Local Density Approximation for Systems with Pairing Correlations

Aurel Bulgac

collaborator/graduate student: Yongle Yu

Transparencies will be available shortly at
http://www.phys.washington.edu/~bulgac
There one can find also transparencies for related talks.

References

A. Bulgac and Y. Yu,	Phys. Rev. Lett. **88**, 0402504 (2002)
A. Bulgac,	Phys. Rev. C **65**, 051305(R) (2002)
A. Bulgac and Y. Yu,	nucl-th/0109083 (Lectures)
Y. Yu and A. Bulgac,	Phys. Rev. Lett. **90**, 222501 (2003)
Y. Yu and A. Bulgac,	nucl-th/0302007 (Appendix to PRL)
Y. Yu and A. Bulgac,	Phys. Rev. Lett. **90**, 161101 (2003)
A. Bulgac and Y. Yu,	cond-mat/0303235, submitted to PRL
Y. Yu,	PhD thesis (2003), almost done.
A. Bulgac and Y. Yu,	in preparation
A. Bulgac	in preparation

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 <u>very lame excuses</u>.
- **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-Ginsburg 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 <u>new qualitative features</u>, 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 **$1/(4e)^{1/3}$** ≈ 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!

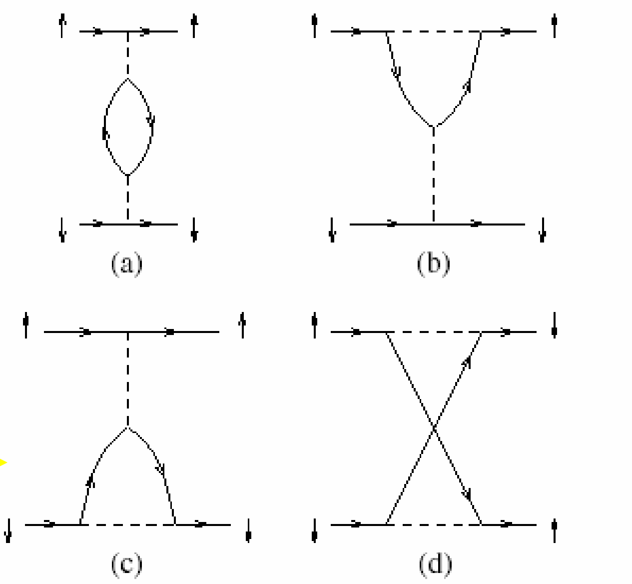
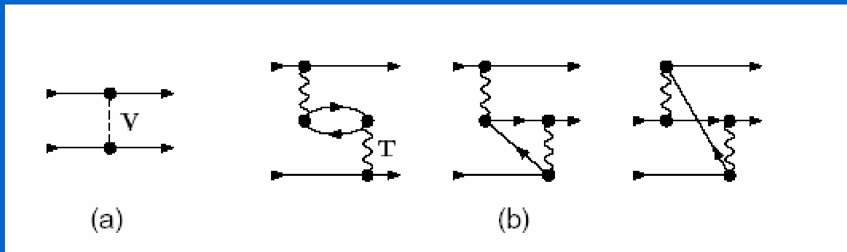
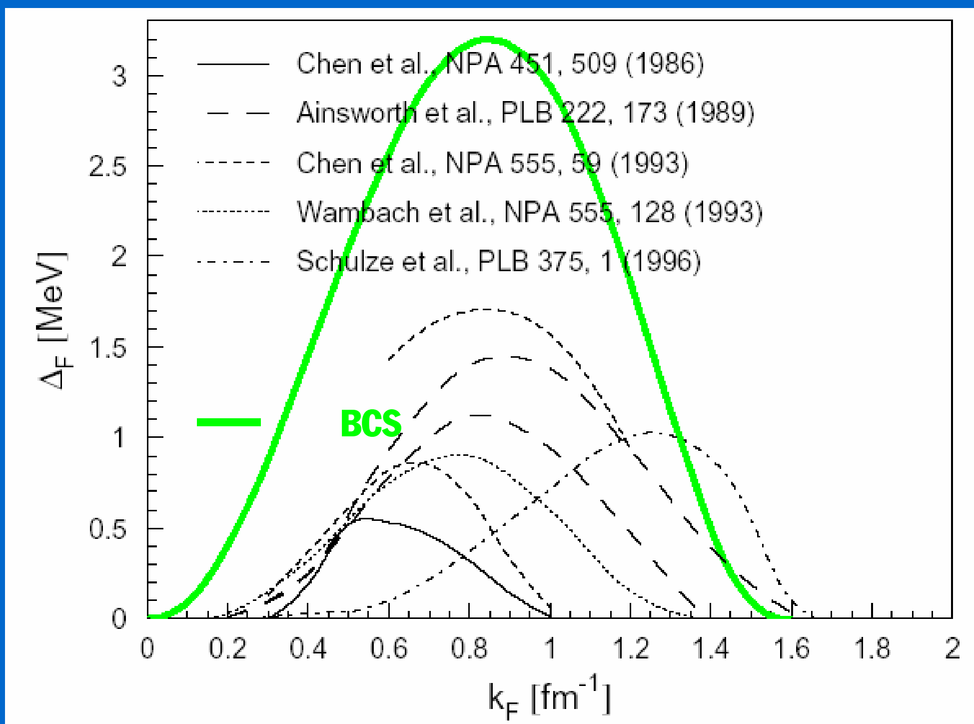


FIG. 1. Diagrams for the induced interactions between two fermions in different internal states to second order in the effective interaction.

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

"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.

LDA (Kohn-Sham) for superfluid fermi systems

(Bogoliubov-de Gennes equations)

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

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

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

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

Mean-field and pairing field are both local fields!

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

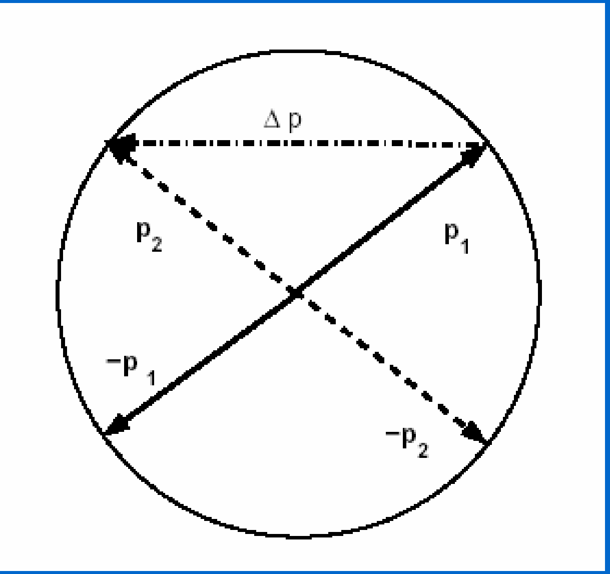
There is a little problem! The pairing field D diverges.

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   interparticle 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 (BCS model)

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

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

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

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)

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

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

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

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

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

The renormalized equations:

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

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

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

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

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

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

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

Typo: replace m by m(r)

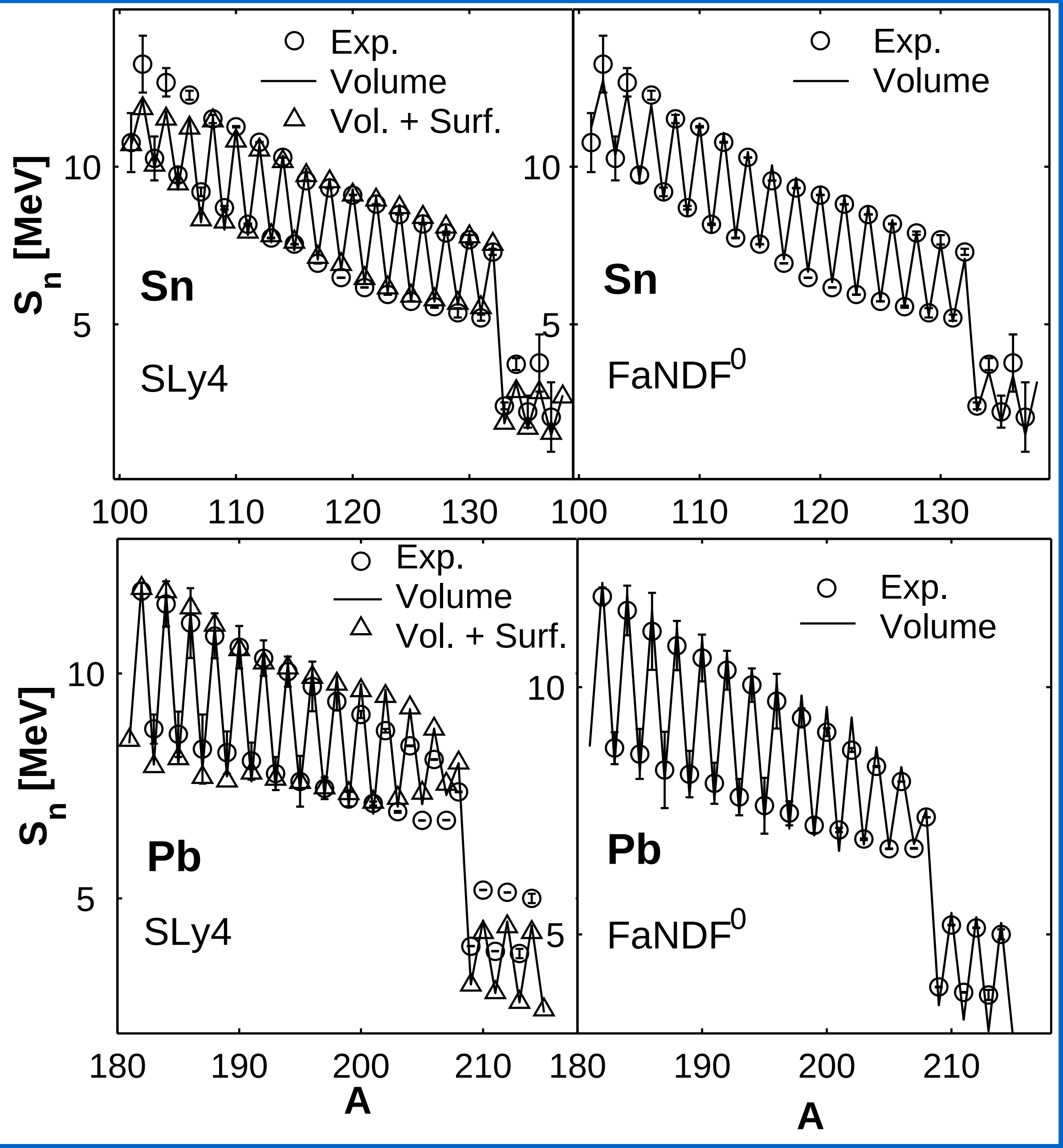
How well does the new approach work?

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

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

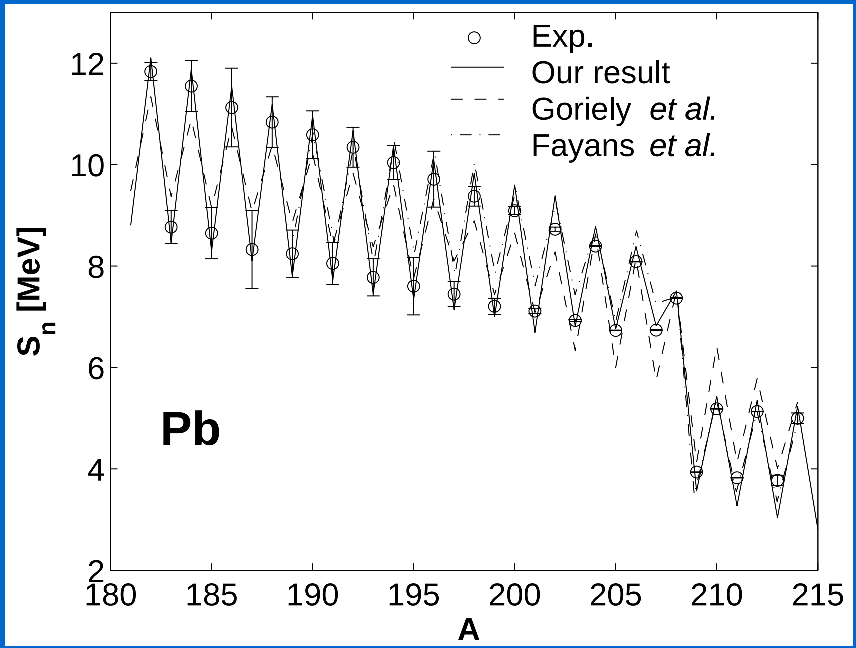
Volume + Surface pairing

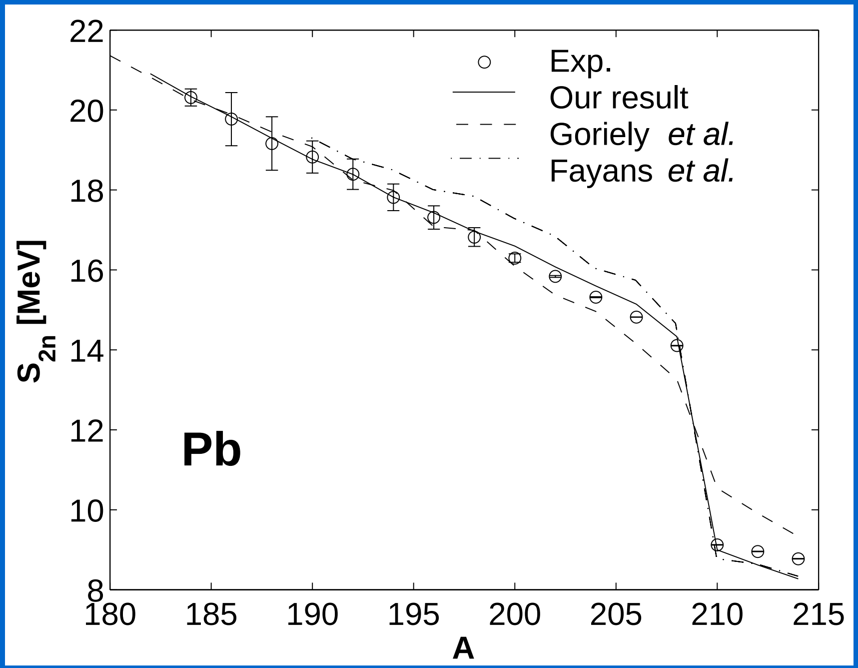
$$g(\vec{r}) = V_0\left(1 - \frac{\rho(\vec{r})}{\rho_c}\right)$$

Normal EDF:

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

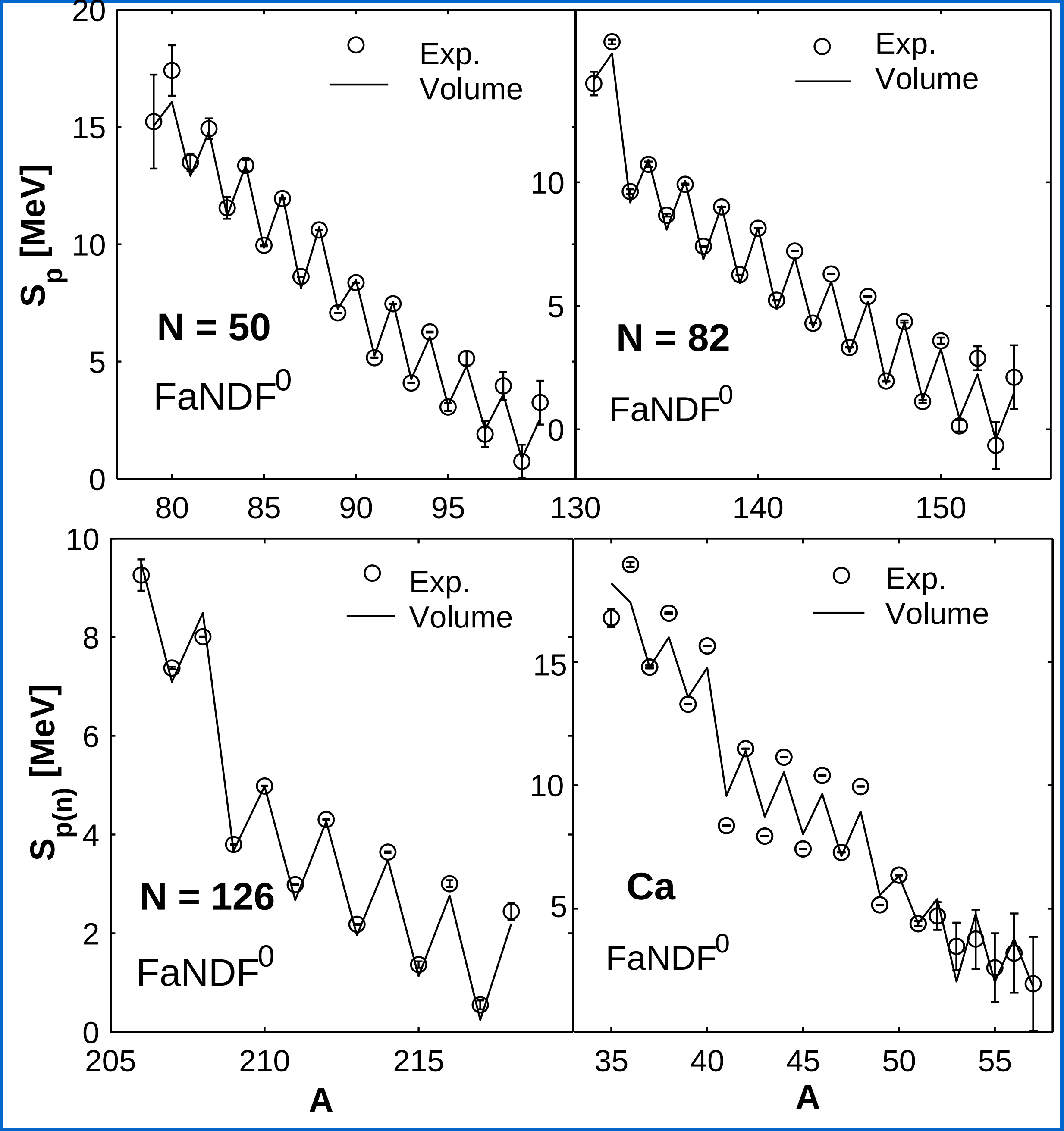
- FaNDF^0 –Fayans
JETP Lett. 68, 169 (1998)





- 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)

One-nucleon separation energies



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

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

$$\begin{cases} \varepsilon_N[\rho_n(\vec{r}), \rho_p(\vec{r})] = \varepsilon_N[\rho_p(\vec{r}), \rho_n(\vec{r})] \\ \varepsilon_S[\rho_n(\vec{r}), \rho_p(\vec{r}), \nu_n(\vec{r}), \nu_p(\vec{r})] = \varepsilon_S[\rho_p(\vec{r}), \rho_n(\vec{r}), \nu_p(\vec{r}), \nu_n(\vec{r})] \end{cases}$$

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 corrrelations are relatively weak.

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

g_0 and g_1 could depend as well on ρ_p and ρ_n

Let us stare at this part of the ED for a moment, … or two.

SU(2) invariant

?

$$\varepsilon_S\left[\nu_p,\nu_n\right]=g_0\,|\,\nu_p+\nu_n\,|^2+g_1\,|\,\nu_p-\nu_n\,|^2$$

$$=g\,[|\,\nu_p\,|^2+|\,\nu_n\,|^2]\;+\;g'\,[\nu_p^*\nu_n+\nu_n^*\nu_p]$$

$$g=g_0+g_1 \qquad g'=g_0-g_1$$

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.

- 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 $\propto |\nu_n|^2 |\nu_p|^2$

- 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:

$$\varepsilon_S\left[\nu_p,\nu_n\right]=g(\rho_p,\rho_n)[|\nu_p|^2+|\nu_n|^2]$$

$$+f(\rho_p,\rho_n)[|\nu_p|^2-|\nu_n|^2]\ \frac{\rho_p-\rho_n}{\rho_p+\rho_n}$$

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

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

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≥8) with an rms better than 0.7 MeV use for pairing couplings:

$$\left.\begin{aligned} V_{pp}^{+} &= -265.3\ \text{MeV} \\ V_{nn}^{+} &= -237.6\ \text{MeV} \end{aligned}\right\}\ \text{for even systems}$$

$$\left.\begin{aligned} V_{pp}^{-} &= -277.8\ \text{MeV} \\ V_{nn}^{-} &= -246.9\ \text{MeV} \end{aligned}\right\}\ \text{for odd systems}$$

$$E_c = 15\ \text{MeV} \qquad \text{cutoff energy}$$

While no other part of their nuclear EDF violates isospin symmetry, and moreover, while they where 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:

$$\varepsilon_S\left[\nu_p,\nu_n\right] = g[|\nu_p|^2 + |\nu_n|^2] + f[|\nu_p|^2 - |\nu_n|^2]\ \frac{\rho_p - \rho_n}{\rho_p + \rho_n}$$

$$\text{where} \quad \underbrace{f \approx -0.39\, g > 0}_{\text{repulsion}} \quad \text{and} \quad \underbrace{g < 0}_{\text{attraction}}$$

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

$$\varepsilon_S\left[\nu_p,\nu_n\right]=g(\rho_p,\rho_n)\,|\,\nu_p\,|^2+g(\rho_n,\rho_p)\,|\,\nu_n\,|^2$$

- ✓ **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 one can 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.

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**

- ✓ 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.