Towards incorporating nuclear pairing on an *ab initio* basis into the nuclear EDF

Aurel Bulgac
University of Washington

Outline:

- A few words about UNEDF
- Very brief/skewed summary of DFT
- Superfluid Local Density Approximation (SLDA) and application for a unitary Fermi gas
- Challenges towards implementation of SLDA in nuclei

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

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- What is UNEDF?
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- Collaborator Access
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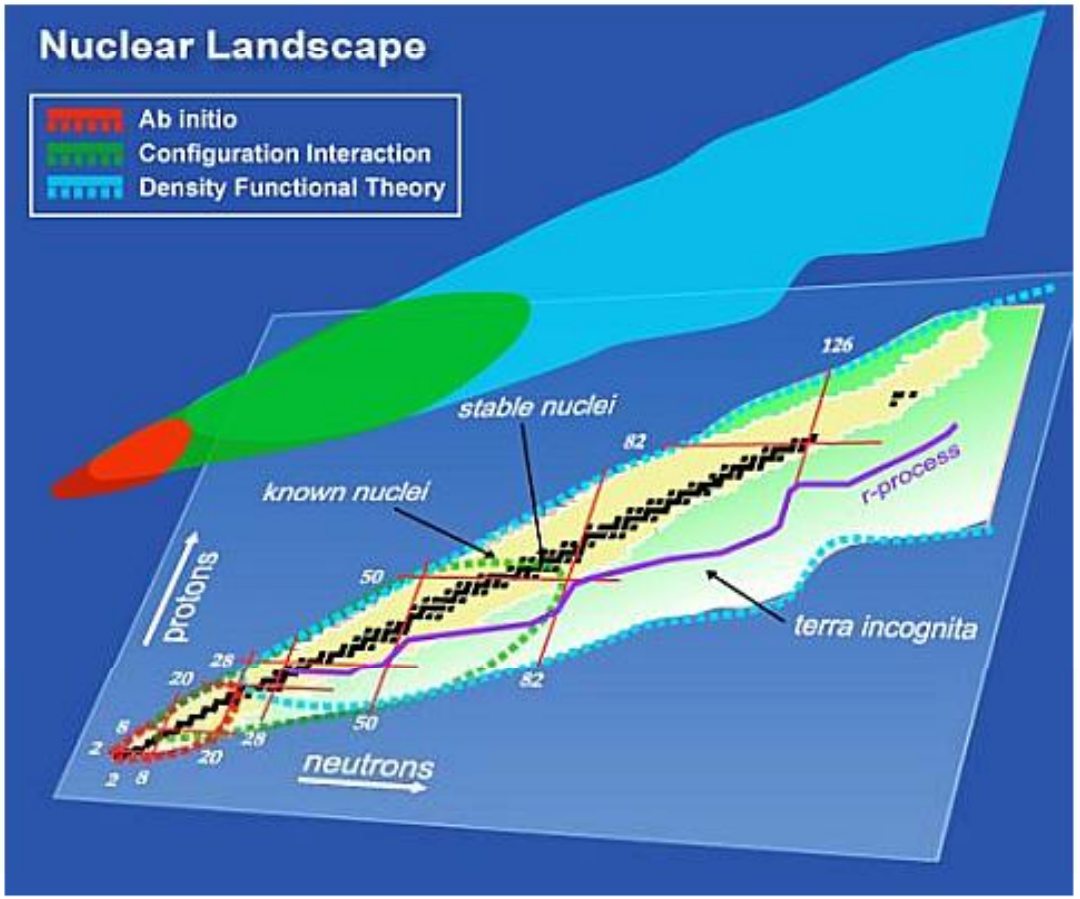
- Council Meetings



http://www.unedf.org

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UNEDF Research Areas

UNEDF has assembled a team of researchers who represent a wide range of intellectual resources, spanning multiple areas of physics, mathematics, and computer science. The main physics areas of UNEDF are:

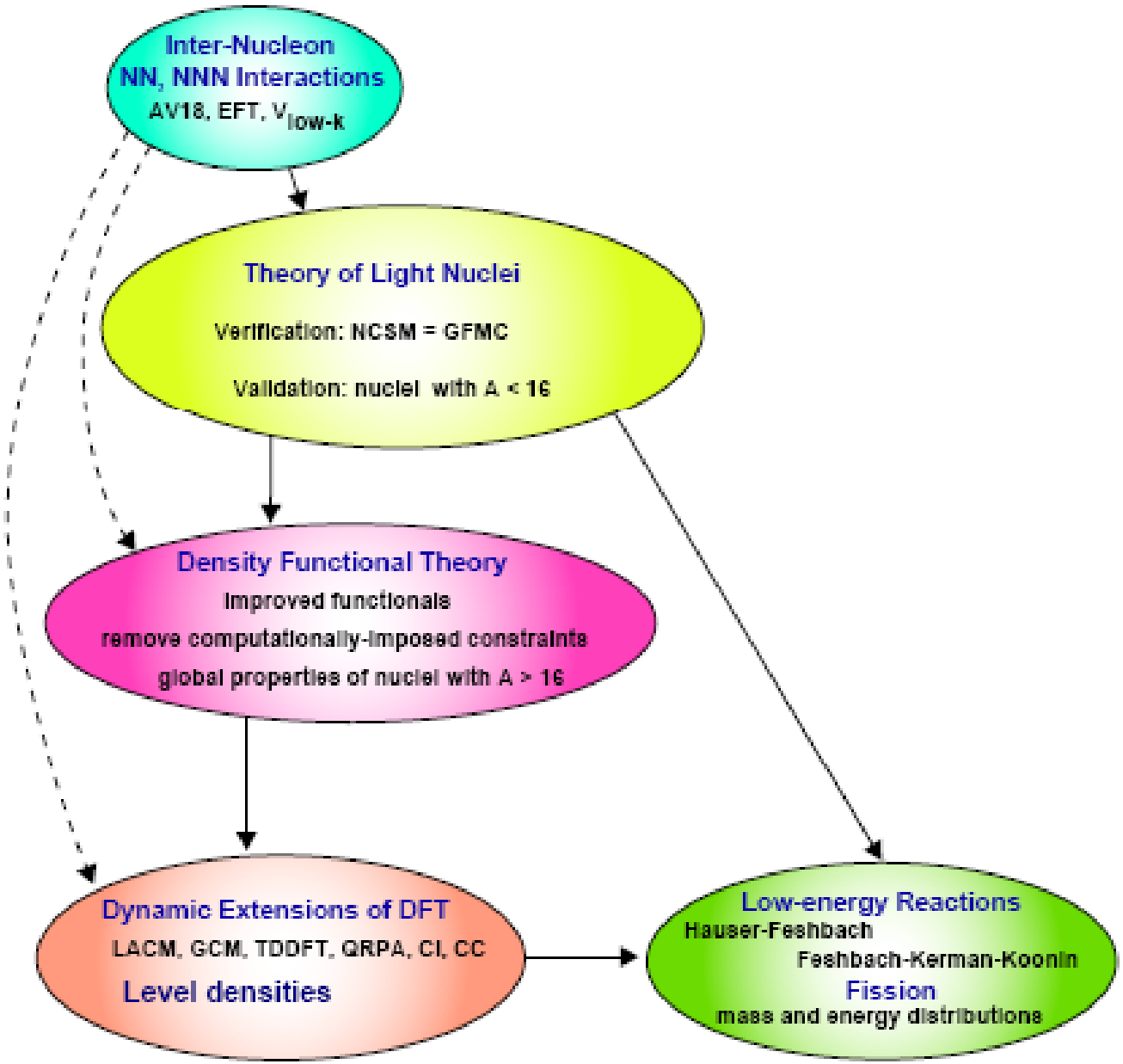
- Ab initio structure
- Ab initio functionals
- DFT applications
- DFT extensions
- Reactions
- Computer Science and Applied Mathematics

In order to ensure the close alignment of the necessary applied mathematics and computer science research with the necessary physics research, partnerships have been formed consisting of computer scientists and mathematicians llinked with specific physicists. In each partnership, the mathematician/computer scientist is addressing a research topic in order to remove a specific barier to progress on the computational/algorithmic physics side.

Ab initio structure

The starting point of nuclear theory is the two-nucleon interaction. Several interactions already in use satisfy the criterion of fitting the two-nucleon

Universal Nuclear Energy Density Functional



Very brief/skewed summary of DFT

Kohn-Sham theorem

$$H = \sum_{i}^{N} T(i) + \sum_{i<j}^{N} U(ij) + \sum_{i<j<k}^{N} U(ijk) + \ldots + \sum_{i}^{N} V_{ext}(i)$$

$$H\Psi_0(1,2,\ldots N) = E_0\Psi_0(1,2,\ldots N)$$

$$n(\vec{r}) = \left\langle \Psi_0 \middle| \sum_{i}^{N} \delta(\vec{r} - \vec{r}_i) \middle| \Psi_0 \right\rangle$$

Injective map (one-to-one)

$$\Psi_0(1,2,\ldots N) \quad \Leftrightarrow \quad V_{ext}(\vec{r}) \quad \Leftrightarrow \quad n(\vec{r})$$

$$E_0 = \min_{n(\vec{r})} \int d^3r \left\{ \frac{\hbar^2}{2m}\tau(\vec{r}) + \varepsilon\left[n(\vec{r})\right] + V_{ext}(\vec{r})n(\vec{r}) \right\}$$

$$n(\vec{r}) = \sum_{i}^{N} \left|\varphi_i(\vec{r})\right|^2, \qquad \tau(\vec{r}) = \sum_{i}^{N} \left|\vec{\nabla}\varphi_i(\vec{r})\right|^2$$

Universal functional of particle density alone

Independent of external potential

How to construct and validate an *ab initio* EDF?

- ❑ **Given a many body Hamiltonian determine the properties of the infinite homogeneous system as a function of density**
- ❑ **Extract the energy density functional (EDF)**
- ❑ **Add gradient corrections, if needed or known how (?)**
- ❑ **Determine in an *ab initio* calculation the properties of a select number of wisely selected finite systems**
- ❑ **Apply the energy density functional to inhomogeneous systems and compare with the *ab initio* calculation, and if lucky declare Victory!**

Extended Kohn-Sham equations

Position dependent mass

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

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

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

Normal Fermi systems only!

However, not everyone is normal!

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)

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

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

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

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

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

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 densities ν and τ diverges!

The SLDA (renormalized) equations

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

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

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

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

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

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

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

Position and momentum dependent running coupling constant

Observables are independent of cut-off energy (when chosen properly).

Superfluid Local Density Approximation (SLDA) for a unitary Fermi gas

What is a unitary Fermi gas and why consider such a system?

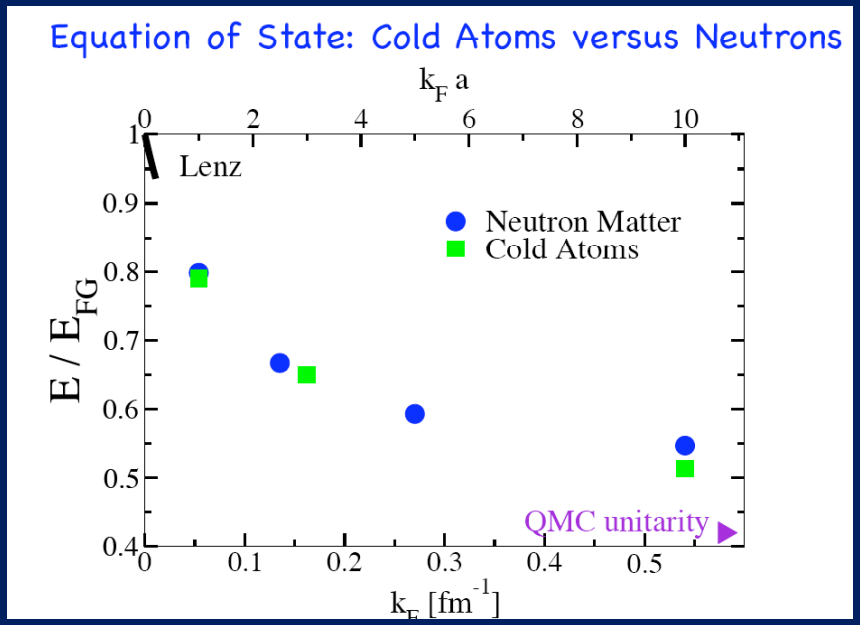
Bertsch Many-Body X challenge, Seattle, 1999

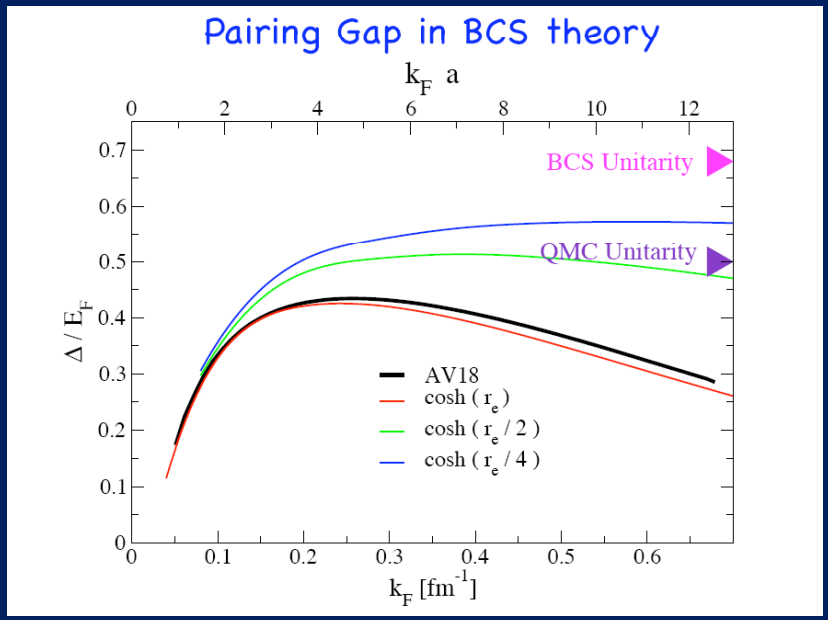
What are the ground state properties of the many-body system composed of spin ½ fermions interacting via a zero-range, infinite scattering-length contact interaction.

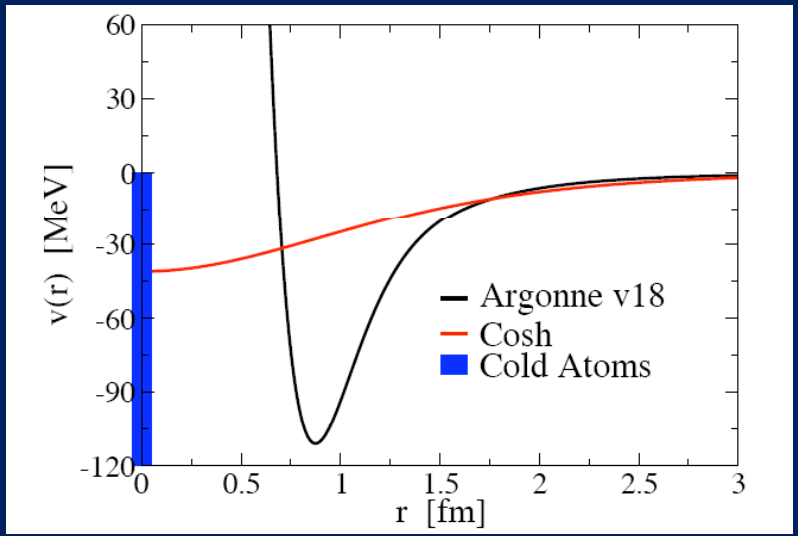
$$|a| \gg \lambda_F \gg r_0$$

In 1999 it was not yet clear, <u>either theoretically or experimentally</u>, whether such fermionic matter is stable or not.

Why a unitary gas?

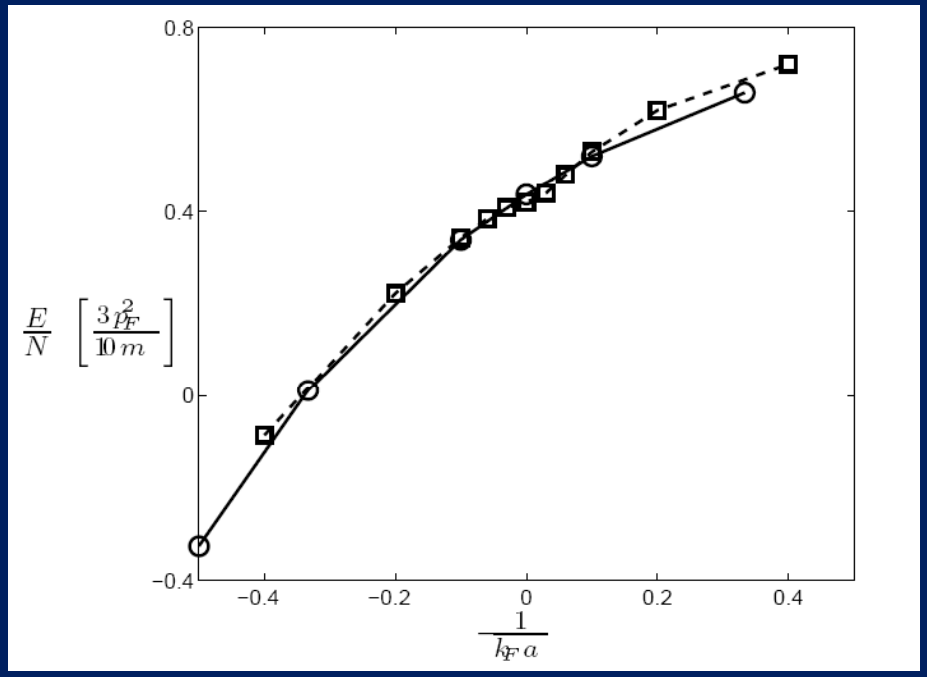


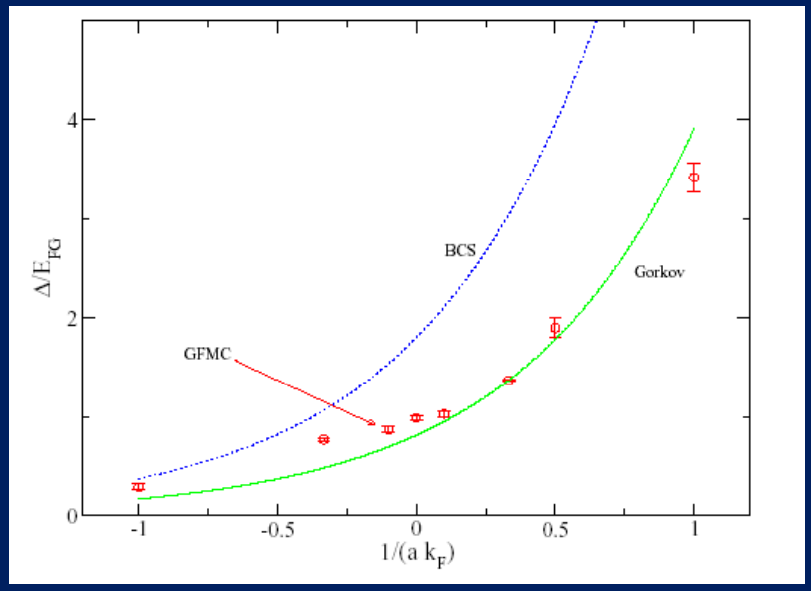




From a talk of J. Carlson, Pack Forrest, WA, August 2007

BEC side BCS side





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

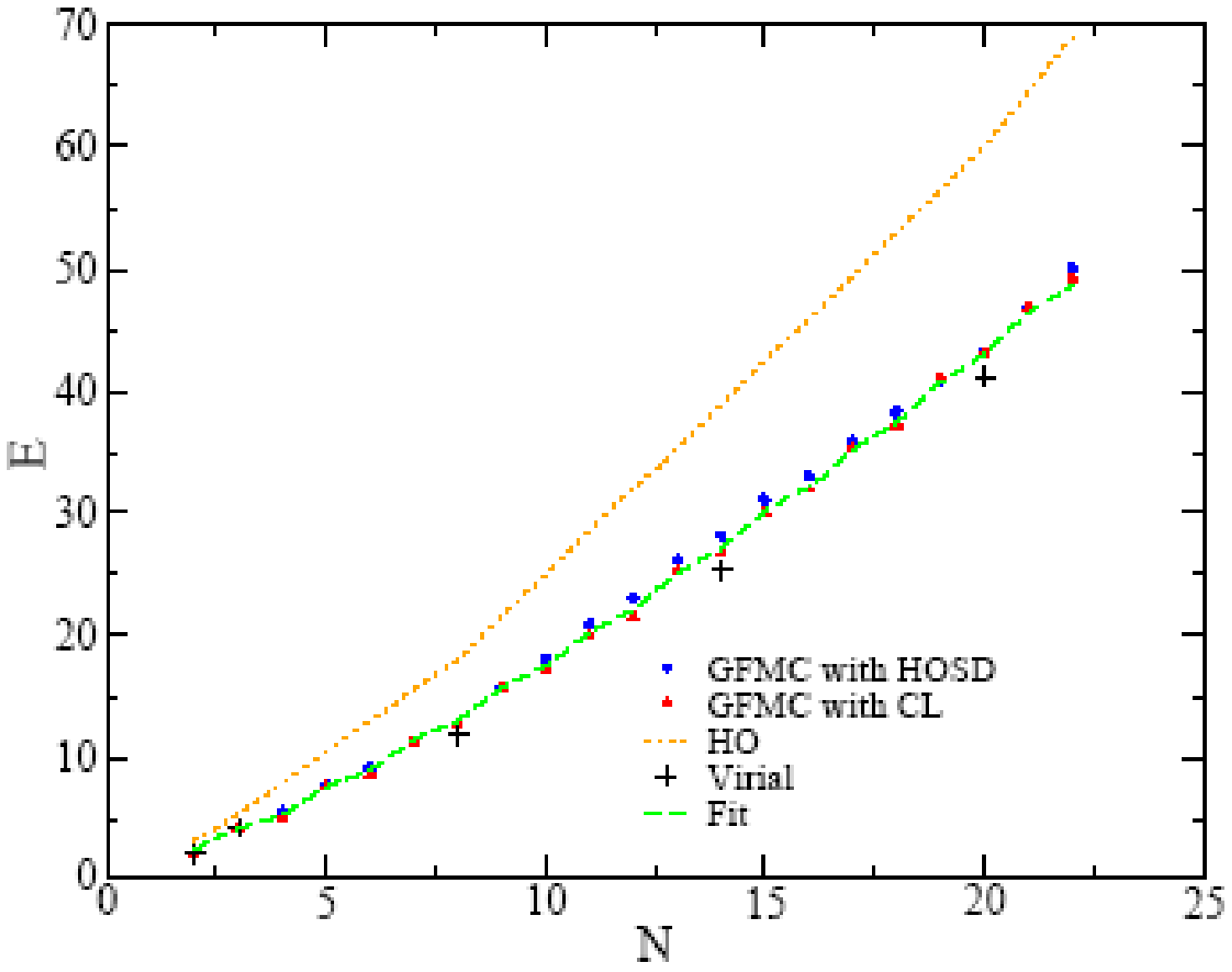
$$\Delta_{BCS} = \frac{8}{e^2} \frac{\hbar^2 k_F^2}{2m} \exp\left(\frac{\pi}{2k_F a}\right)$$

open circles – Chang *et al.* PRA, 70, 043602 (2004)
squares - Astrakharchik *et al.* PRL 93, 200404 (2004)

FN-GFMC, S.-Y. Chang *et al.* PRA 70, 043602 (2004)

Unitary Fermi gas in a harmonic trap

Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)



The renormalized SLDA energy density functional

Only this combination is cutoff independent

$$\varepsilon(\vec{r}) = \left[\alpha\frac{\tau_c(\vec{r})}{2} - \Delta(\vec{r})\nu_c(\vec{r})\right] + \beta\frac{3(3\pi^2)^{2/3}n^{5/3}(\vec{r})}{5}$$

$$n(\vec{r}) = 2\sum_k \left|\mathrm{v}_\mathrm{k}(\vec{r})\right|^2, \quad \tau_c(\vec{r}) = 2\sum_{E<E_c}\left|\vec{\nabla}\mathrm{v}_\mathrm{k}(\vec{r})\right|^2, \quad \nu_c(\vec{r}) = \sum_{E<E_c}\mathrm{u}_\mathrm{k}(\vec{r})\mathrm{v}_\mathrm{k}^*(\vec{r})$$

$$\frac{1}{g_{eff}(\vec{r})} = \frac{n^{1/3}(\vec{r})}{\gamma} - \frac{k_c(\vec{r})}{2\pi^2\alpha}\left[1 - \frac{k_0(\vec{r})}{2k_c(\vec{r})}\ln\frac{k_c(\vec{r})+k_0(\vec{r})}{k_c(\vec{r})-k_0(\vec{r})}\right]$$

$$E_c + \mu = \alpha\frac{k_c^2(\vec{r})}{2} + U(\vec{r}), \qquad \mu = \alpha\frac{k_0^2(\vec{r})}{2} + U(\vec{r})$$

$$U(\vec{r}) = \beta\frac{(3\pi^2)^{2/3}n^{2/3}(\vec{r})}{2} - \frac{\left|\Delta(\vec{r})\right|^2}{3\gamma n^{2/3}(\vec{r})} + V_{ext}(\vec{r}) + \text{small correction}$$

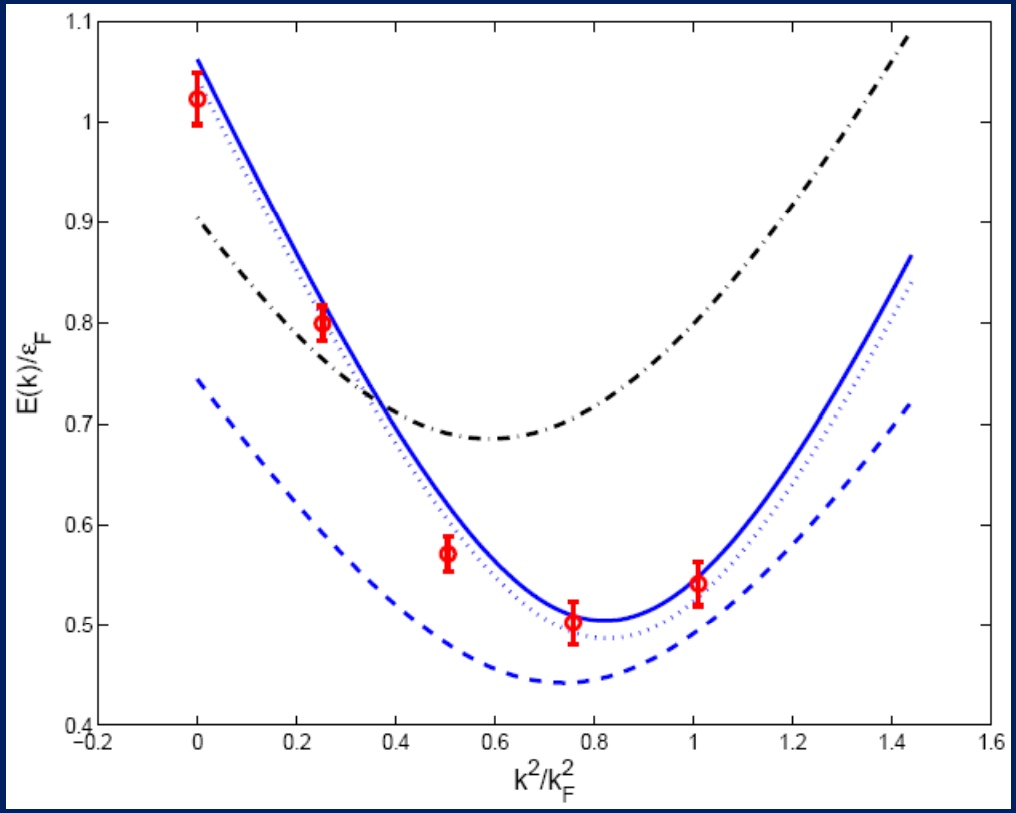
$$\Delta(\vec{r}) = -g_{eff}(\vec{r})\nu_c(\vec{r})$$

Parameters defining SLDA functional for a unitary gas:

$$\begin{cases} \xi_s = \dfrac{5E}{3N\varepsilon_F} = 0.42(2) \\ \eta = \dfrac{\Delta}{\varepsilon_F} = 0.504(24) \\ \varsigma = \dfrac{\mu}{\varepsilon_F} = 0.42(2) \end{cases} \Rightarrow \begin{cases} \alpha = 1.14 \\ \beta = -0.553 \\ \dfrac{1}{\gamma} = -0.0906 \end{cases}$$

Bonus!

Quasiparticle spectrum in homogeneous matter



solid/dotted blue line - SLDA, homogeneous GFMC due to Carlson et al
red circles - GFMC due to Carlson and Reddy
dashed blue line - SLDA, homogeneous MC due to Juillet
black dashed-dotted line - meanfield at unitarity

Extra Bonus!

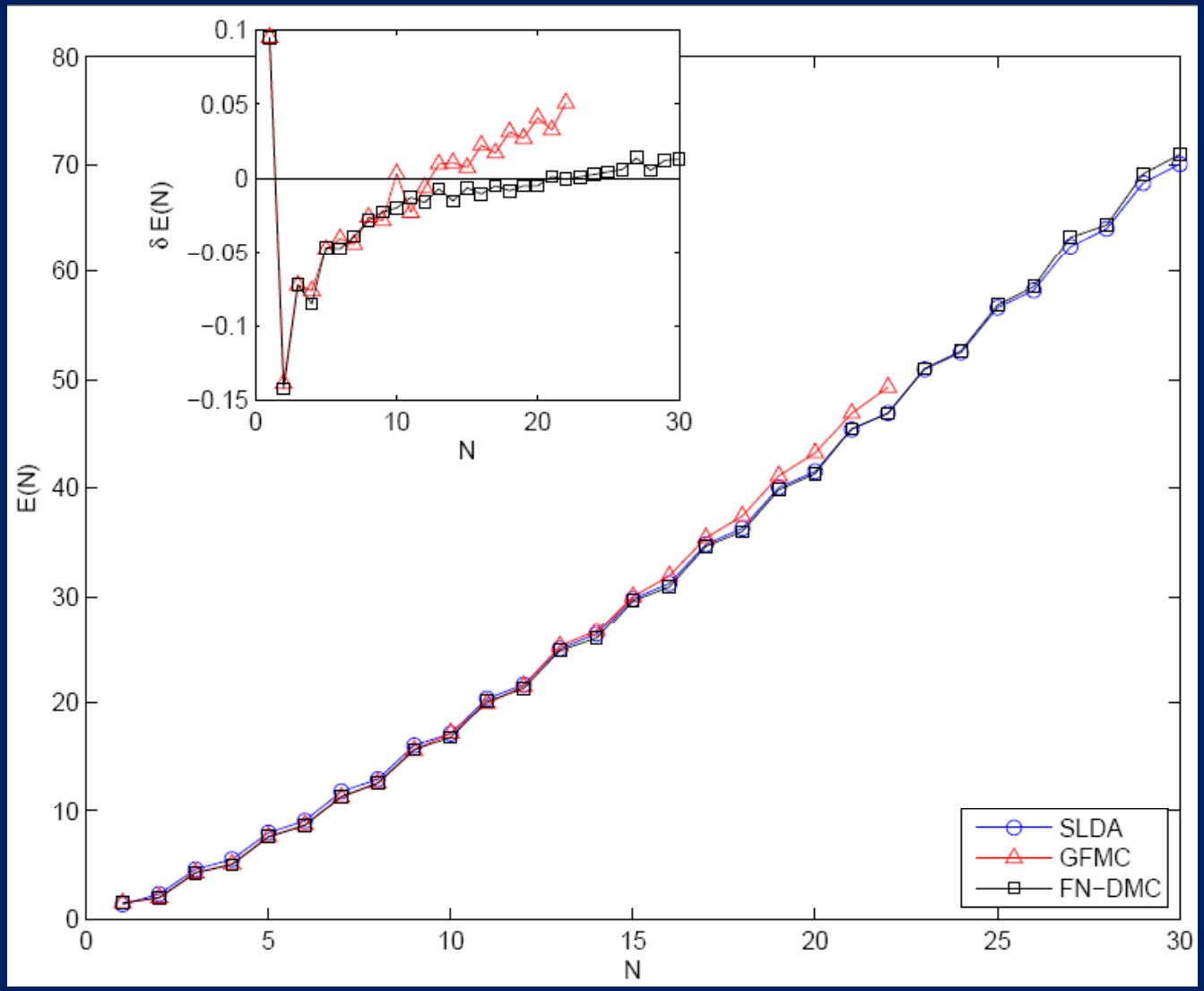
The normal state has been also determined in GFMC

$$\xi_N = \frac{5E}{3N\varepsilon_F} = 0.55(2)$$

SLDA functional predicts

$$\xi_N = \alpha + \beta = 0.59$$

Fermions at unitarity in a harmonic trap



GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)

FN-DMC - von Stecher, Greene and Blume, PRL 99, 233201 (2007)

PRA 76, 053613 (2007)

TABLE I: Table I. The energies $E(N)$ calculated within the GFMC [14], FN-DMC [15] and SLDA. When two numbers are present the first was calculated as the expectation value of the Hamiltonian/functional, while the second is the value obtained using the virial theorem, namely $E(N) = m\omega^2 \int d^3r n(\mathbf{r}) r^2$ [23].

N	E_{GFMC}	E_{FN-DMC}	E_{SLDA}
1	1.5		1.37
2	2.01/1.95	2.002	2.33/2.34
3	4.28/4.19		4.62/4.62
4	5.10	5.069	5.52/5.56
5	7.60		7.98/8.02
6	8.70	8.67	9.07/9.14
7	11.3		11.83/11.91
8	12.6/11.9	12.57	12.94/13.06
9	15.6		16.06/16.20
10	17.2	16.79	17.15/17.33
11	19.9		20.36/20.56
12	21.5	21.26	21.63/21.88
13	25.2		24.96/25.23
14	26.6/26.0	25.90	26.32/26.65
15	30.0		29.78/30.14
16	31.9	30.92	31.21/31.62
17	35.4		34.81/35.26
18	37.4	36.00	36.27/36.78
19	41.1		40.02/40.58
20	43.2/40.8	41.35	41.51/42.12
21	46.9		45.42/46.10
22	49.3		46.92/47.64

NB Particle projection neither required nor needed in SLDA!!!

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

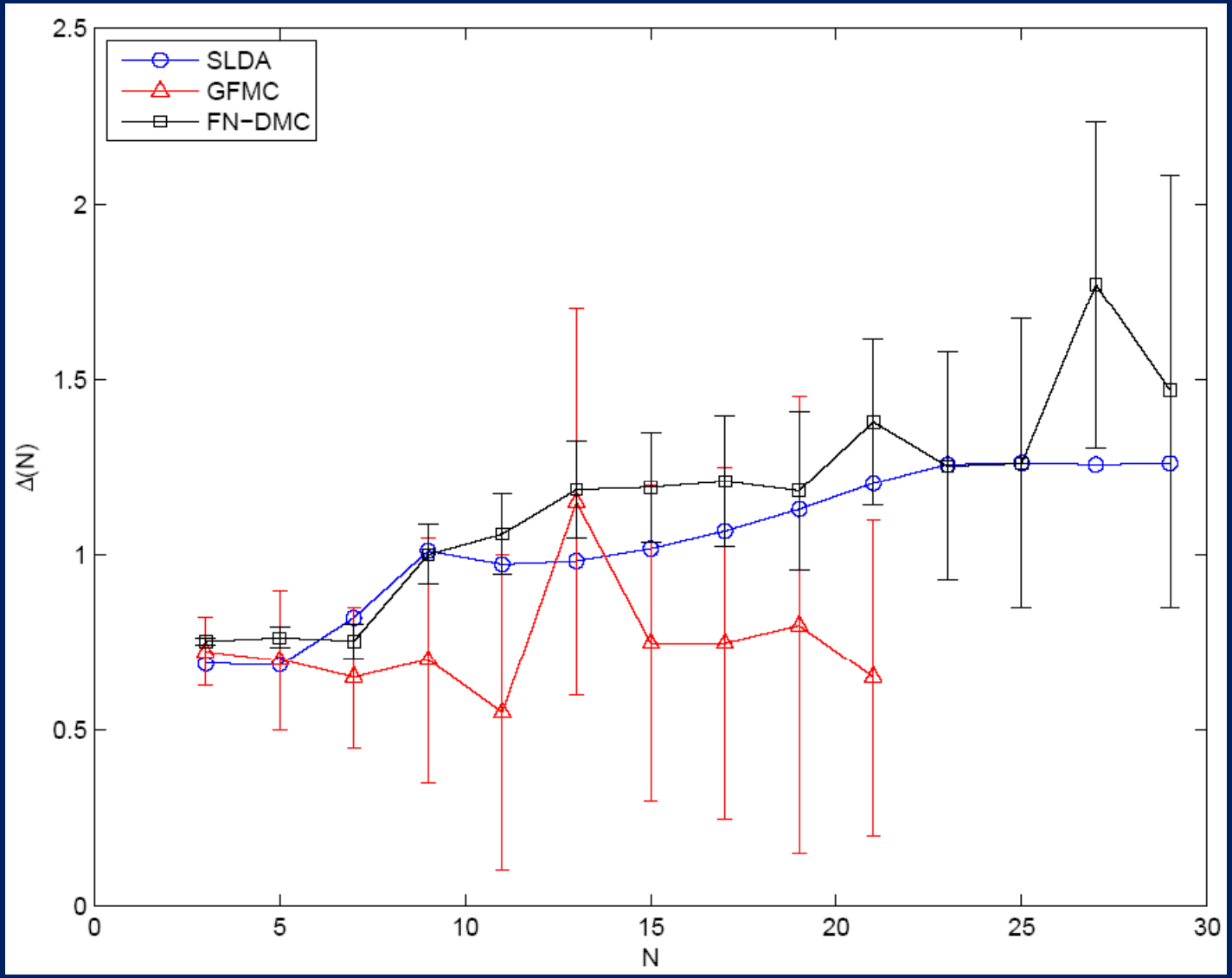
$$E_{gs} = \int d^3r \Big\{ \varepsilon(n(\vec{r}), \tau(\vec{r}), \nu(\vec{r})) + V_{ext}(\vec{r}) n(\vec{r}) + \Delta_{ext}(\vec{r}) \nu(\vec{r}) + \Delta^*_{ext}(\vec{r}) \nu^*(\vec{r}) \Big\}$$

universal functional
(independent of external potential)

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

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

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



GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)

FN-DMC - von Stecher, Greene and Blume, PRL 99, 233201 (2007)

PRA 76, 053613 (2007)

- **Agreement between GFMC/FN-DMC and SLDA extremely good, a few percent (at most) accuracy**

Why not better?
A better agreement would have really signaled big troubles!

- **Energy density functional is not unique,**
in spite of the strong restrictions imposed by unitarity

- **Self-interaction correction neglected**
smallest systems affected the most

- **Absence of polarization effects**
spherical symmetry imposed, odd systems mostly affected

- **Spin number densities not included**
extension from SLDA to SLSD(A) needed
***ab initio* results for asymmetric system needed**

- **Gradient corrections not included, … but very likely small!!!**

Challenges towards implementation of SLDA in nuclei

JETP LETTERS VOLUME 68, NUMBER 3 10 AUGUST 1998

Towards a universal nuclear density functional

S. A. Fayans
Kurchatov Institute Russian Science Center, 123182 Moscow, Russia

The total energy density of a nuclear system is represented as

$$\varepsilon = \varepsilon_{\rm kin} + \varepsilon_v + \varepsilon_s + \varepsilon_{\rm Coul} + \varepsilon_{sl} + \varepsilon_{\rm anom}, \qquad (1)$$

where $\varepsilon_{\rm kin}$ is the kinetic energy term which, since we are constructing a Kohn–Sham type functional, is taken with the free operator $t = p^2/2m$, i.e., with the effective mass $m^* = m$; all the other terms are discussed below.

The volume term in (1) is chosen to be in the form

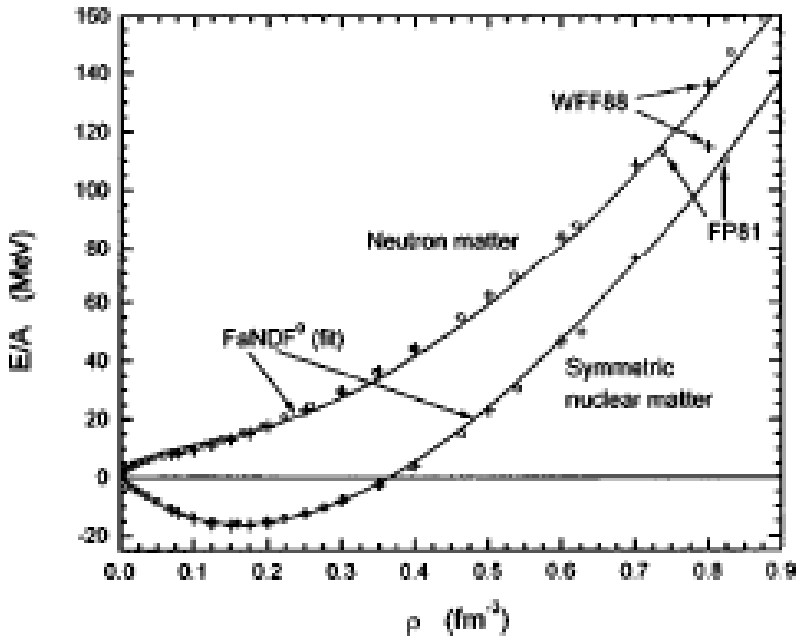
$$\varepsilon_v = \frac{2}{3}\epsilon_F^0 \rho_0 \left[a_+^v \frac{1 - h_{1+}^v x_+^\sigma}{1 + h_{2+}^v x_+^\sigma} x_+^2 + a_-^v \frac{1 - h_{1-}^v x_+}{1 + h_{2-}^v x_+} x_-^2 \right].$$

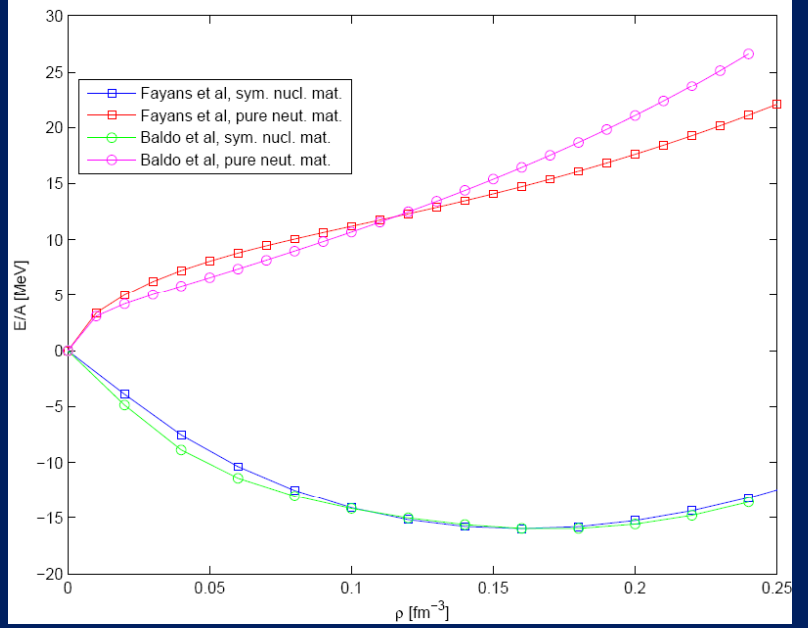
Here and in the following $x_\pm = (\rho_n \pm \rho_p)/2\rho_0$, $\rho_{n(p)}$ is the neutron ($2\rho_0$ is the equilibrium density of symmetric nuclear matter wit

The surface part in Eq. (1) is meant to describe the finite-range and nonlocal in-medium effects which may presumably be incorporated phenomenologically within the EDF framework in a localized form by introducing a dependence on density gradients. It is taken as follows:

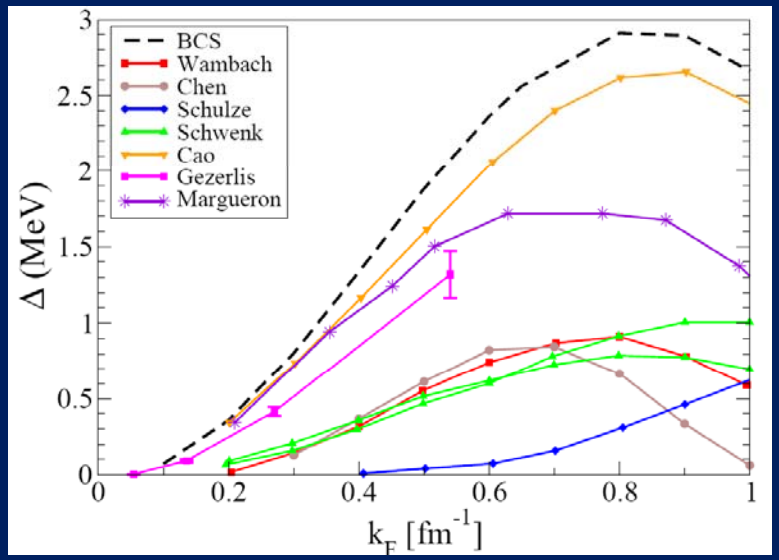
$$\varepsilon_s = \frac{2}{3}\epsilon_F^0 \rho_0 \frac{a_+^s r_0^2 (\nabla x_+)^2}{1 + h_+^s x_+^\sigma + h_\nabla^s r_0^2 (\nabla x_+)^2}, \qquad (3)$$

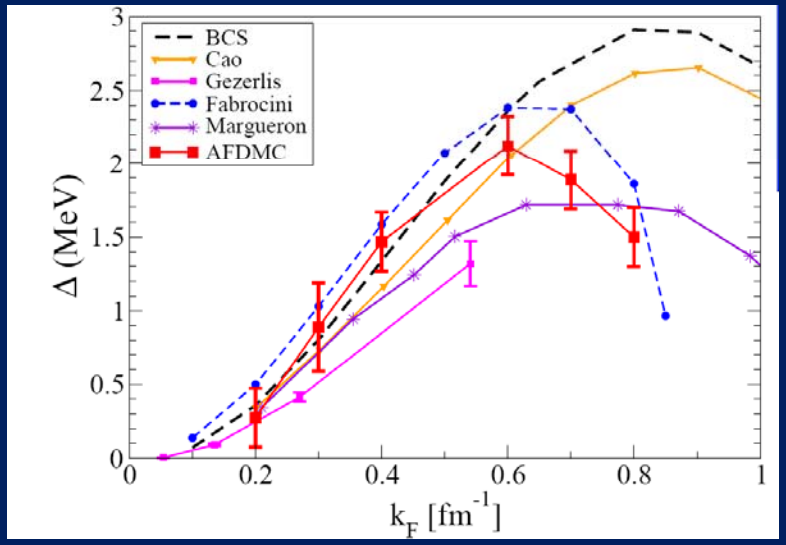
with $h_+^s = h_2^v$, , a_-^s and h_-^s the two free parameters. Such a form is obtained by adding



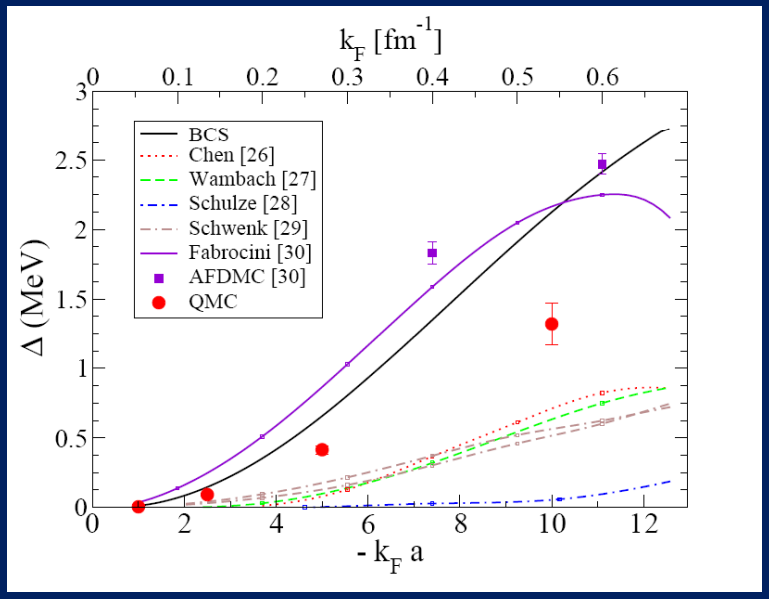


Baldo, Schuck, and Vinas, arXiv:0706.0658

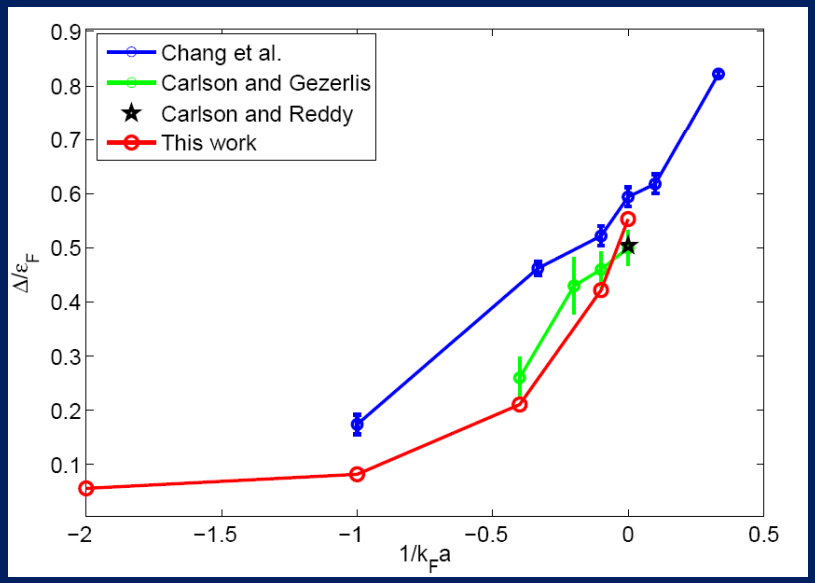




Gandolfi et al. arXiv:0805.2513



Gezerlis and Carlson, PRC 77, 032801 (2008)



Bulgac et al. arXiv:0801.1504, arXiv:0803.3238

Let us summarize some of the ingredients of the SLDA in nuclei

Energy Density (ED) describing the normal system

ED contribution due to superfluid correlations

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

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

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.

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

g_0 and g_1 could depend as well on ρ_p and ρ_n

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

SU(2) invariant

?

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

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

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

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.

In the end one finds that a suitable superfluid nuclear EDF has the following structure:

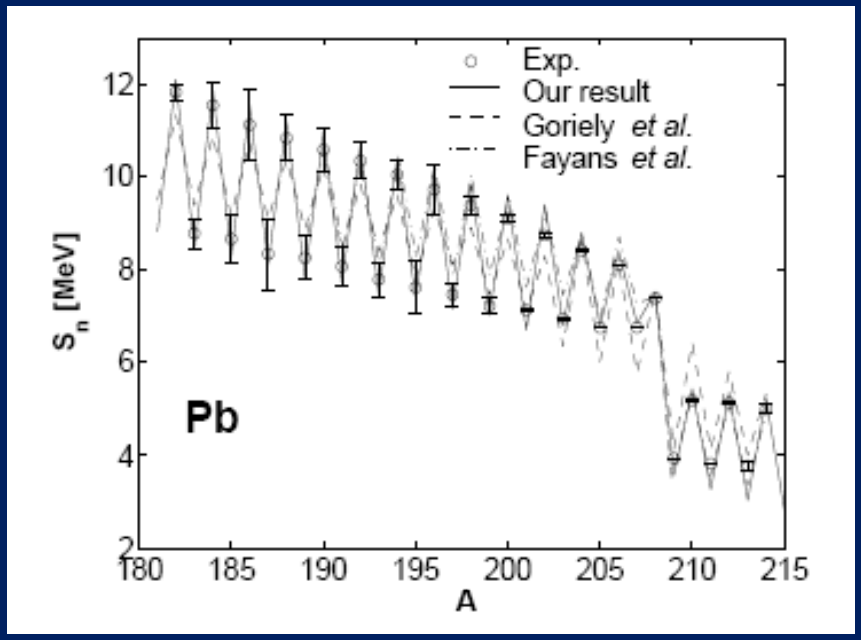
Isospin symmetric

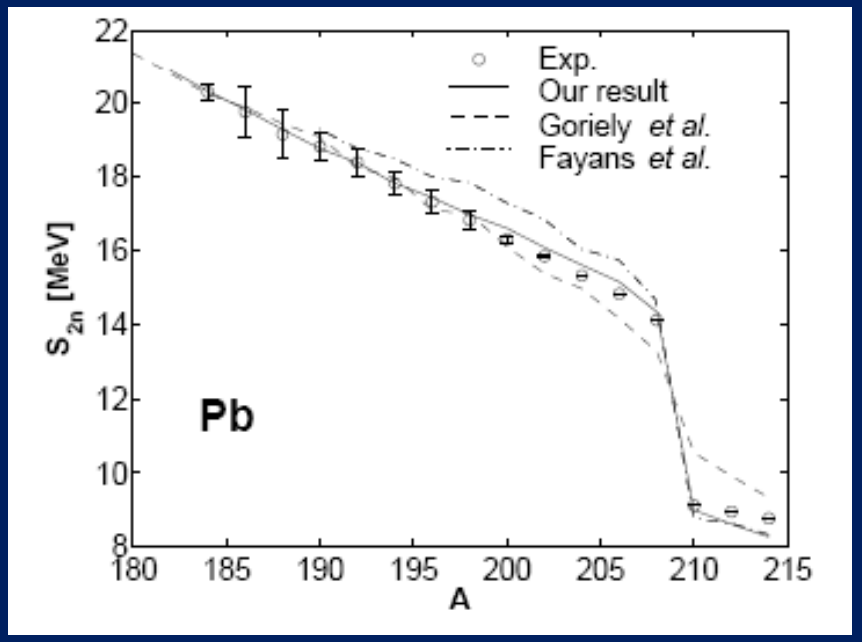
$$\varepsilon_S[\nu_p,\nu_n] = g(\rho_p,\rho_n)[|\nu_p|^2 + |\nu_n|^2] + f(\rho_p,\rho_n)[|\nu_p|^2 - |\nu_n|^2]\ \frac{\rho_p - \rho_n}{\rho_p + \rho_n}$$

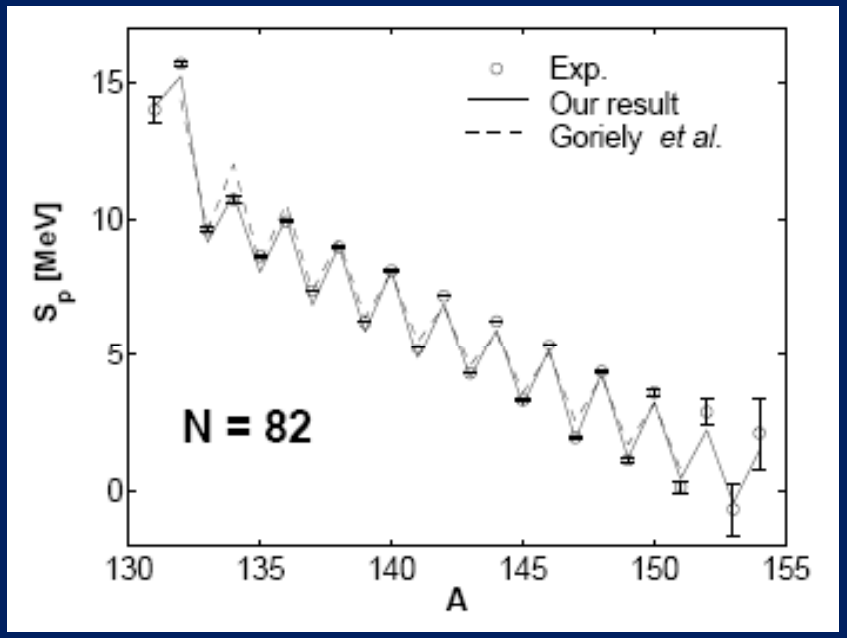
where $g(\rho_p,\rho_n) = g(\rho_n,\rho_p)$

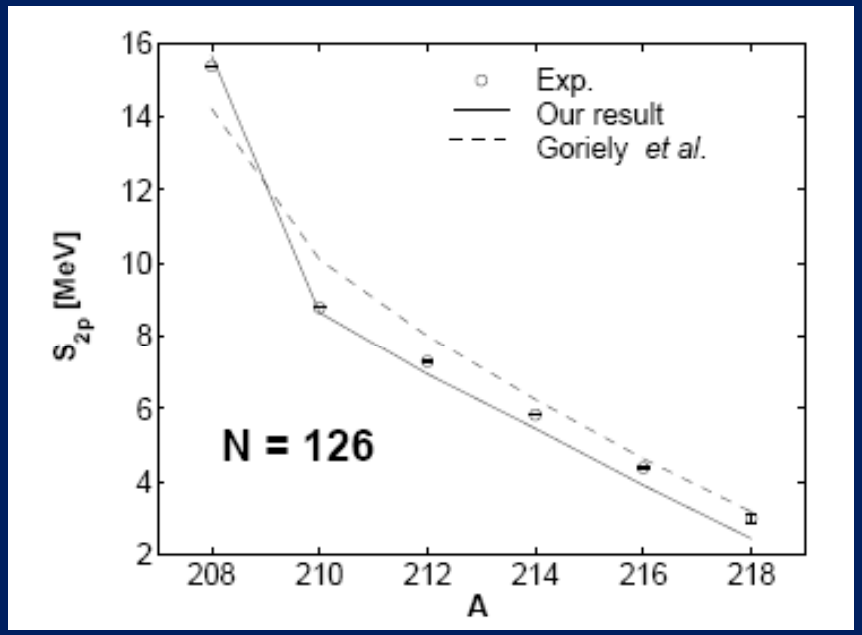
and $f(\rho_p,\rho_n) = f(\rho_n,\rho_p)$

The same coupling constant for both even and odd neutron/proton numbers!!!









A single universal parameter for pairing!

Conclusions

The future looks promising and there is light of the end of the tunnel!