 1, \quad \varepsilon_\mathrm{k} = \frac{\hbar^2\vec{k}^2}{2m} + U, \quad \Delta = \frac{\hbar^2\delta}{2m}$$

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

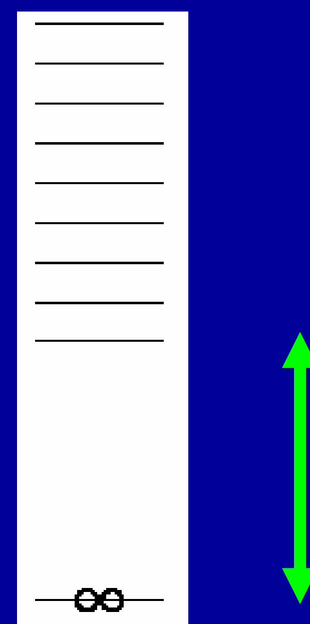
How pairing emerges?

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)

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

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

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

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

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

The SLDA (renormalized) equations

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

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

$$\begin{cases} [h(\vec r)-\mu]\mathrm{u}_{\mathrm{i}}(\vec r)+\Delta(\vec r)\mathrm{v}_{\mathrm{i}}(\vec r) = E_i\mathrm{u}_{\mathrm{i}}(\vec r) \\ \Delta^*(\vec r)\mathrm{u}_{\mathrm{i}}(\vec r)-[h(\vec r)-\mu]\mathrm{v}_{\mathrm{i}}(\vec r) = E_i\mathrm{v}_{\mathrm{i}}(\vec r) \end{cases}$$

$$\begin{cases} h(\vec r) = -\vec\nabla \dfrac{\hbar^2}{2m(\vec r)}\vec\nabla + U(\vec r) \\ \Delta(\vec r) = -g_{\text{eff}}(\vec r)\nu_c(\vec r) \end{cases}$$

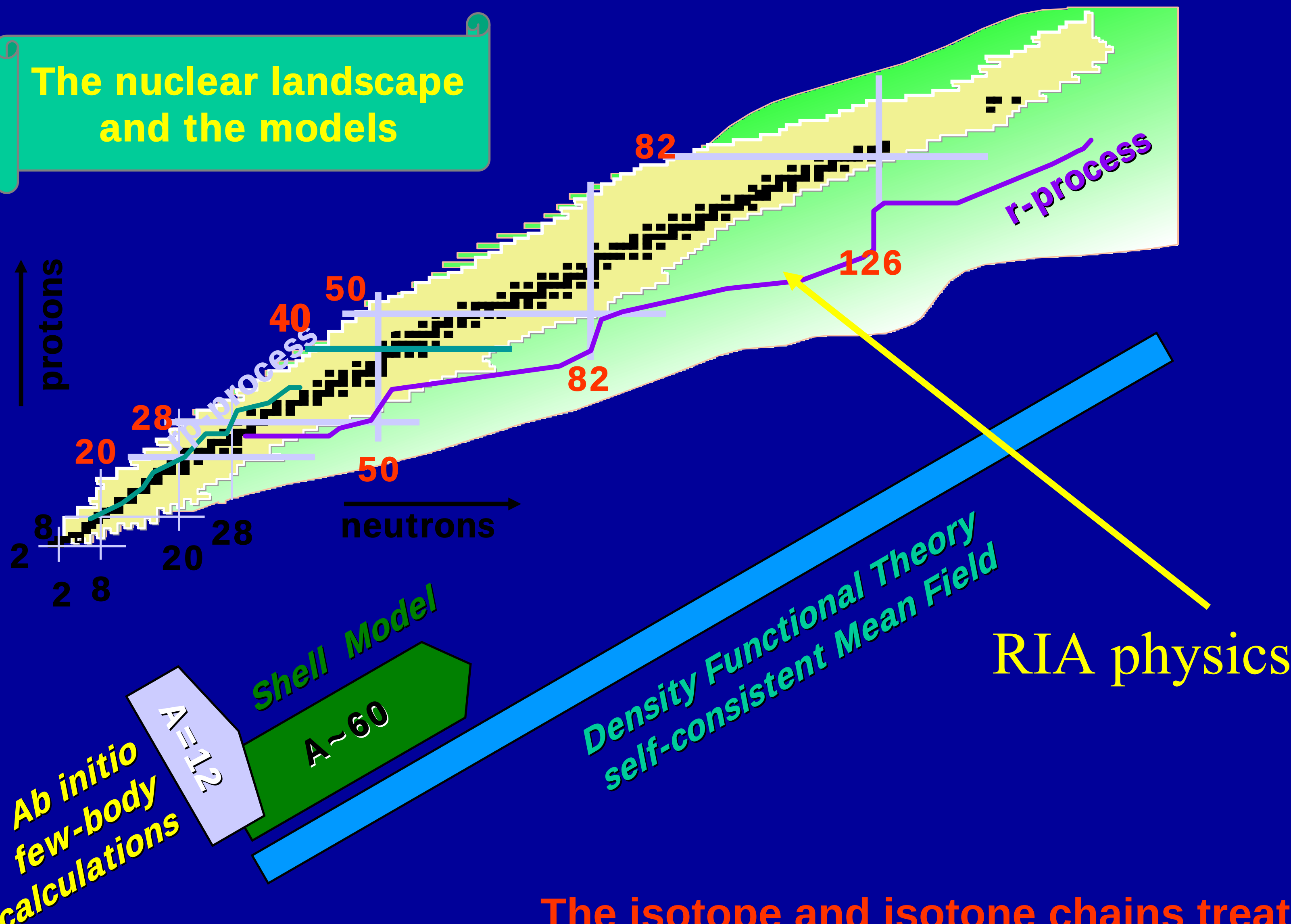
$$\boxed{\frac{1}{g_{eff}(\vec r)} = \frac{1}{g[\rho(\vec r)]} - \frac{m(\vec r)k_c(\vec r)}{2\pi^2\hbar^2}\left\{1-\frac{k_F(\vec r)}{2k_c(\vec r)}\ln\frac{k_c(\vec r)+k_F(\vec r)}{k_c(\vec r)-k_F(\vec r)}\right\}}$$

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

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

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

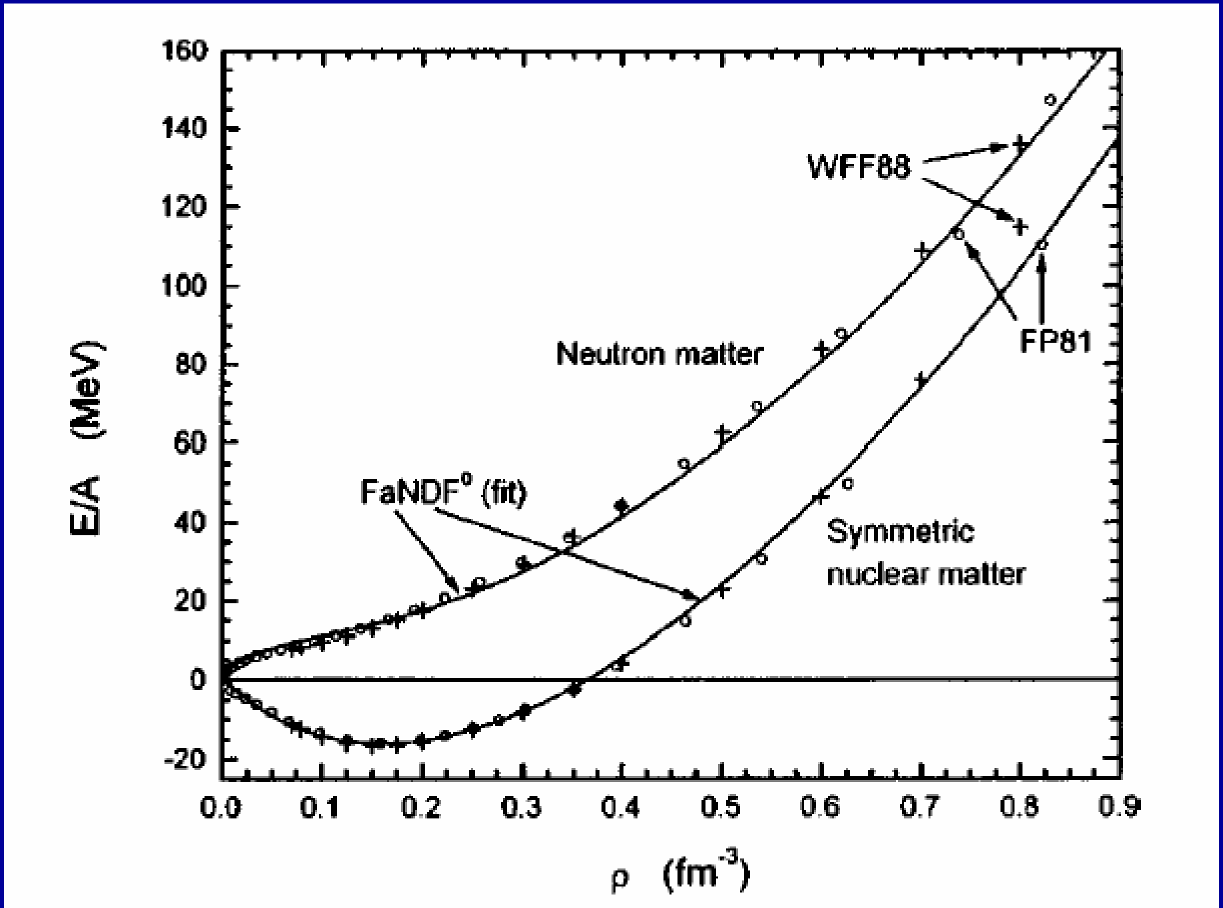
The nuclear landscape and the models



Courtesy of Mario Stoitsov

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

How to describe nuclei?

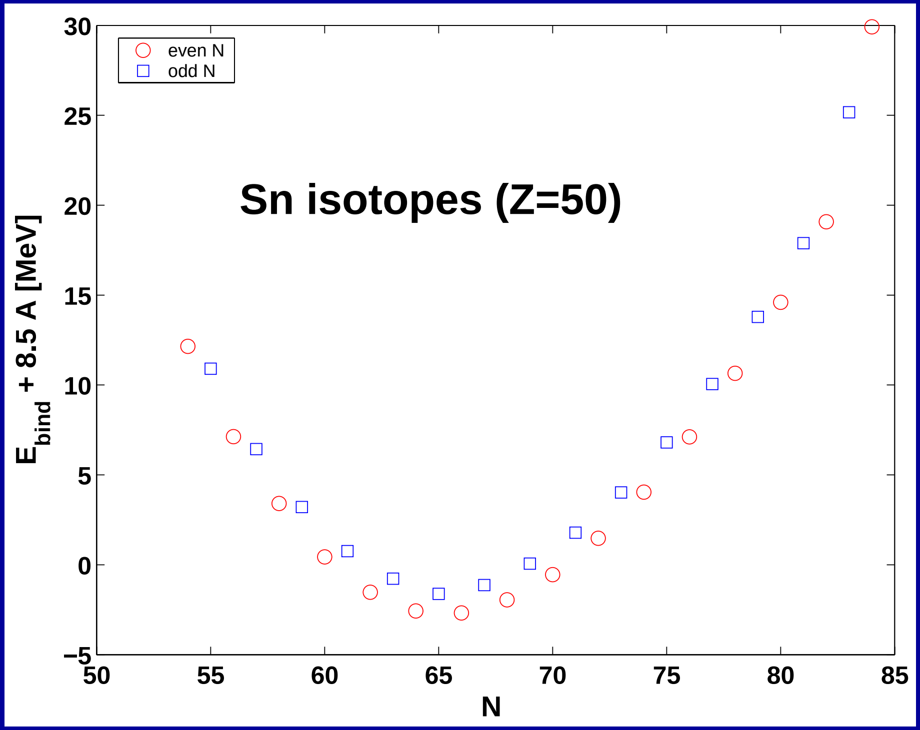


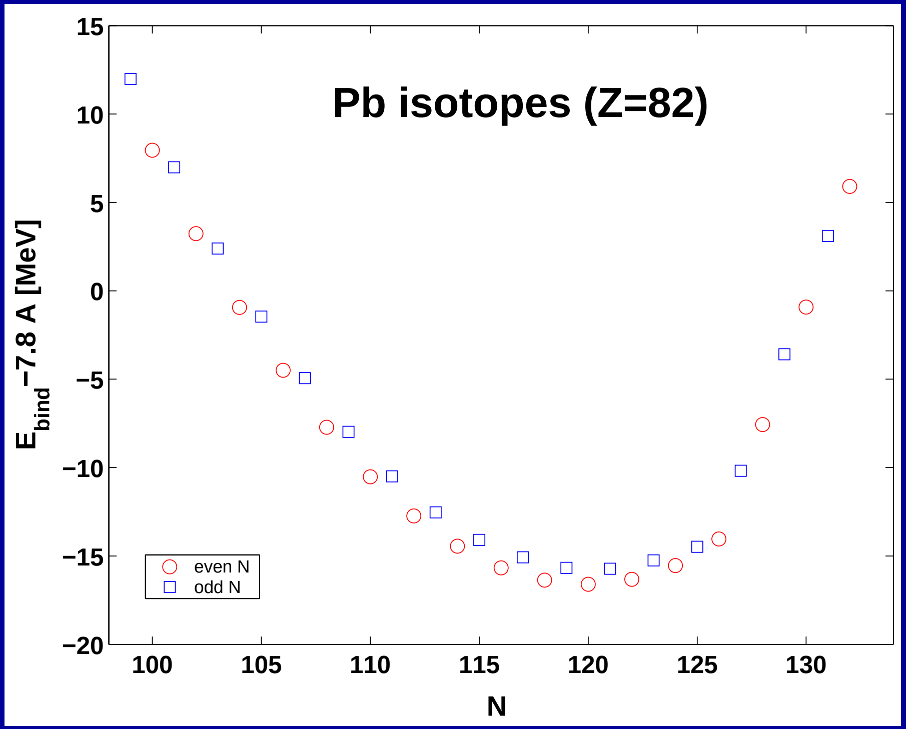
Fayans parameterization of the infinite matter calculations
Wiringa, Fiks and Fabrocini, Phys. Rev. **38**, 1010 (1988)
Friedman and Pandharipande, Nucl. Phys. A **361**, 502 (1981)

This defines the normal part of the EDF.

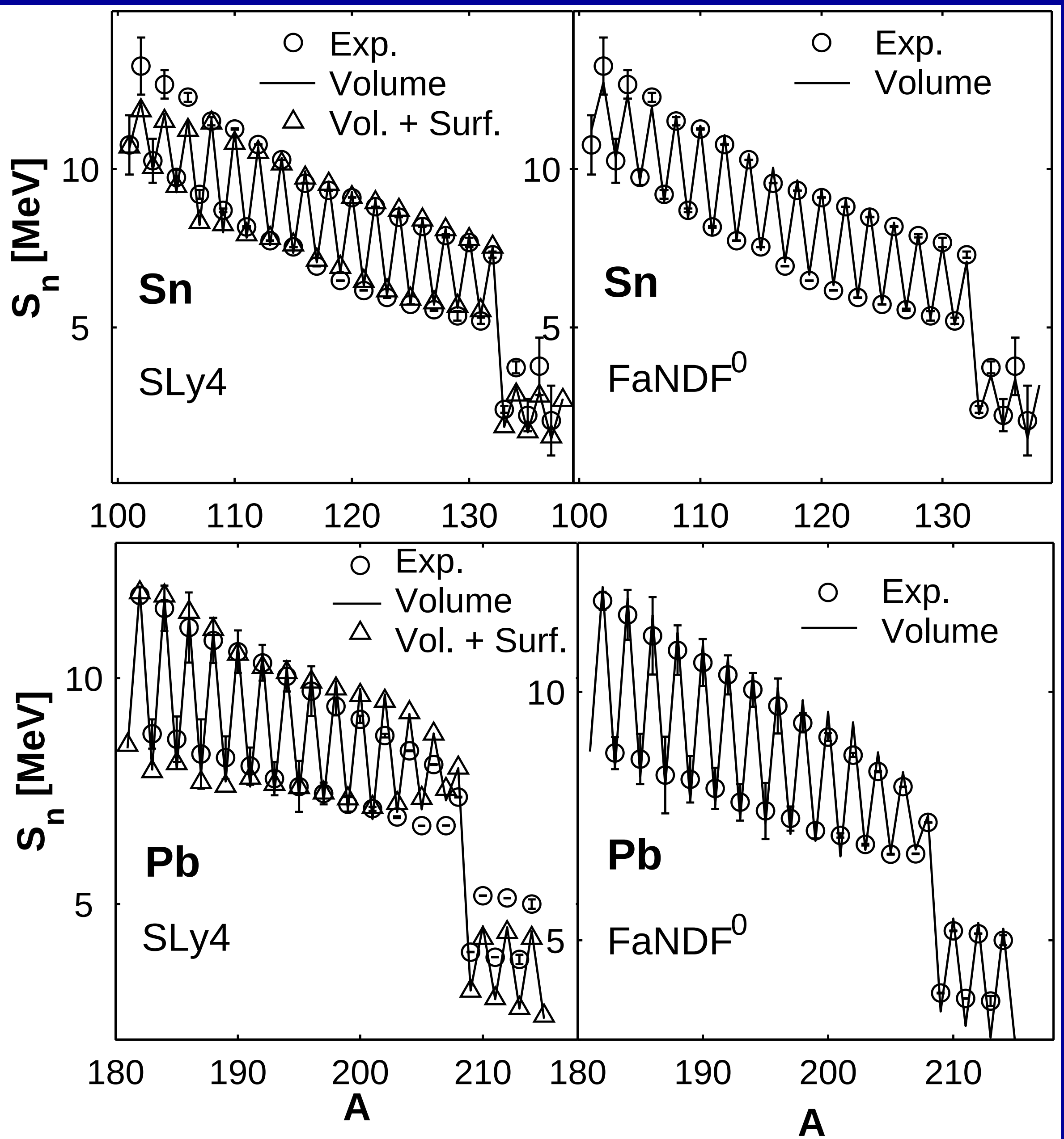
Pairing correlations show prominently in the staggering of the binding energies.

Systems with odd particle number are less bound than systems with even particle number.





One-neutron separation energies



Volume pairing

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

Volume + Surface pairing

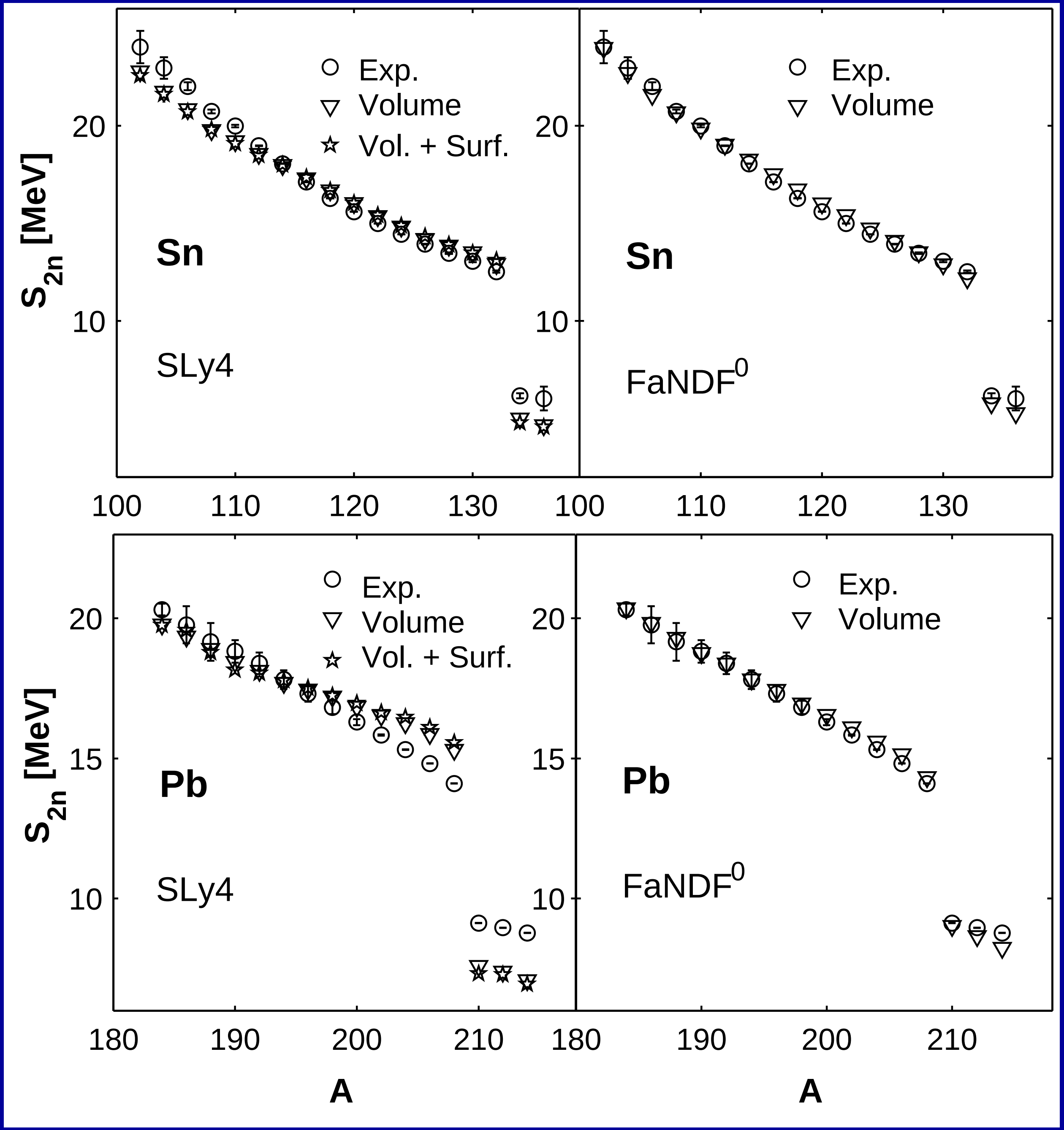
$$g(\vec{r}) = V_0\left(1 - \frac{\rho(\vec{r})}{\rho_c}\right)$$

Normal EDF:

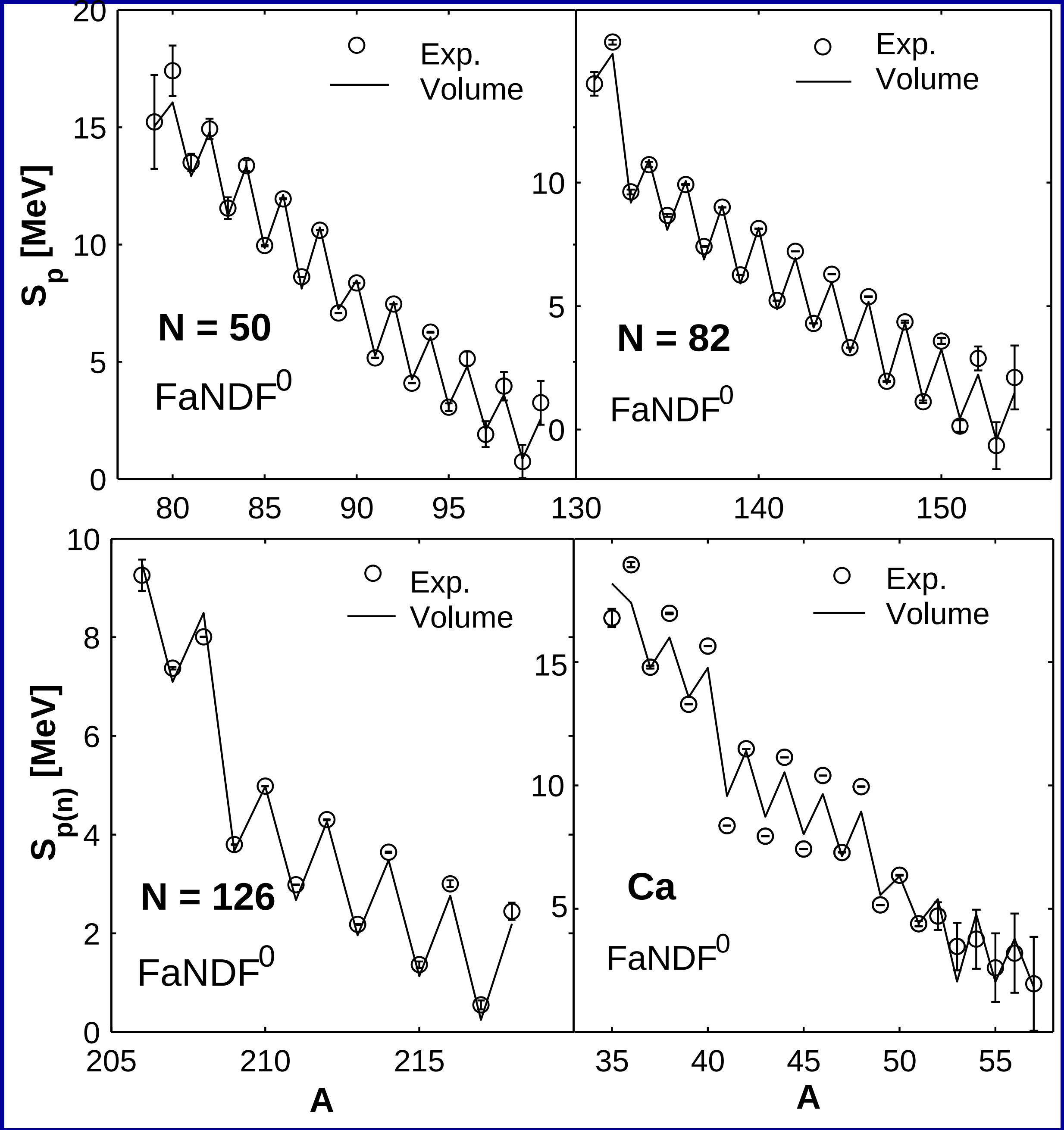
- **SLy4** - Chabanat et al.
Nucl. Phys. **A627**, 710 (1997)
Nucl. Phys. **A635**, 231 (1998)
Nucl. Phys. **A643**, 441(E)(1998)

- FaNDF^0 – Fayans
JETP Lett. **68**, 169 (1998)

Two-neutron separation energies



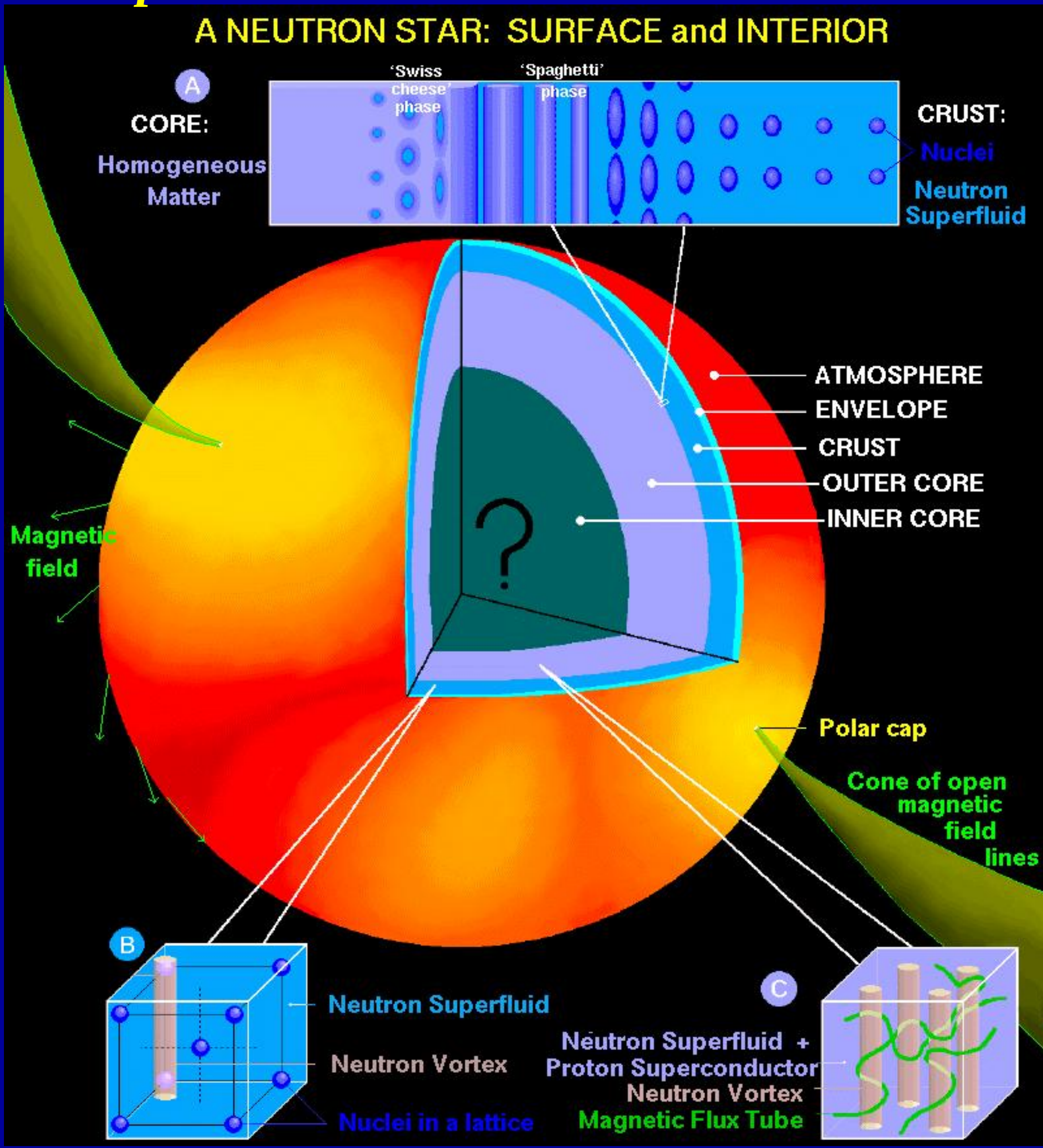
One-nucleon separation energies



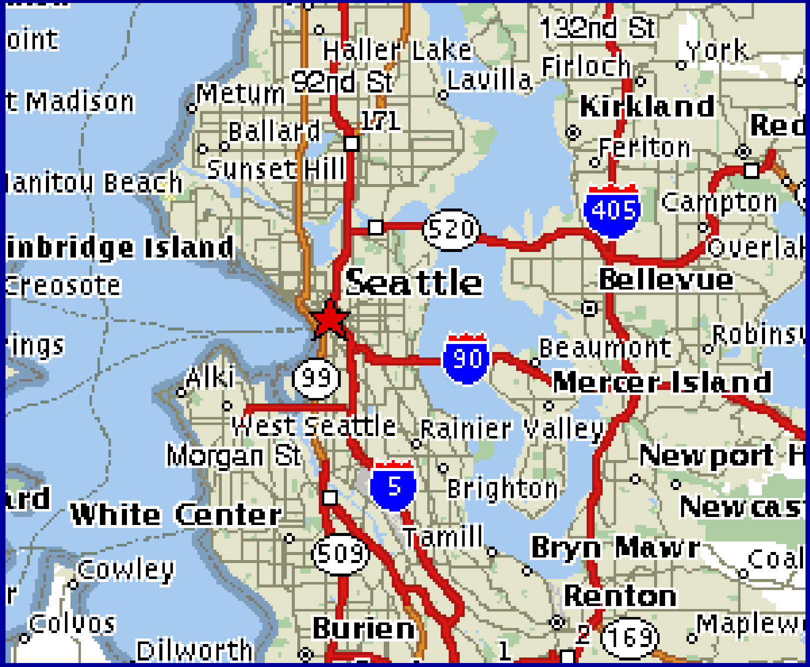
Anderson and Itoh, Nature, 1975

“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/cm^3**



Author: Dany Page

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

$$\varepsilon_S\left[\rho(\vec{r}),\nu(\vec{r})\right]=g[\rho(\vec{r})]\,|\,\nu(\vec{r})\,|^2$$

← **Superfluid contribution to EDF**

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

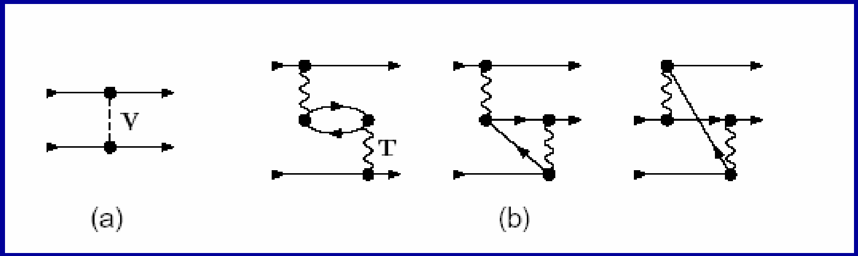
$$\Delta=\left(\frac{2}{e}\right)^{7/3}\frac{\hbar^2k_F^2}{2m}\exp\left(\frac{\pi}{2k_Fa}\right)$$

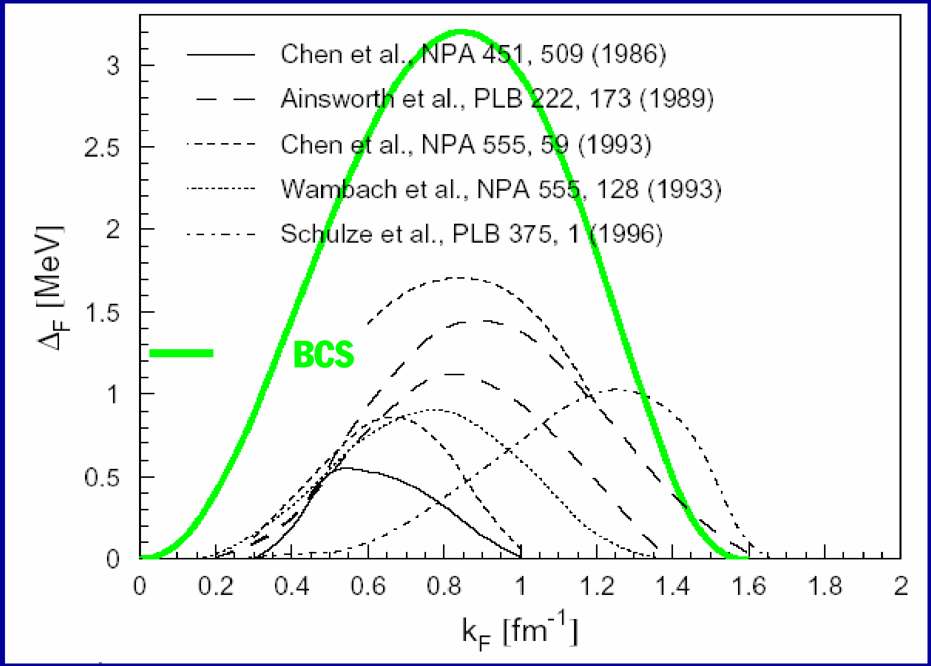
Gorkov and Melik-Barkhudarov, 1961

✓ **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.

“Screening effects” are significant!

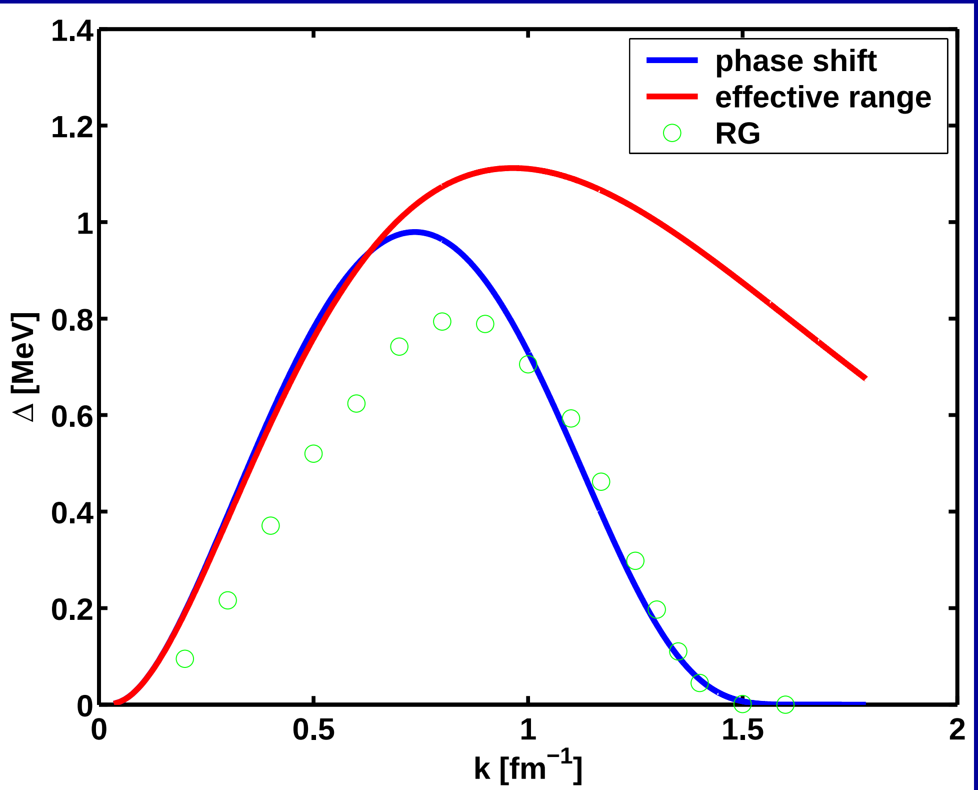


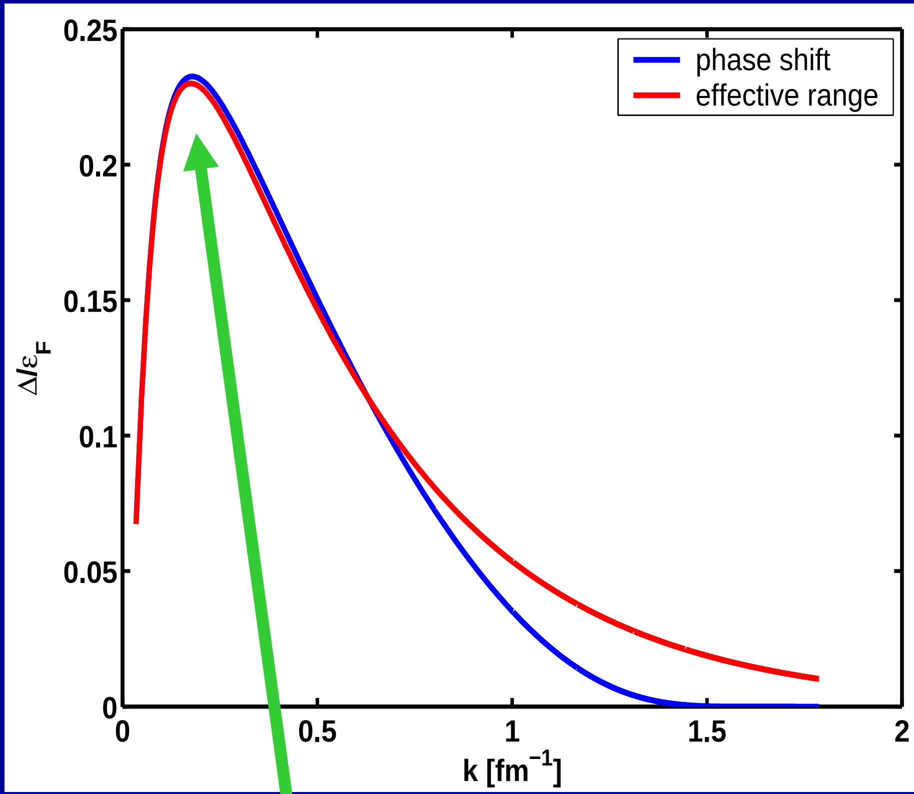


s-wave pairing gap in infinite neutron matter with realistic NN-interactions

from Lombardo and Schulze astro-ph/0012209

These are major effects beyond the naïve HFB when it comes to describing pairing correlations.





NB! Extremely high relative T_c

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

Corrected Emery formula (1960)

NN-phase shift

RG- renormalization group calculation

Schwenk, Friman, Brown, Nucl. Phys. A713, 191 (2003)

Vortex in neutron matter

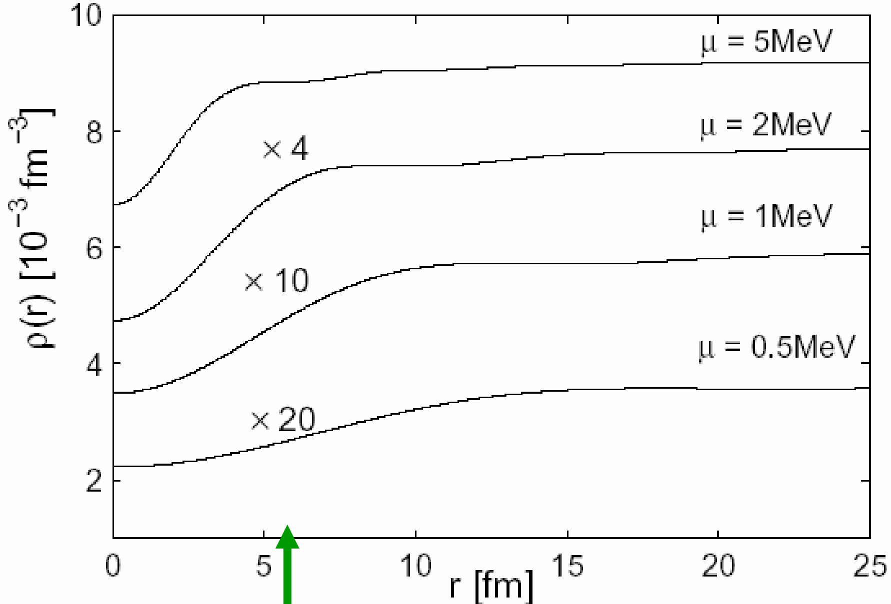
$$\begin{pmatrix} \mathrm{u}_{\alpha\,\mathrm{kn}}(\vec{r}) \\ \mathrm{v}_{\alpha\,\mathrm{kn}}(\vec{r}) \end{pmatrix} = \begin{pmatrix} \mathrm{u}_{\alpha}(r)\exp[i(n+1/2)\phi - ikz] \\ \mathrm{v}_{\alpha}(r)\exp[i(n-1/2)\phi - ikz] \end{pmatrix}, \quad \text{n - half-integer}$$

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

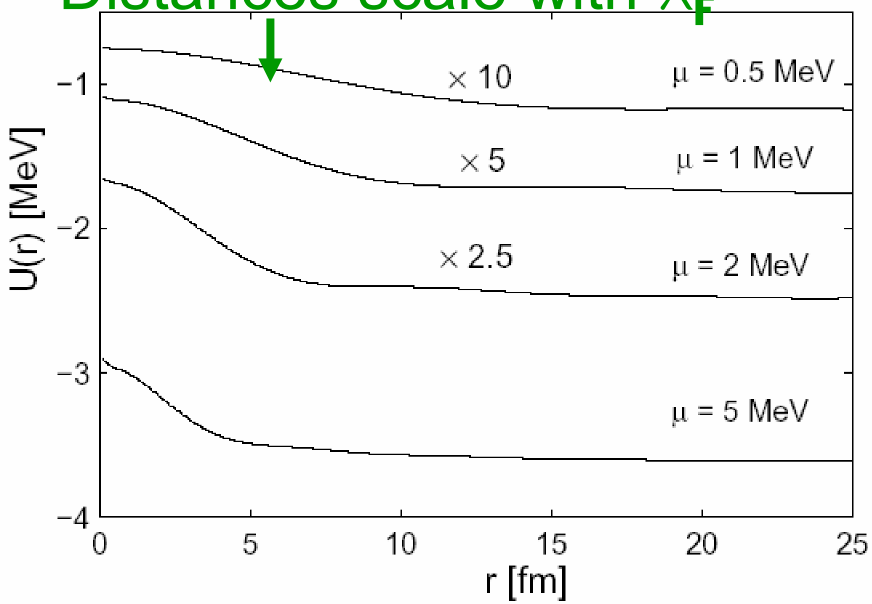
Oz - vortex symmetry axis

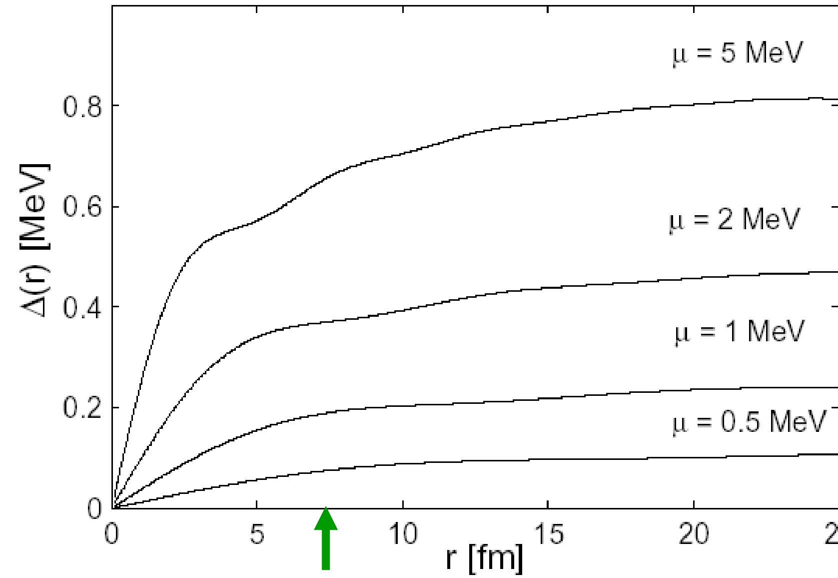
Ideal vortex, Onsager's quantization (one $\hbar$ per Cooper pair)

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

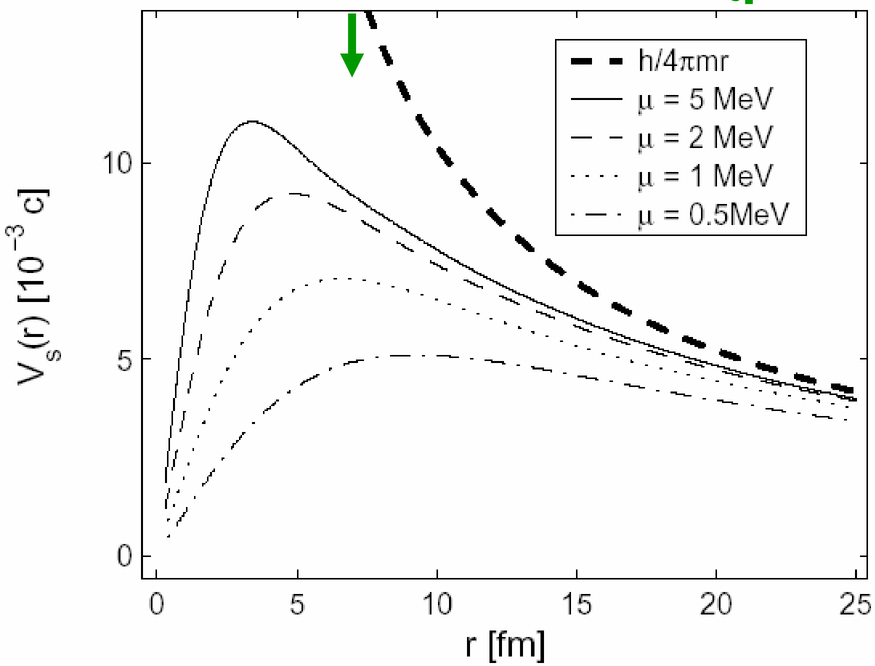


Distances scale with λ_F





Distances scale with ξ_F



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

- $\frac{v_S}{v_F} \leq \left.\frac{\Delta}{2\varepsilon_F}\right|_{max} \approx 0.12,$ extremely fast vortical motion,

  $\frac{\lambda_F}{\xi} \propto \frac{\Delta}{\varepsilon_F}$

- In low density region $\varepsilon(\rho_{out})\rho_{out} > \varepsilon(\rho_{in})\rho_{in}$

which thus leads to a large anti-pinning energy $E^V_{pin} > 0$:

$$E^V_{pin} = \left[\varepsilon(\rho_{out})\rho_{out} - \varepsilon(\rho_{in})\rho_{in}\right]V$$

- The energy per unit length is going to be changed dramatically

when compared to previous estimates, by

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

- 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).

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

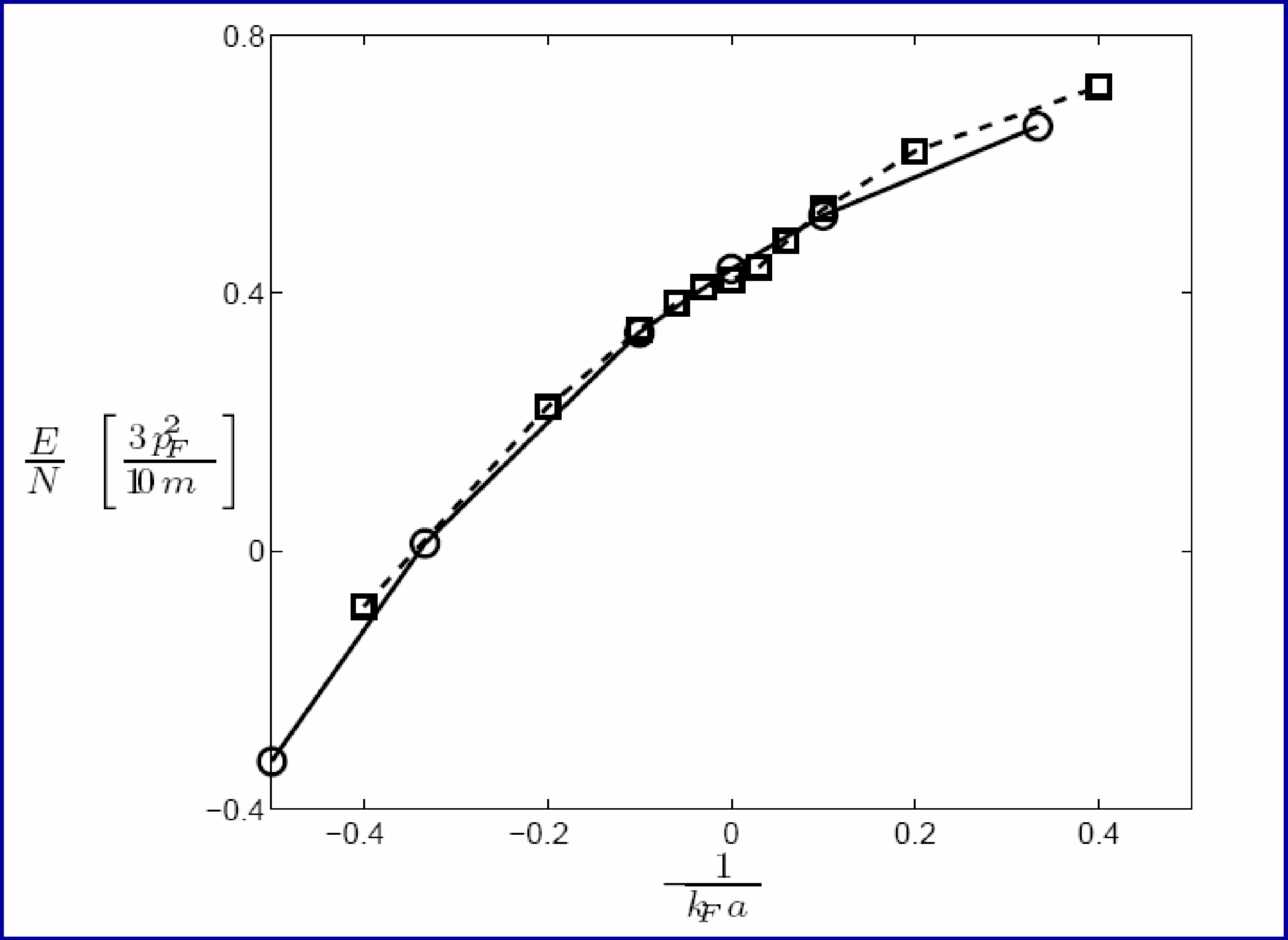
- Carlson, Chang, Pandharipande and Schmidt, PRL 91, 050401 (2003), with GFMC

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

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.

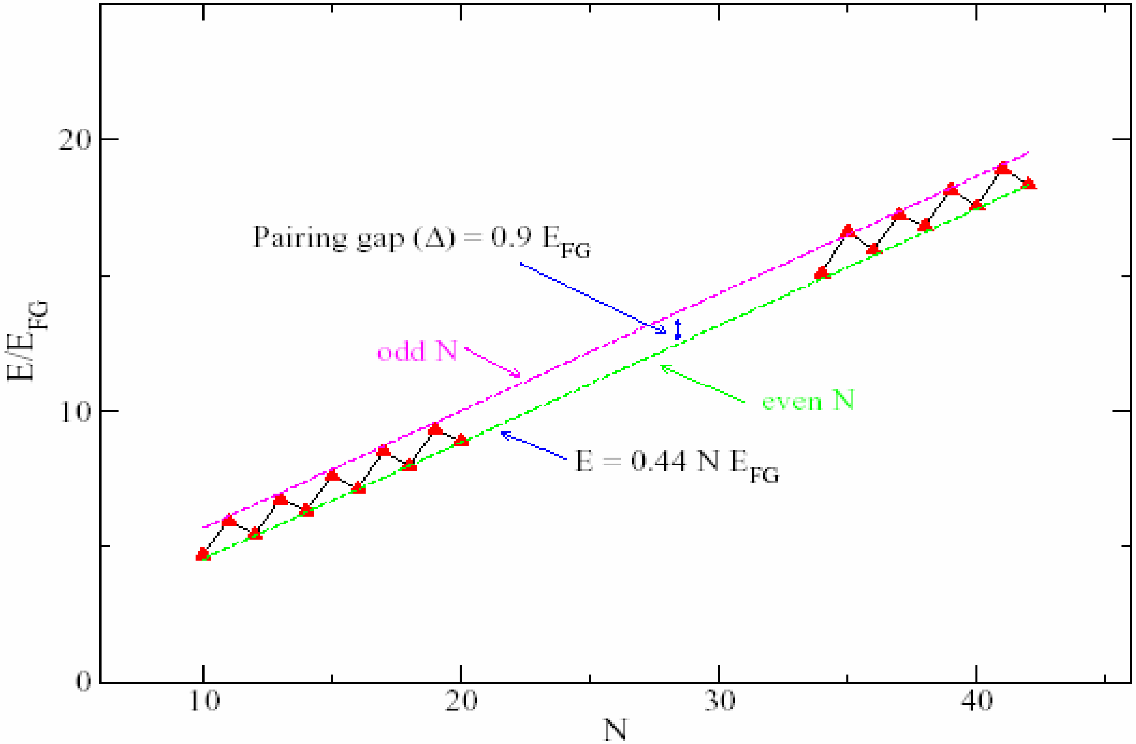
BEC side **BCS side**



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

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

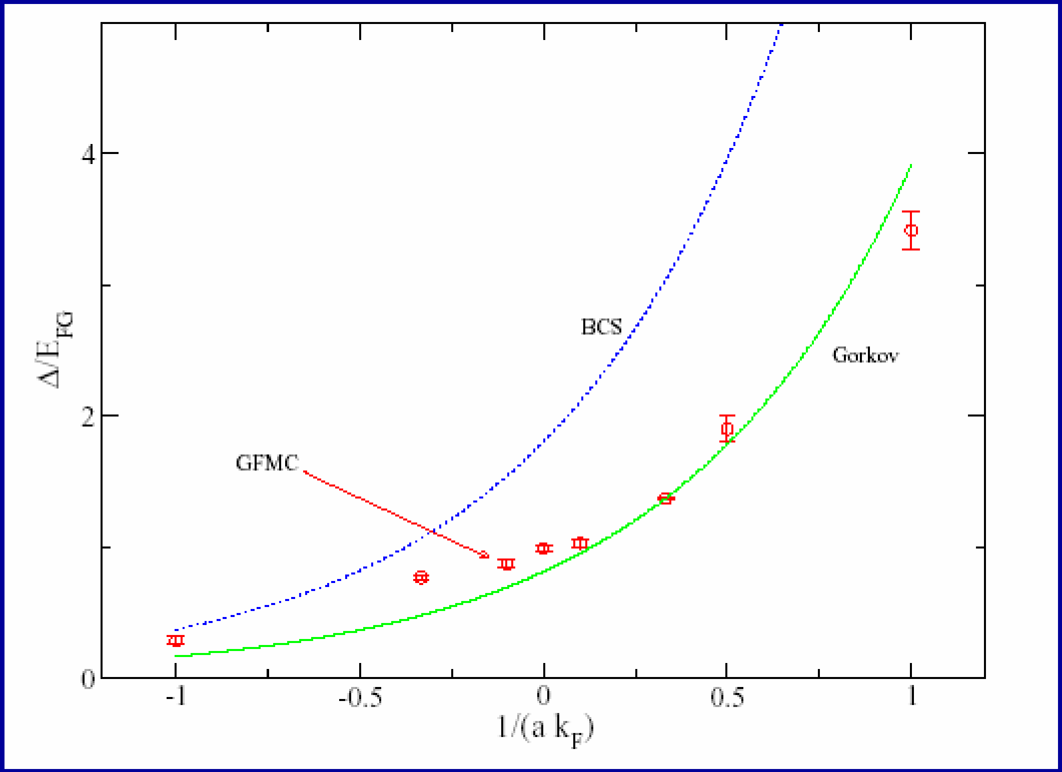
$$\Delta(2n+1) = E(2n+1) - \frac{1}{2}(E(2n) + E(2n+2))$$



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)

BCS $\rightarrow$BEC crossover

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

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

SLDA for dilute atomic Fermi gases

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

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

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

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

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

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!

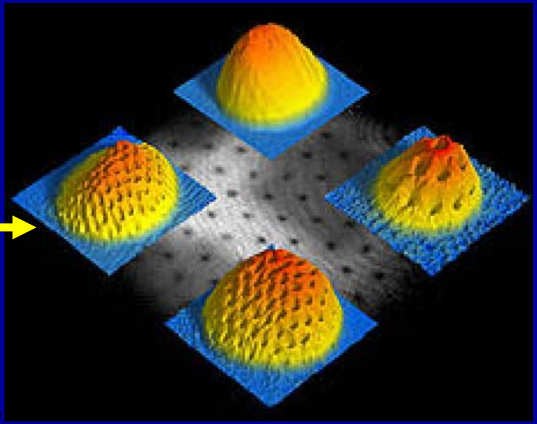
How can one put in evidence a vortex in a Fermi superfluid?

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!

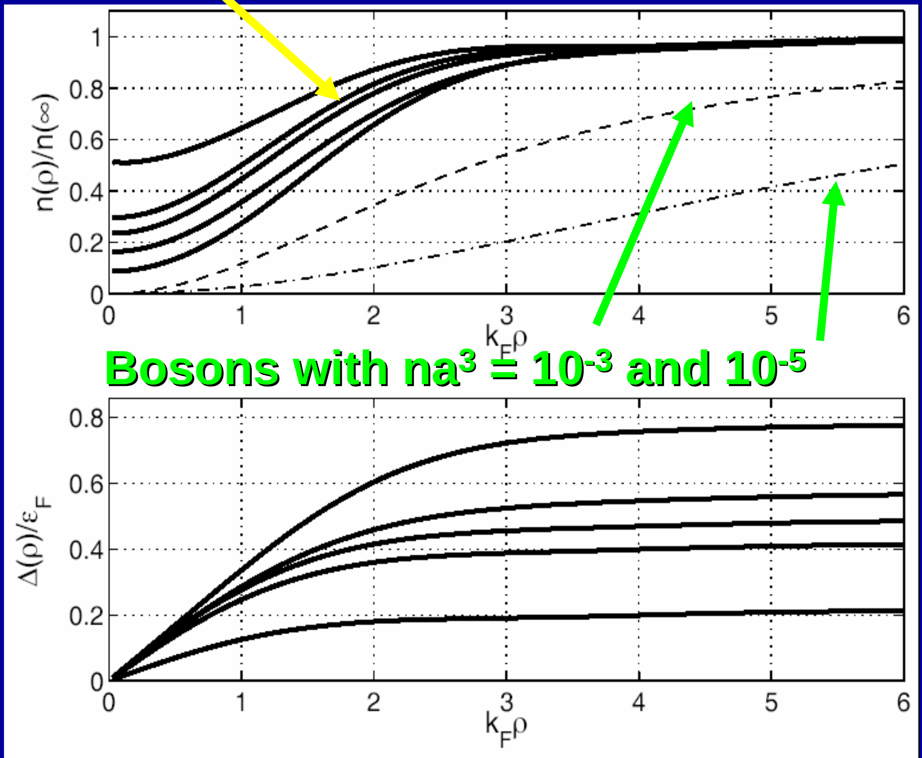
One can change the magnitude of the gap by altering the scattering length between two atoms with magnetic fields by means of a Feshbach resonance.

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.

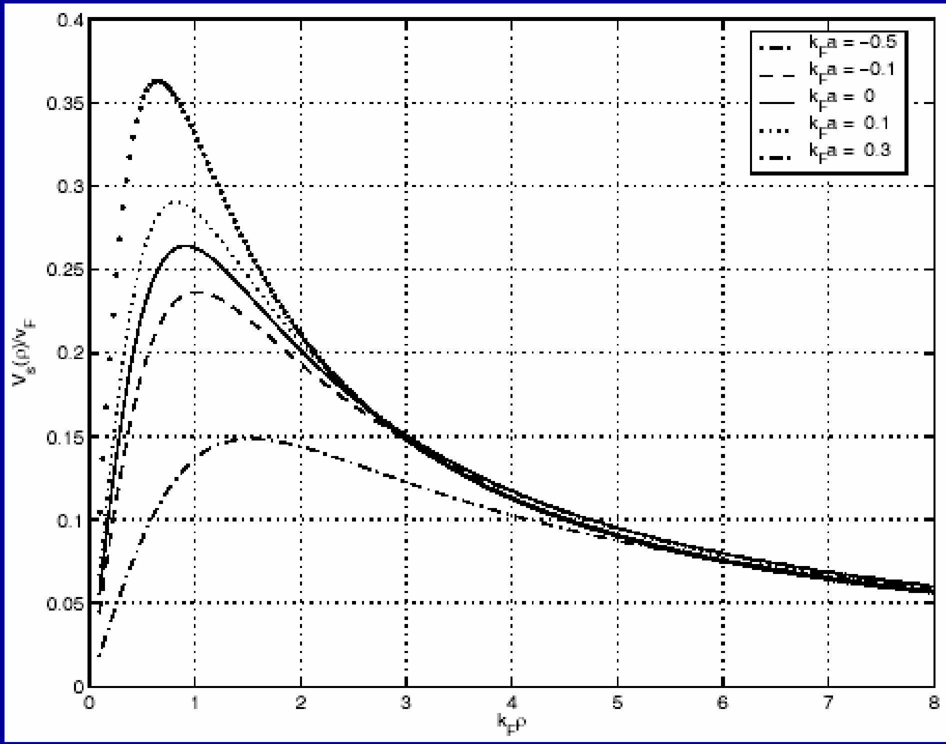


From Ketterle's group

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

- ✓ …
- ✓ …
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