Static Properties and Dynamics of Strongly Interacting Many Fermion Systems

Aurel Bulgac
University of Washington, Seattle, USA

Collaborators:

M.M. Forbes, P. Magierski, Y.-L. (Alan) Luo, K.J. Roche, I. Stetcu, S. Yoon, Y. Yu

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Slides to be posted at: http://www.phys.washington.edu/users/bulgac/

I will discuss properties of two different systems, which surprisingly share a lot in common:

- ✓ **Cold atomic gases**
- ✓ **Nuclear systems**

I am in big trouble:

I have too many slides!

I do not have enough slides!!!

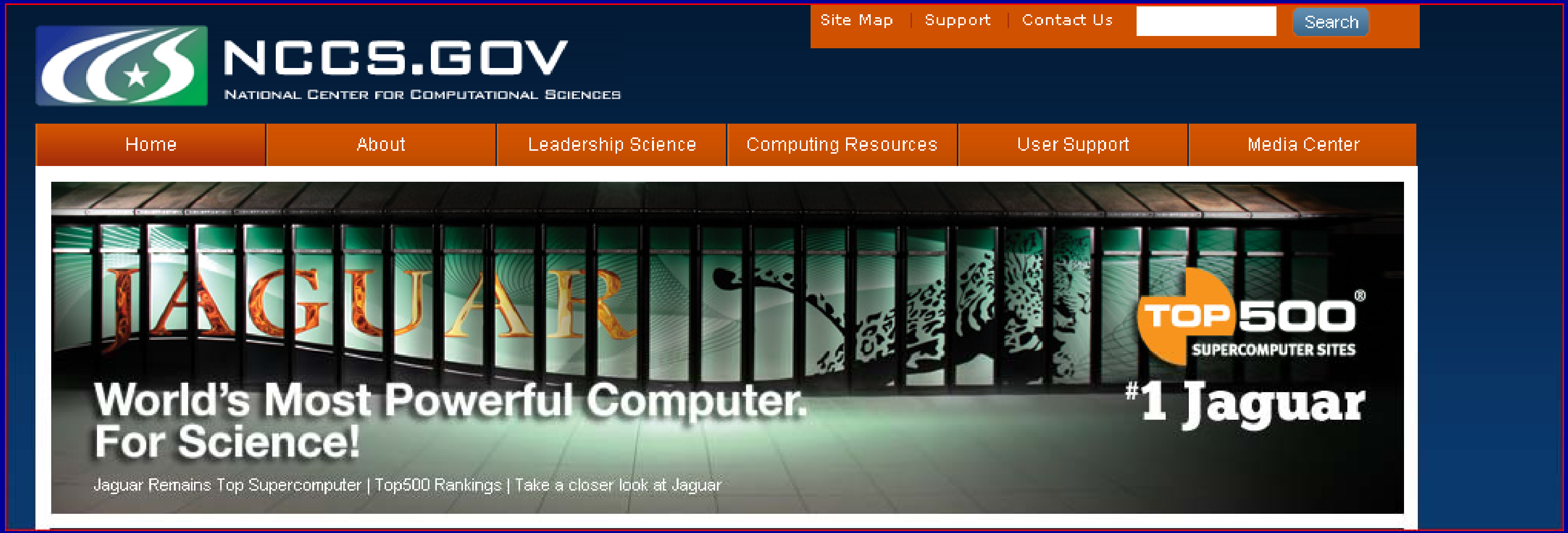
Both statements are correct!!!!!

First lecture – Static properties

How to implement Density Functional Theory (DFT) in the Case of Superfluid Fermion Systems

Second Lecture **- Implementation of Time-Dependent DFT for Superfluid Fermion Systems in 3D**

Applications to unitary gas and nuclei and how all this was implemented on JaguarPf (the largest supercomputer in the world)



Outline:

- **What is a unitary Fermi gas**

- **Very brief/skewed summary of DFT**

- **Bogoliubov-de Gennes equations, renormalization**

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

- **Fermions at unitarity in a harmonic trap within SLDA and comparison with *ab intio* results**

- **Challenges one has to face in order to implement DFT in nuclei**

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Jaguar Explores Carbon-Water Union

Water is everywhere, as is carbon. Big deal, right? Actually, it is. Understanding the adsorption, or accumulation, of a water molecule on graphene could influence everything from hydrogen storage to astrophysics to corrosion to geology.

Full story

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UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

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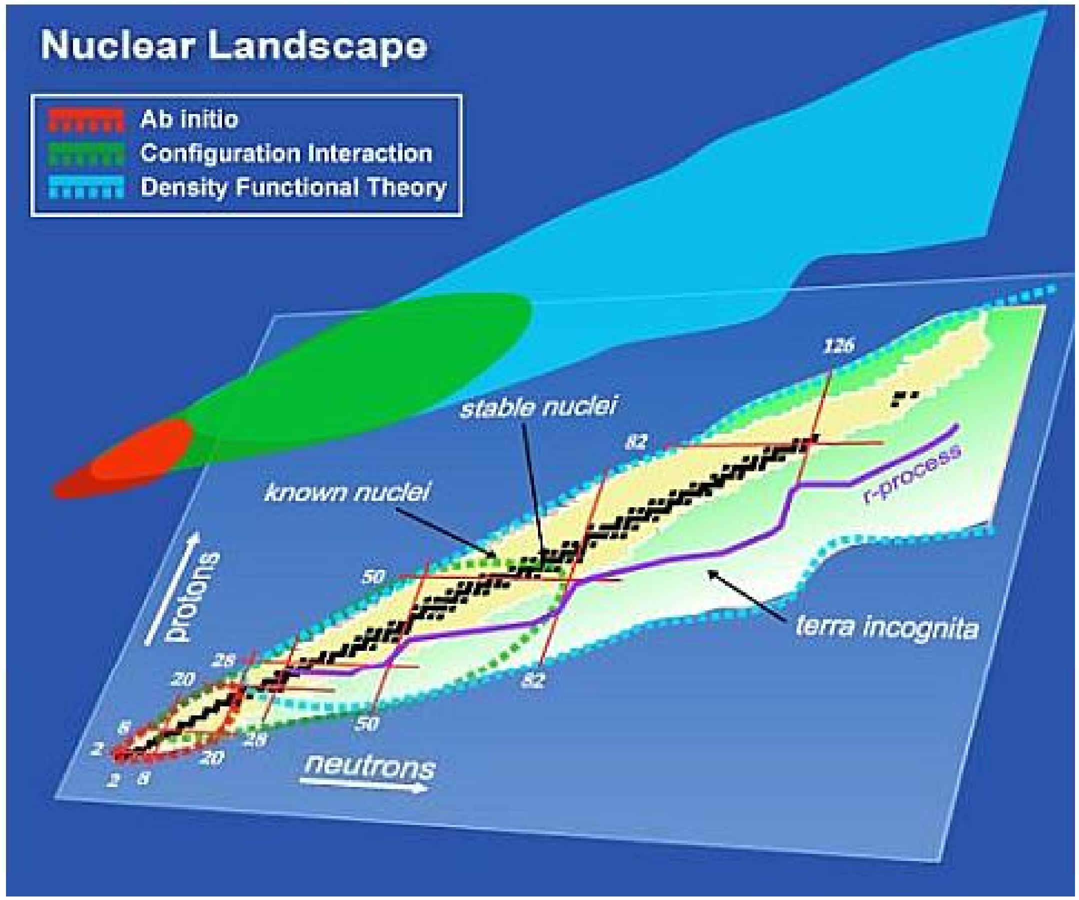

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UNEDF Research Areas

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:

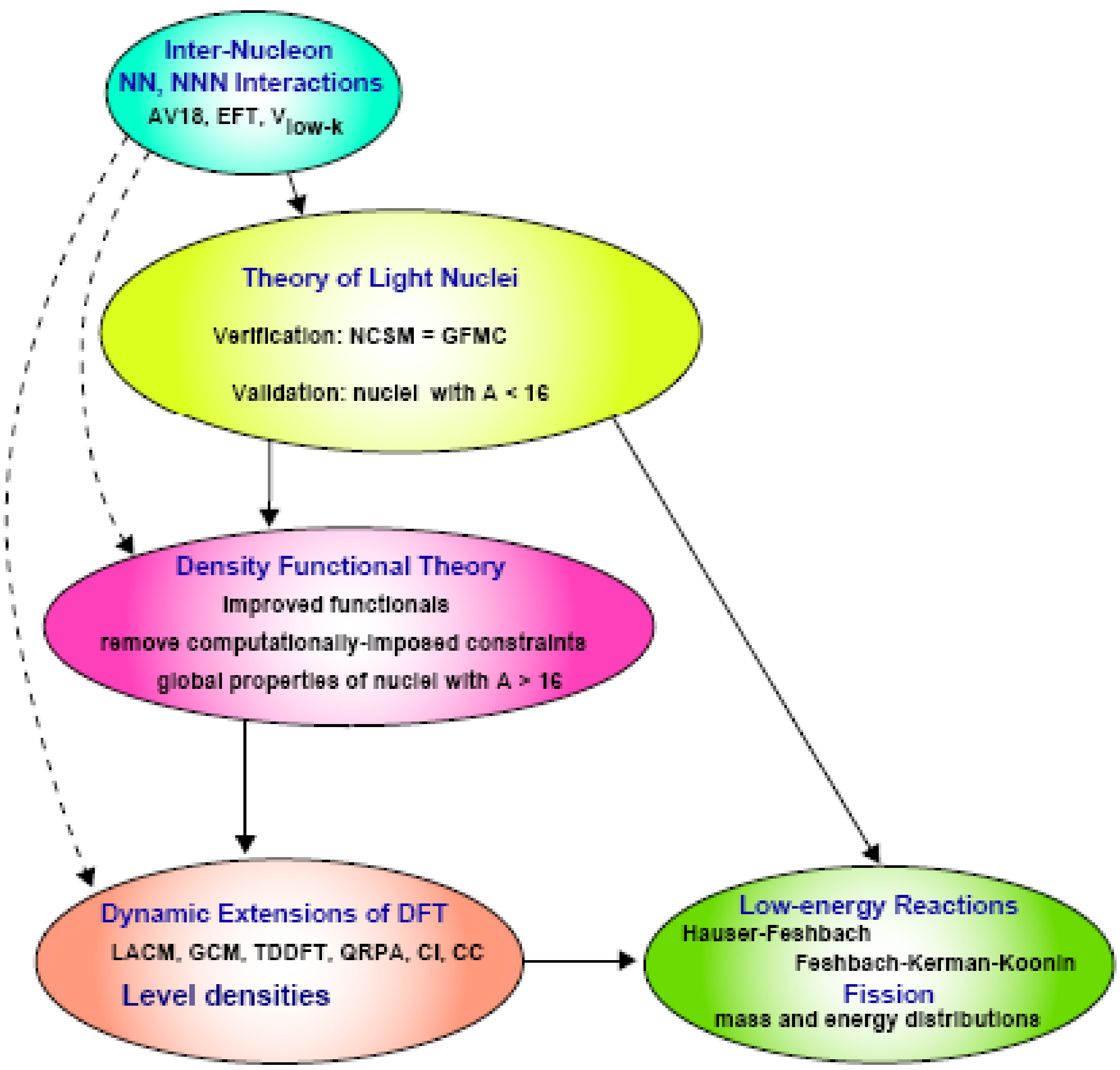
- Ab initio structure
- Ab initio functionals
- DFT applications
- DFT extensions
- Reactions
- Computer Science and Applied Mathematics

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

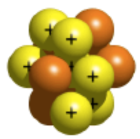
Universal Nuclear Energy Density Functional



What are models good for?

Step 3 - Build the Nucleus

The nucleus, the central part of the atom, is made from protons and neutrons. All of your atom's protons and neutrons go in the nucleus. For nitrogen, the nucleus would look something like this:



escape of any of them.

N. Bohr (1937)

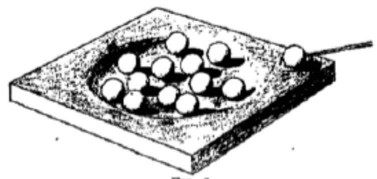


FIG. 1

Models:
-capture the essential phenomena
-are simple, at least in formulation

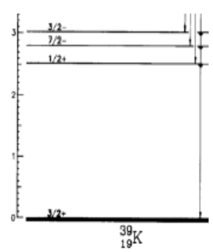
Characteristics of good theories

-need only a small set of parameters
-have wide predictive power
-have intrinsic criteria for limits of validity

Examples of informative nuclear models

1. The shell model

$$H = -\frac{\hbar^2\nabla^2}{2m} - V_0 f(r) + V_{\ell s}\frac{1}{r}\frac{df}{dr}\ell \cdot s$$



2. Seniority model for pairing SU(2)

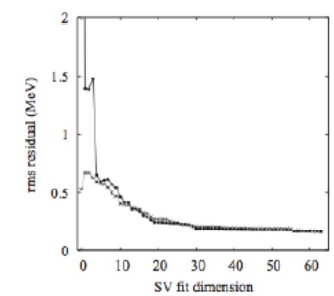
$$E_v(N) = -\frac{1}{4}G(N-v)(2\Omega - N - v + 2)$$

Error assessment

INT09-1: Effective field theories and the many-body problem

Example: intrinsic error from shell truncation in CI fits

PHYSICAL REVIEW C **80**, 027302 (2009)



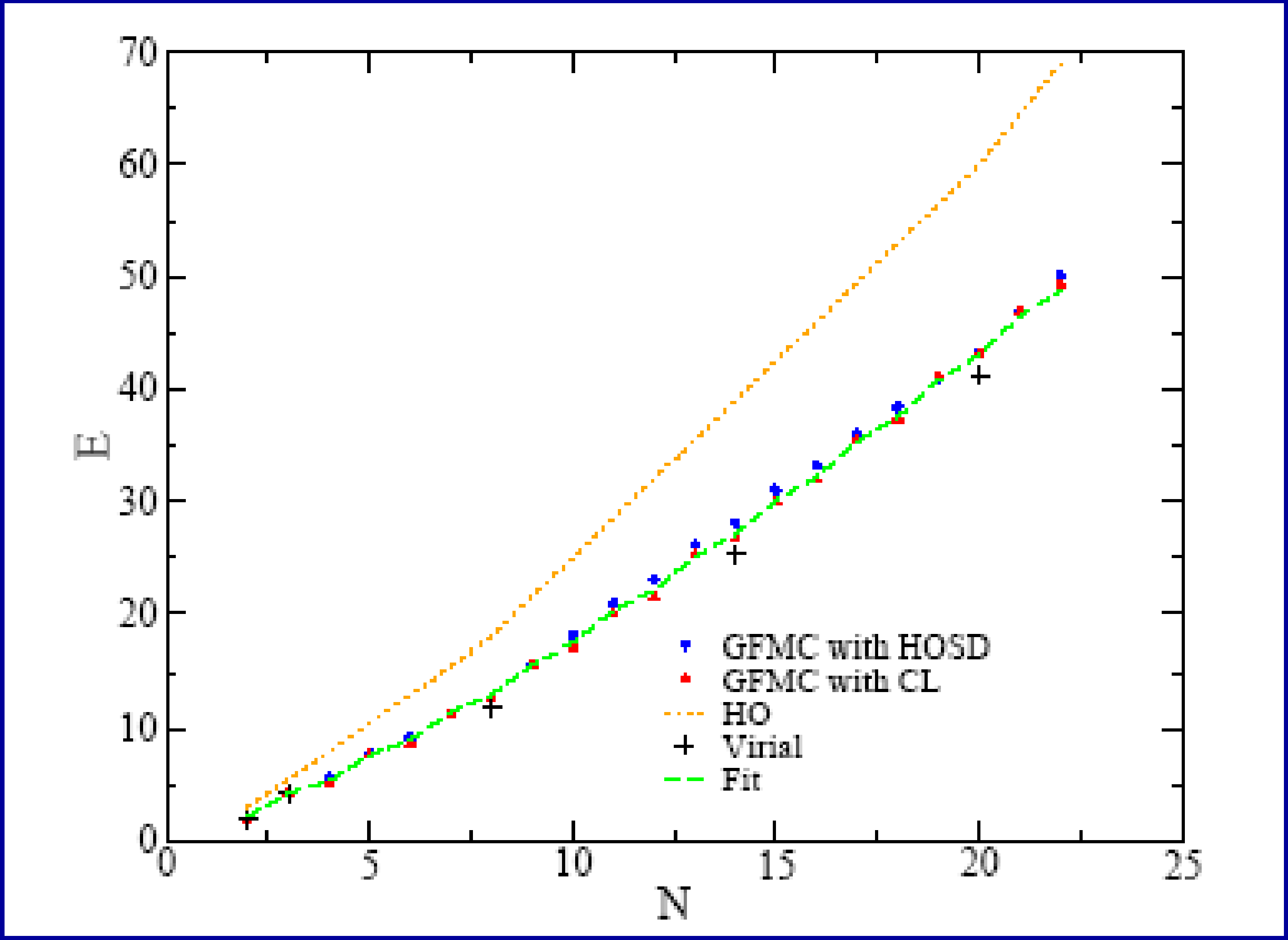
Estimated error of 0.2 MeV is close to actual value.

From a talk given by G.F. Bertsch, INT at 20, July 1-2, 2010

Part I

Unitary Fermi gas in a harmonic trap

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



Why would one want to study this system?

One reason:

(for the nerds, I mean the hard-core theorists,
not for the phenomenologists)

Bertsch's 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.

What are the scattering length and the effective range?

$$k \ \text{cotan}\ \delta_0 = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + \cdots$$

$$\sigma = \frac{4\pi}{k^2} \sin^2 \delta_0 + \cdots = 4\pi a^2 + \cdots$$

If the energy is small only the s-wave is relevant.

Let us consider a very old example: the hydrogen atom.

The ground state energy could only be a function of:

- ✓ **Electron charge**
- ✓ **Electron mass**
- ✓ **Planck's constant**

and then trivial dimensional arguments lead to

$$E_{gs} = \frac{e^4 m}{\hbar^2} \times \frac{1}{2}$$

Only the factor ½ requires some hard work.

Let us turn now to dilute fermion matter

The ground state energy is given by a function:

$$E_{gs} = f(N, V, \hbar, m, a, r_0)$$

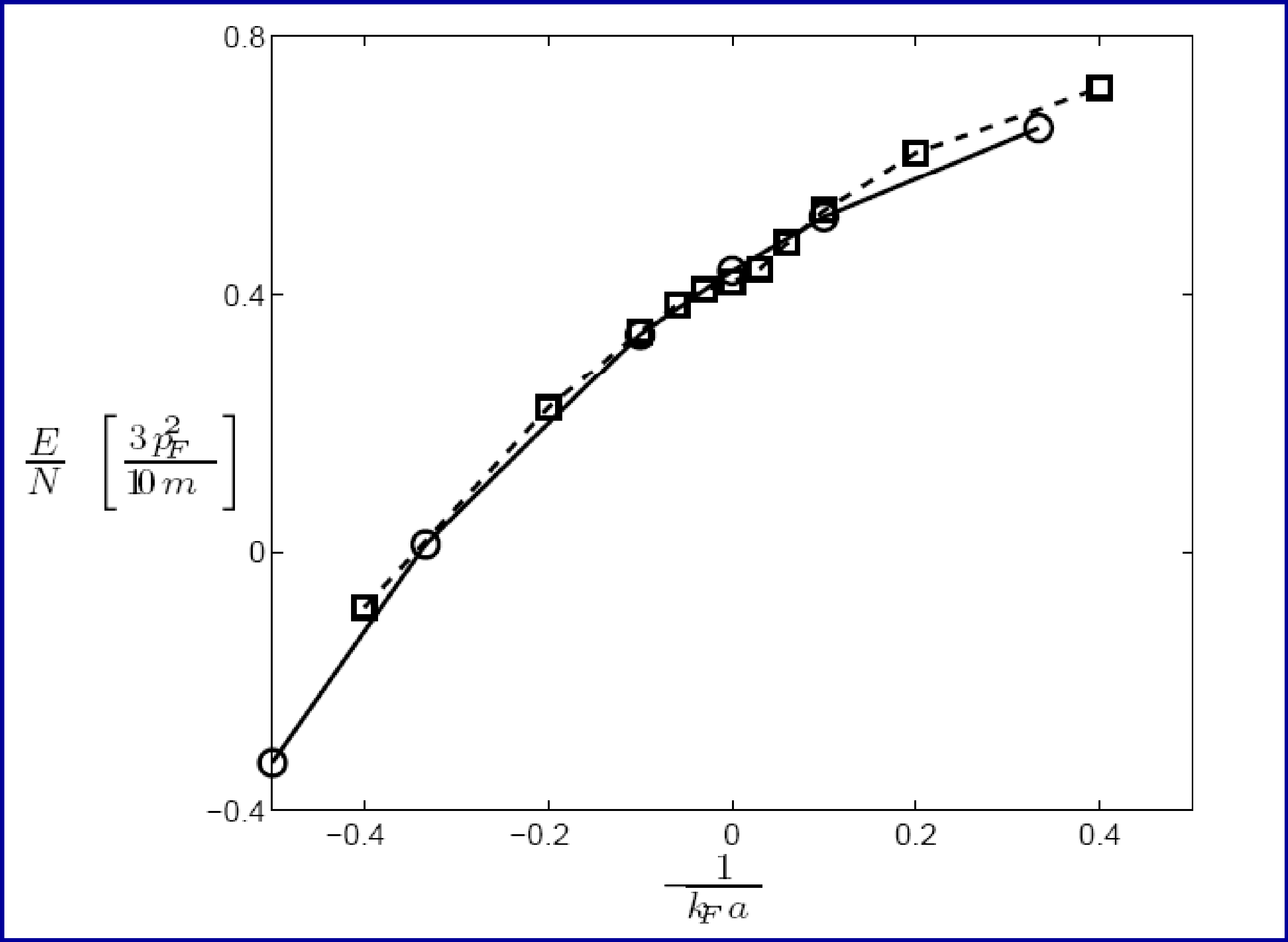
Taking the scattering length to infinity and the range of the interaction to zero, we are left with:

$$E_{gs} = F(N, V, \hbar, m) = \frac{3}{5}\varepsilon_F N \times \xi$$

$$\frac{N}{V} = \frac{k_F^3}{3\pi^2}, \qquad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

Pure number (dimensionless)

BEC side **BCS side**



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

What is a unitary Fermi gas

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, <u>either theoretically or experimentally</u>, 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

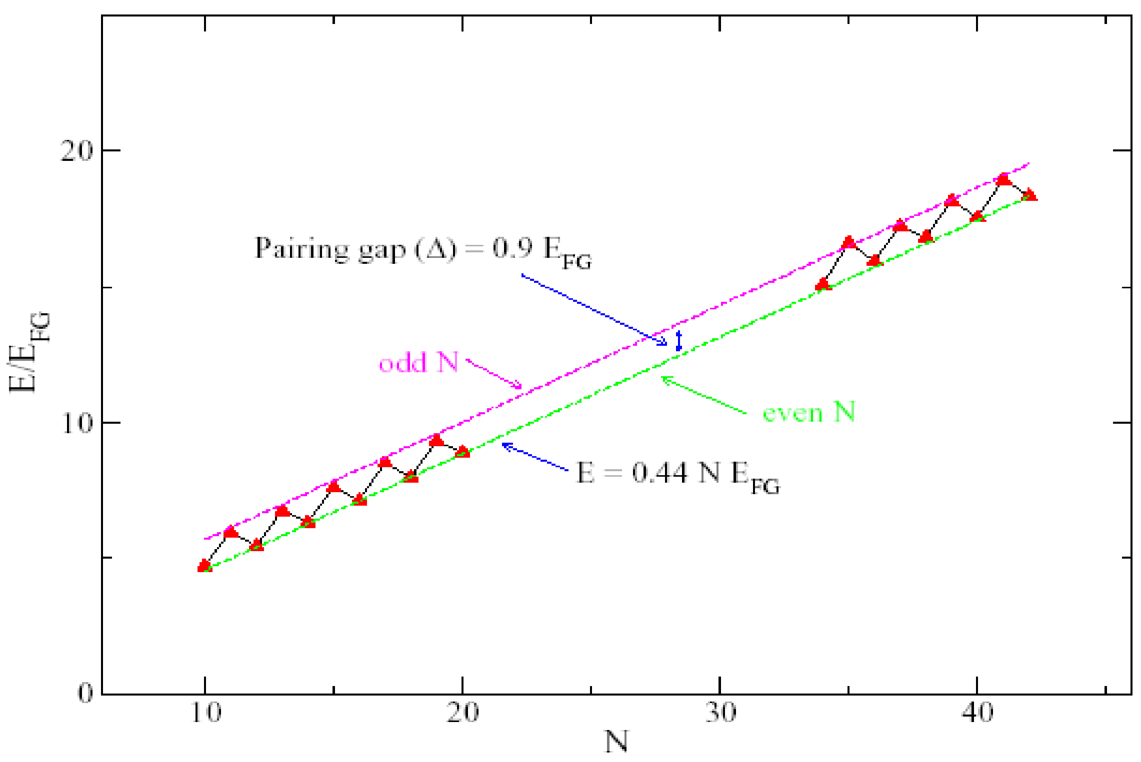
- Carlson, Chang, Pandharipande and Schmidt, PRL 91, 050401 (2003), with GFMC

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

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.

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

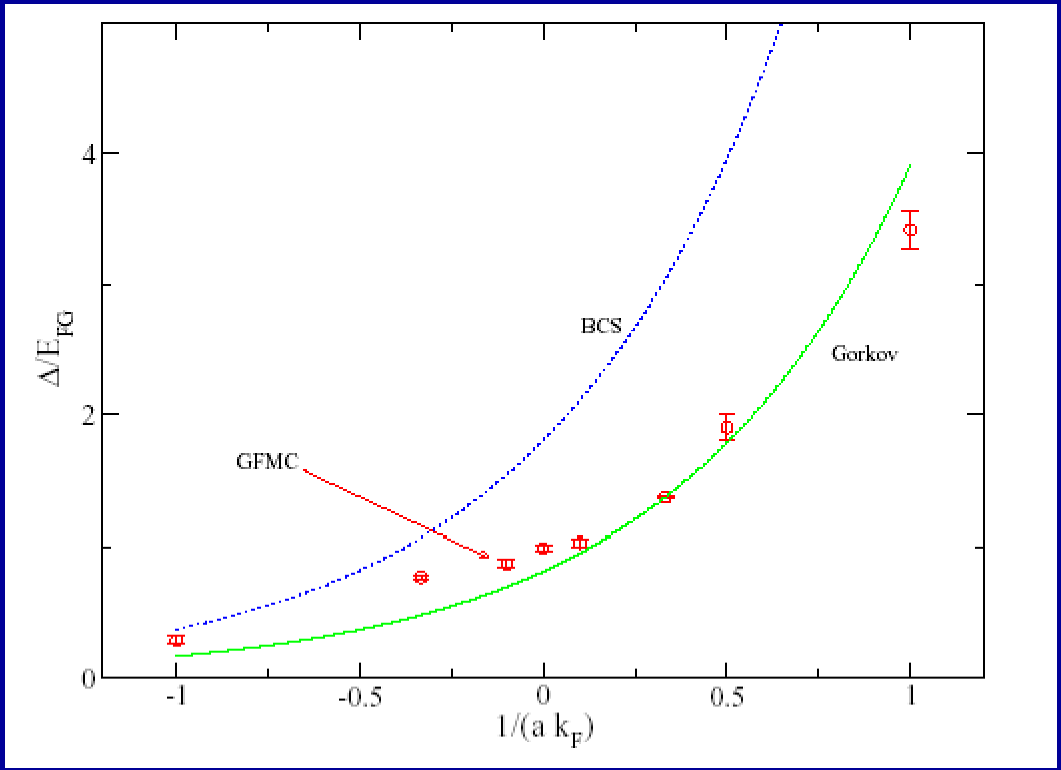


Result for $ak_F = -\infty$

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

Green Function Monte Carlo with Fixed Nodes

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



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

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

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

BCS →BEC crossover

Eagles (1960), Leggett (1980), Nozieres and Schmitt-Rink (1985), Randeria *et al.* (1993),…

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

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

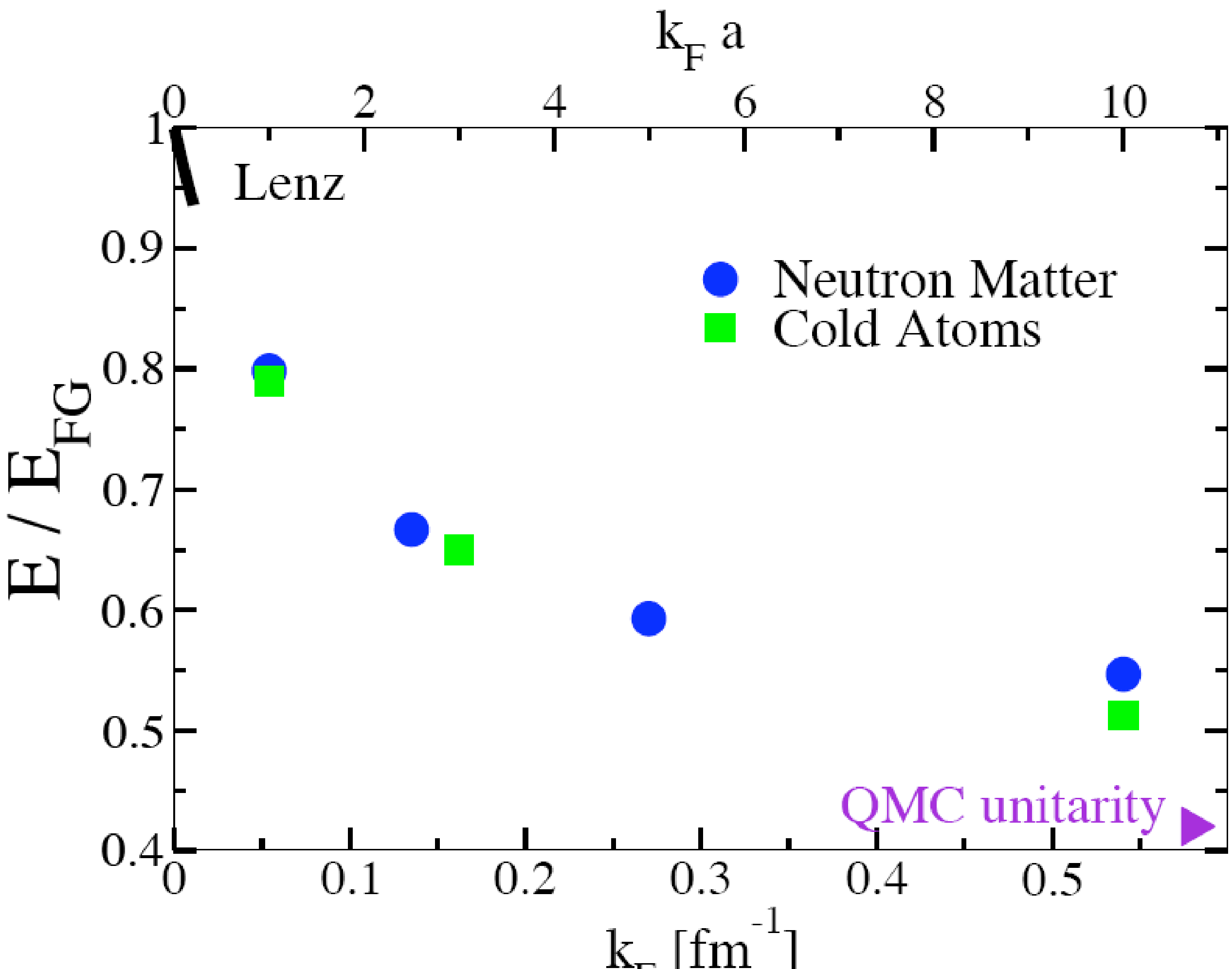
If |a|=∞ and $nr_0^3 \ll 1$ a Fermi system is strongly coupled and its properties are universal. Carlson *et al*. PRL 91, 050401 (2003)

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

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

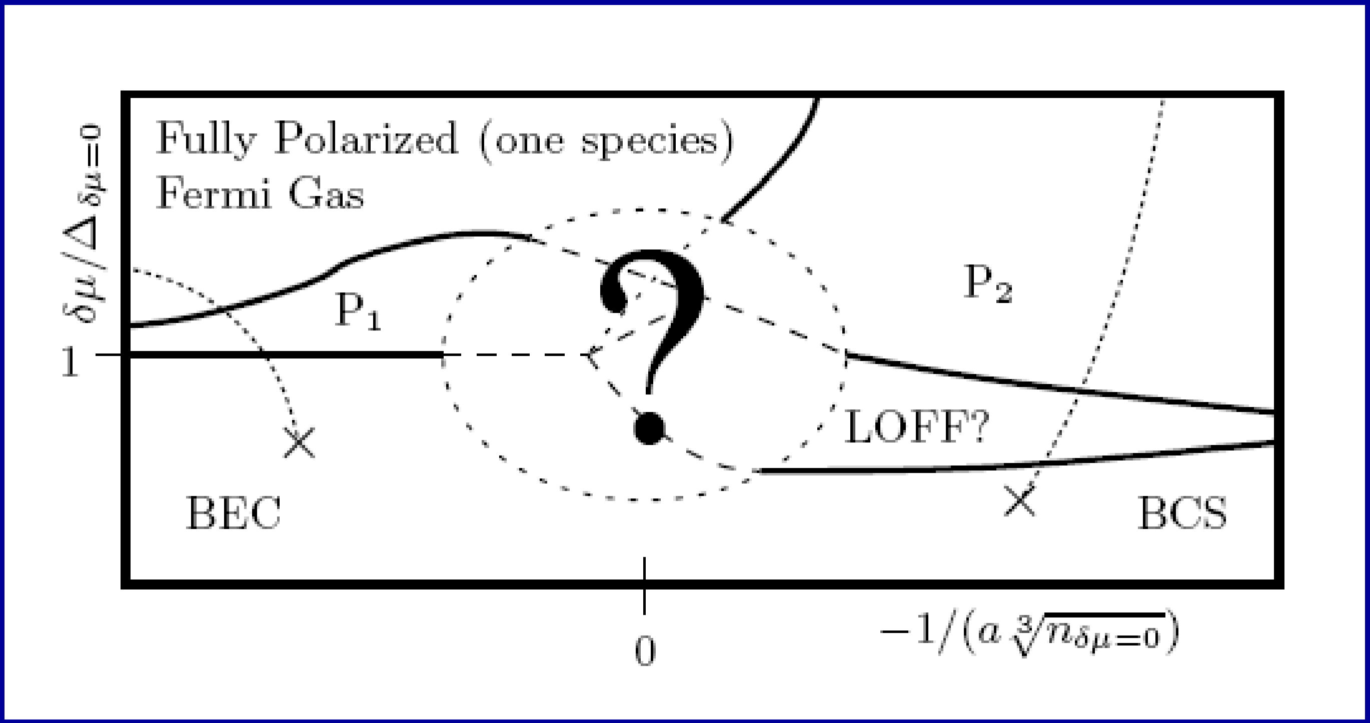
$$\varepsilon_2 = -\frac{\hbar^2}{ma^2} \quad \text{and} \quad n_b a^3 << 1, \quad \text{where} \quad n_b = \frac{n_f}{2} \text{ and } a_{bb} = 0.6a > 0$$

Equation of State: Cold Atoms versus Neutrons



Carlson's talk at UNEDF meeting, Pack Forest, WA, August, 2007

Fermi gas near unitarity has a very complex phase diagram (T=0)



Bulgac, Forbes, Schwenk, PRL 97, 020402 (2007)

Very brief/skewed summary of DFT

Density Functional Theory (DFT)
Hohenberg and Kohn, 1964

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

particle density only!

Local Density Approximation (LDA) Kohn and Sham, 1965

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

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

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

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

Kohn-Sham equations

Kohn-Sham theorem

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

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

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

Injective map (one-to-one)

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

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

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

Universal functional of density 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**

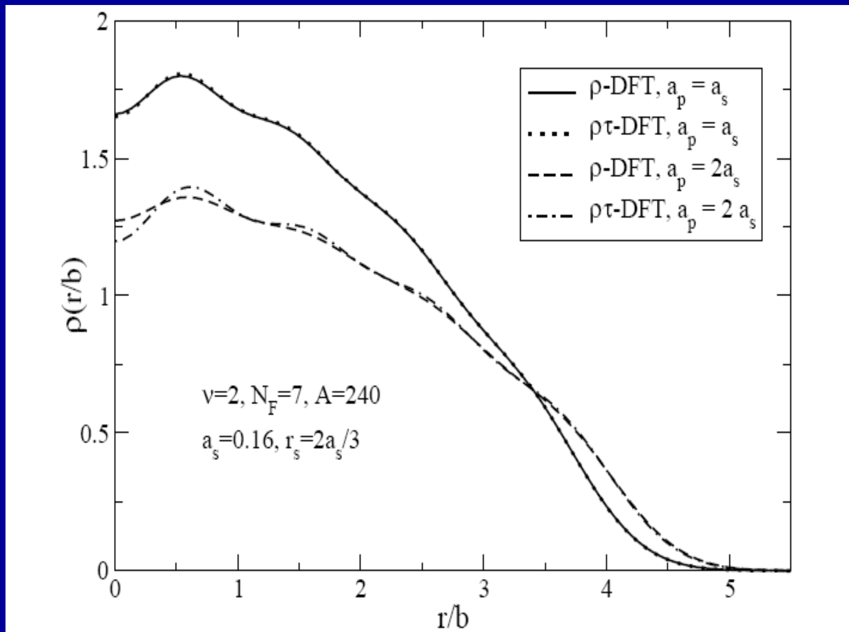
- ❑ **Apply the energy density functional to inhomogeneous systems and compare with the *ab initio* calculation, and if lucky declare Victory!**

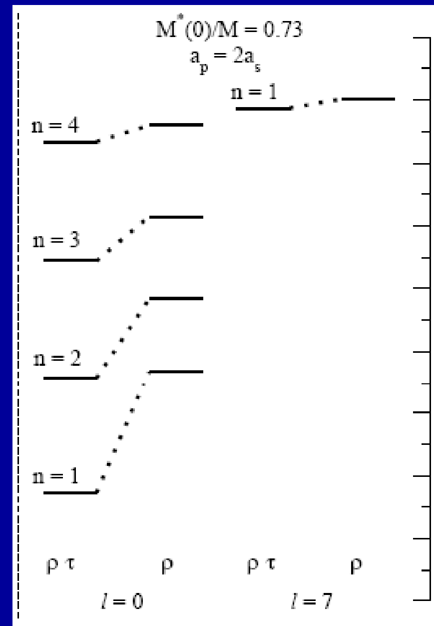
One can construct however an EDF which depends both on particle density and kinetic energy density and use it in a extended Kohn-Sham approach (perturbative result)

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

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. A 747, 268 (2005)





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	$\langle k_F \rangle$	$\sqrt{\langle r^2 \rangle}$	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)

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 ^3He** $T_c \approx 10^{-7}$ 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)

Bogoliubov-de Gennes equations and renormalization

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

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

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

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

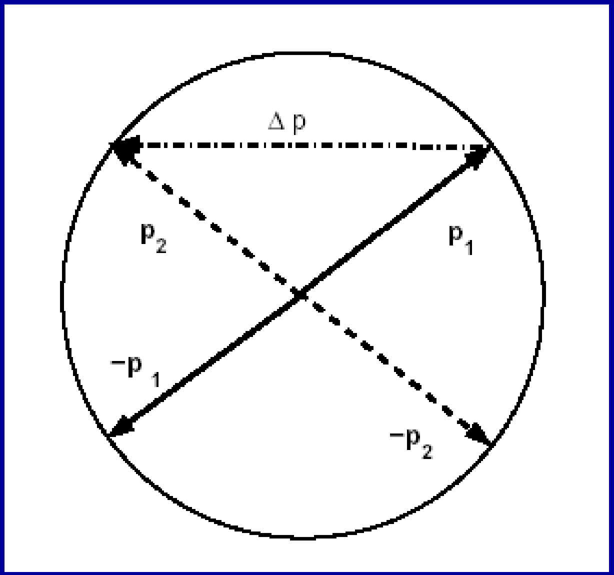
$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix}$$

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

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

$$\Delta(\vec{r}_1,\vec{r}_2) = -V(\vec{r}_1,\vec{r}_2)\nu(\vec{r}_1,\vec{r}_2)$$

at small separations

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

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

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

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

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)

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

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

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

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

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

The SLDA (renormalized) equations

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

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

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

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

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

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

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

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

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

The naïve SLDA energy density functional suggested by dimensional arguments

$$\varepsilon(\vec{r}) = \alpha \frac{\tau(\vec{r})}{2} + \beta \frac{3(3\pi^2)^{2/3} n^{5/3}(\vec{r})}{5} + \gamma \frac{\left|\nu(\vec{r})\right|^2}{n^{1/3}(\vec{r})}$$

$$n(\vec{r}) = 2\sum_k \left|\mathrm{v}_\mathrm{k}(\vec{r})\right|^2$$

$$\tau(\vec{r}) = 2\sum_k \left|\vec{\nabla}\mathrm{v}_\mathrm{k}(\vec{r})\right|^2$$

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

The SLDA energy density functional at unitarity for equal numbers of spin-up and spin-down fermions

$$\varepsilon(\vec{r}) = \overbrace{\left[\alpha\frac{\tau_c(\vec{r})}{2} - \Delta(\vec{r})\nu_c(\vec{r})\right]}^{\text{Only this combination is cutoff independent}} + \beta\frac{3(3\pi^2)^{2/3}n^{5/3}(\vec{r})}{5}$$

$$n(\vec{r}) = 2\sum_{0<E_k<E_c}\left|\mathrm{v}_{\mathrm{k}}(\vec{r})\right|^2, \quad \tau_c(\vec{r}) = 2\sum_{0<E_k<E_c}\left|\vec{\nabla}\mathrm{v}_{\mathrm{k}}(\vec{r})\right|^2,$$

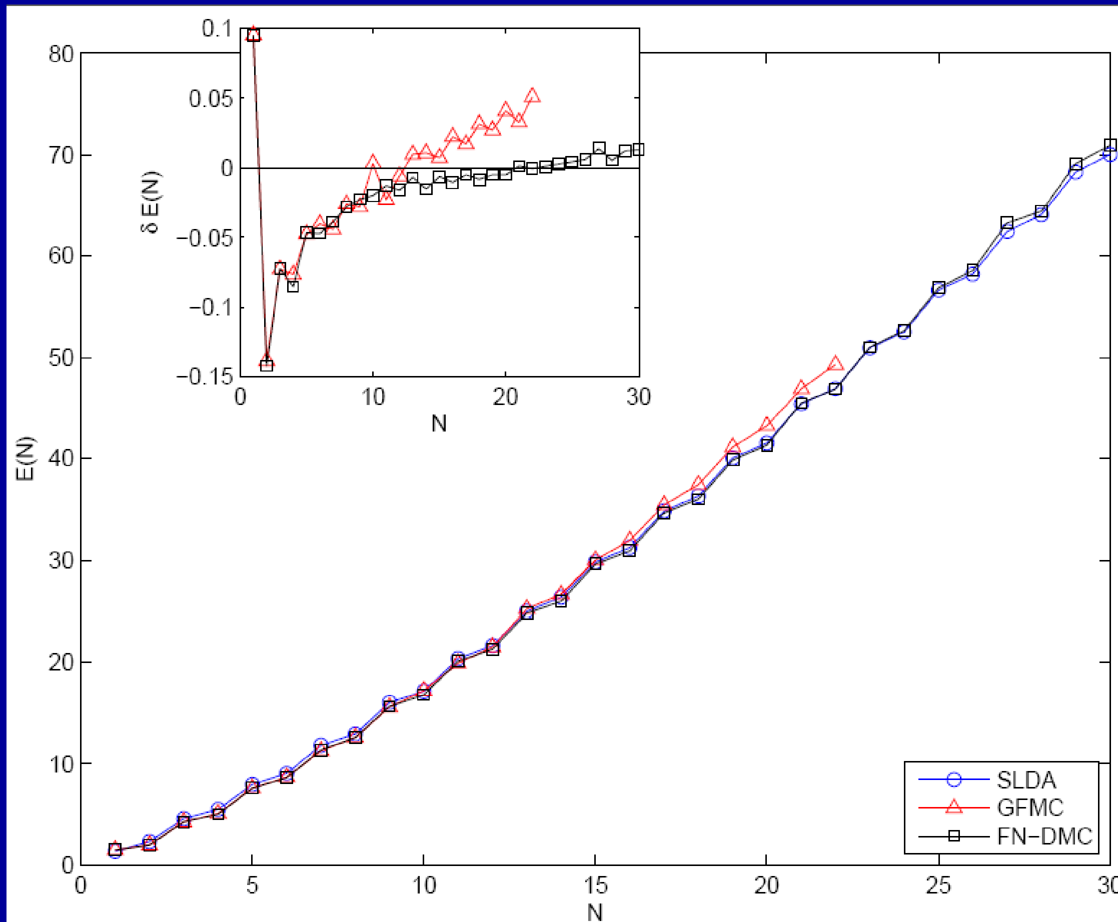
$$\nu_c(\vec{r}) = \sum_{0<E<E_c}\mathrm{u}_{\mathrm{k}}(\vec{r})\mathrm{v}^*_{\mathrm{k}}(\vec{r})$$

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

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

α can take any positive value,
but the best results are obtained when α is fixed by the qp-spectrum

Fermions at unitarity in a harmonic trap
Total energies E(N)



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)

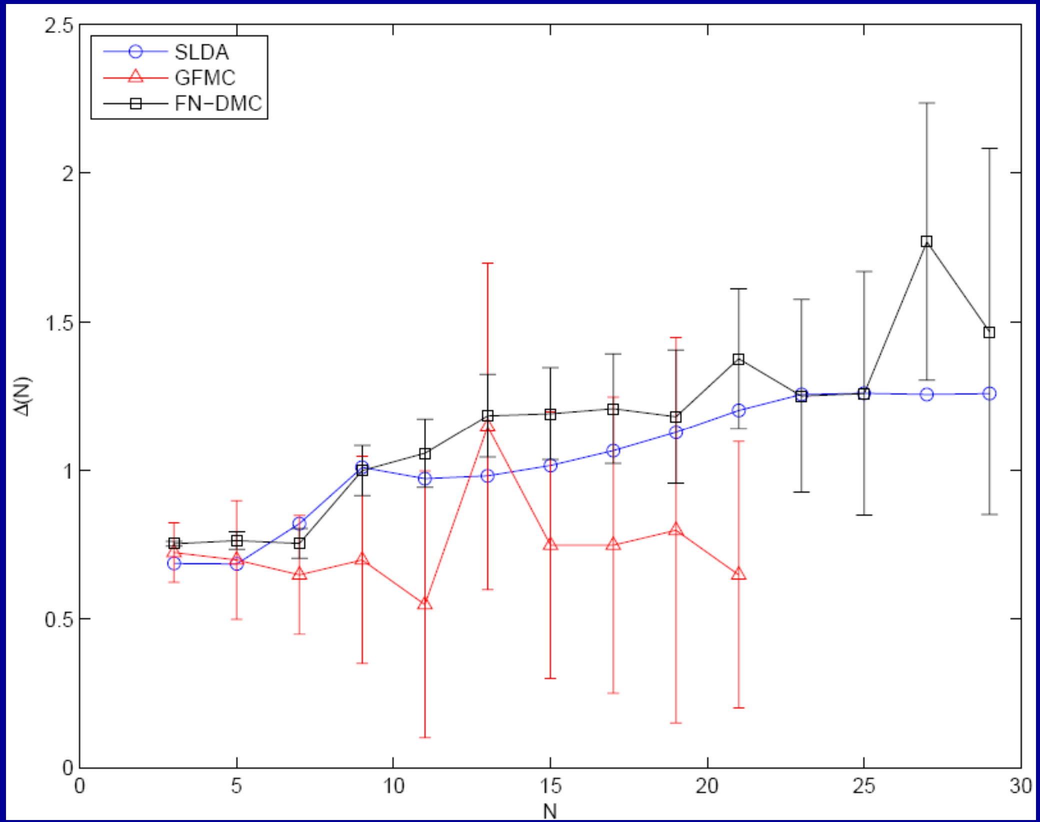
Bulgac, PRA 76, 040502(R) (2007)

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!!!

Fermions at unitarity in a harmonic trap
Pairing gaps



$$\Delta(N) = \frac{E(N+1) - 2E(N) + E(N-1)}{2}, \quad \text{for odd } N$$

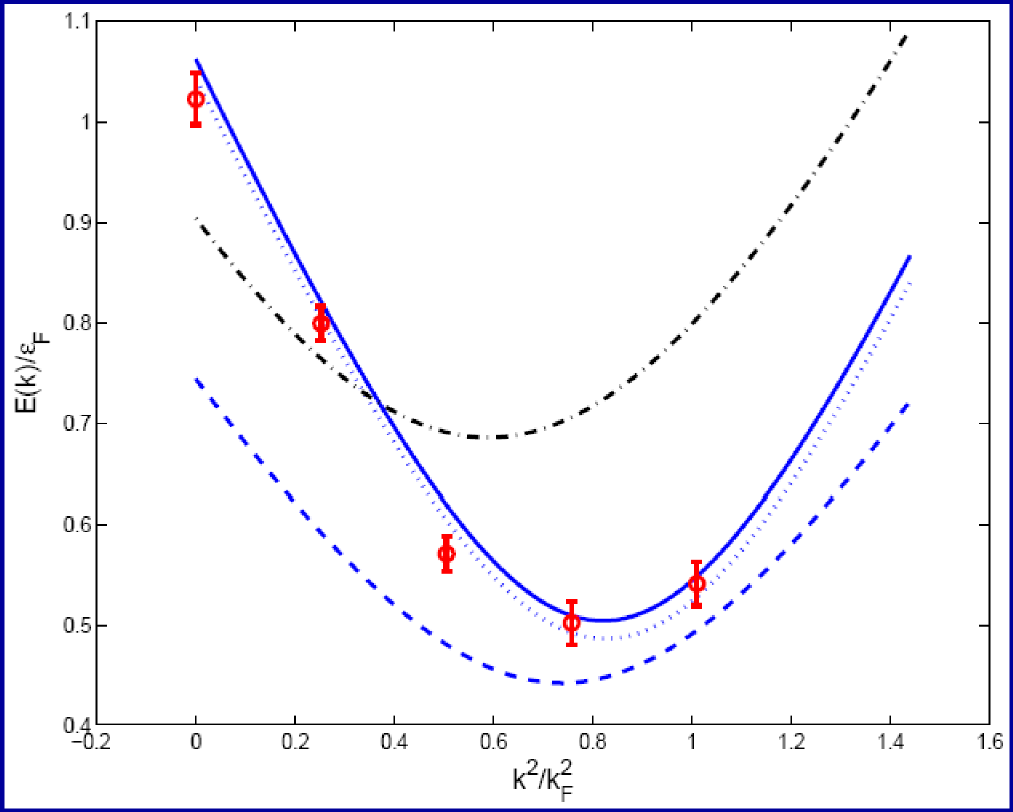
GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)

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

PRA 76, 053613 (2007)

Bulgac, PRA 76, 040502(R) (2007)

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

Two more universal parameter characterizing the unitary Fermi gas and its excitation spectrum:
effective mass, meanfield potential

Bulgac, PRA 76, 040502(R) (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**

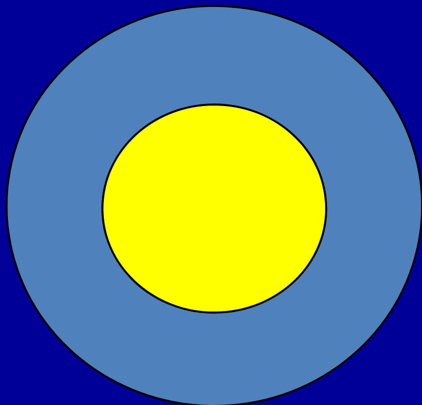
- **Gradient corrections not included**

Until now we kept the numbers of spin-up and spin-down equal.

What happens when there are not enough partners for everyone to pair with?

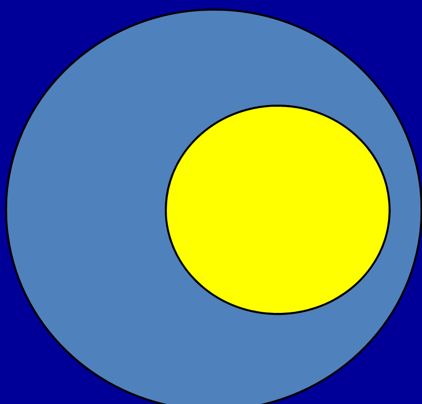
(In particular this is what one expects to happen in color superconductivity, due to a heavier strange quark)

What theory tells us?

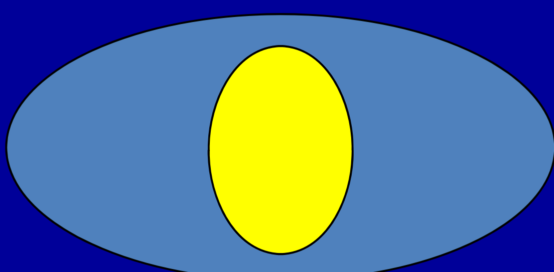


Green – Fermi sphere of spin-up fermions
Yellow – Fermi sphere of spin-down fermions

$$\text{If} \quad \left|\mu_\uparrow - \mu_\downarrow\right| < \frac{\Delta}{\sqrt{2}} \quad \text{the same solution as for } \mu_\uparrow = \mu_\downarrow$$



LOFF/FFLO solution (1964)
Pairing gap becomes a spatially varying function
Translational invariance broken

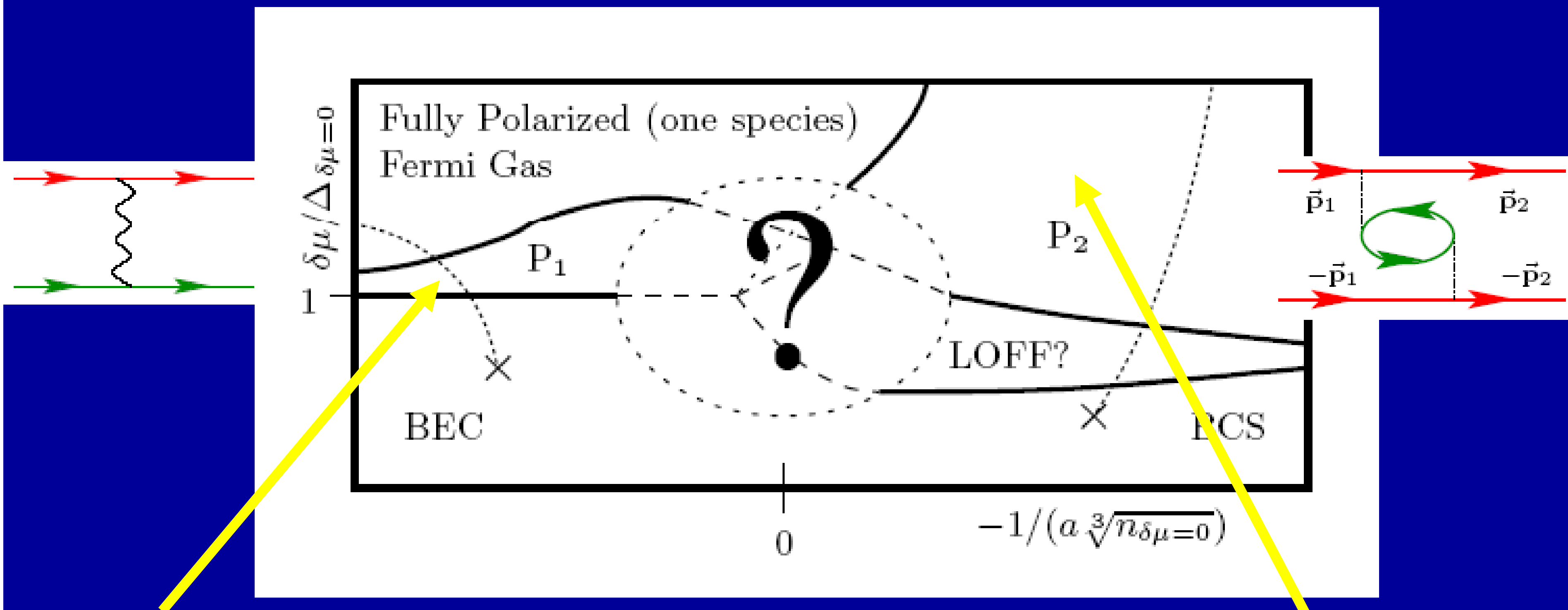


Muether and Sedrakian (2002)
Translational invariant solution
Rotational invariance broken

What we think is happening in spin imbalanced systems?

Induced P-wave superfluidity

Two new superfluid phases where before they were not expected

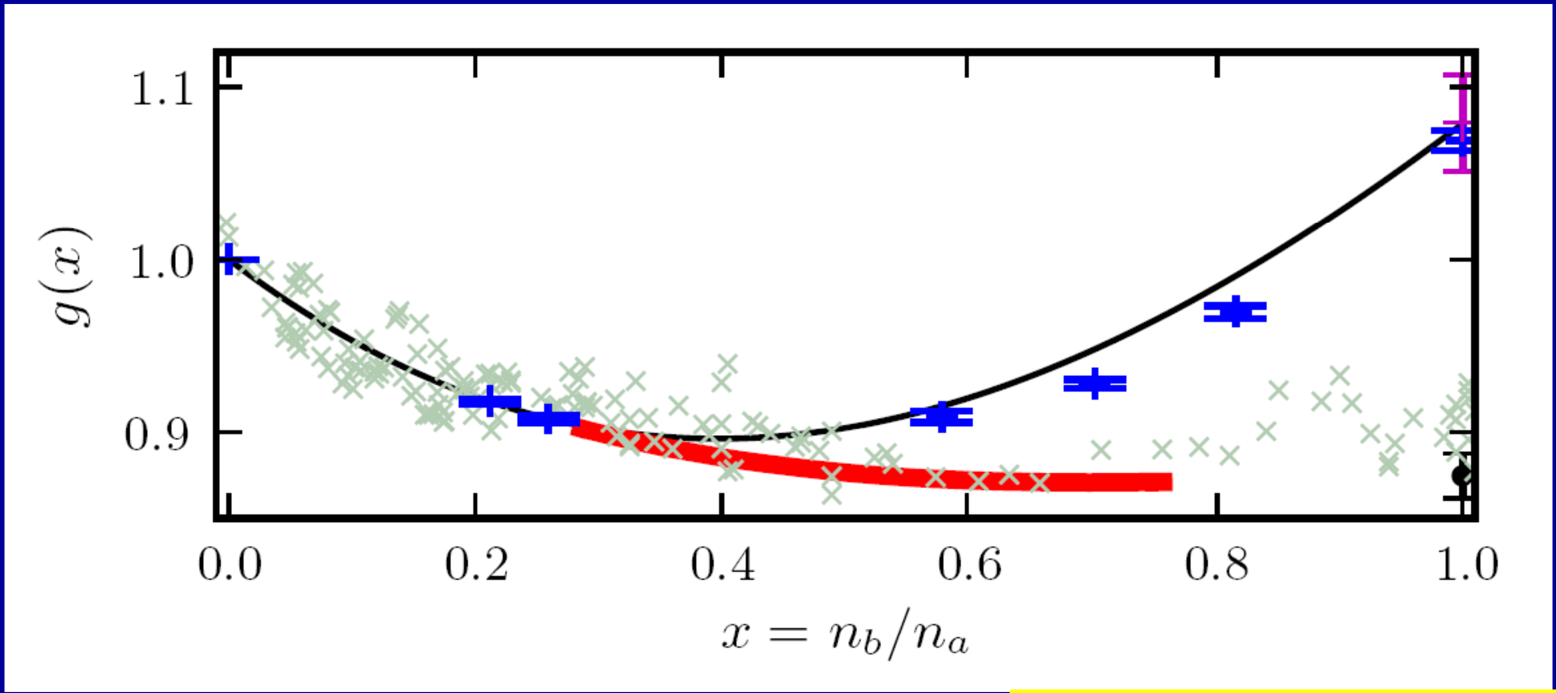


One Bose superfluid coexisting with one P-wave Fermi superfluid

Two coexisting P-wave Fermi superfluids

Bulgac, Forbes, Schwenk, Phys. Rev. Lett. 97, 020402 (2006)

A refined EOS for spin unbalanced systems



Bulgac and Forbes,
Phys. Rev. Lett. 101, 215301 (2008)

Red line: Larkin-Ovchinnikov phase

Black line: normal part of the energy density
Blue points: DMC calculations for normal state, Lobo et al, PRL 97, 200403 (2006)
Gray crosses: experimental EOS due to Shin, Phys. Rev. A 77, 041603(R) (2008)

$$E(n_a, n_b) = \frac{3}{5}\frac{(6\pi^2)^{2/3}\hbar^2}{2m}\left[n_a g\left(\frac{n_b}{n_a}\right)\right]^{5/3}$$

Asymmetric SLDA (ASLDA)

$$n_a(\vec{r}) = \sum_{E_n<0} \left|\mathrm{u}_n(\vec{r})\right|^2, \qquad n_b(\vec{r}) = \sum_{E_n>0} \left|\mathrm{v}_n(\vec{r})\right|^2,$$

$$\tau_a(\vec{r}) = \sum_{E_n<0} \left|\vec{\nabla}\mathrm{u}_n(\vec{r})\right|^2, \qquad \tau_b(\vec{r}) = \sum_{E_n>0} \left|\vec{\nabla}\mathrm{v}_n(\vec{r})\right|^2,$$

$$\nu(\vec{r}) = \frac{1}{2}\sum_{E_n} \mathrm{sign}(E_n)\mathrm{u}_n(\vec{r})\mathrm{v}_n^*(\vec{r}),$$

$$\mathrm{E}(\vec{r}) = \frac{\hbar^2}{2m}\left[\alpha_a(\vec{r})\tau_a(\vec{r}) + \alpha_b(\vec{r})\tau_b(\vec{r})\right] - \Delta(\vec{r})\nu(\vec{r}) +$$

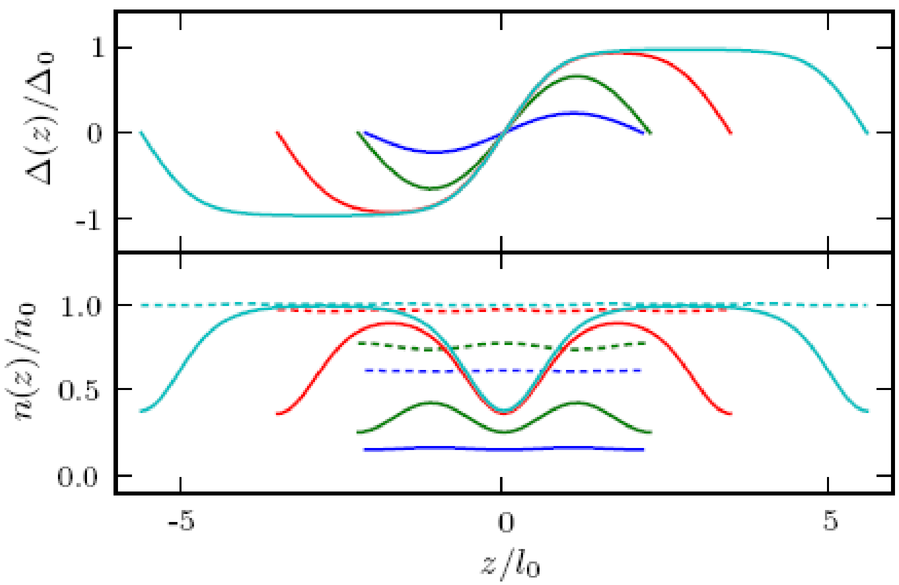
$$+\frac{3\left(3\pi^2\right)^{2/3}\hbar^2}{10m}\left[n_a(\vec{r}) + n_b(\vec{r})\right]^{5/3}\beta[x(\vec{r})],$$

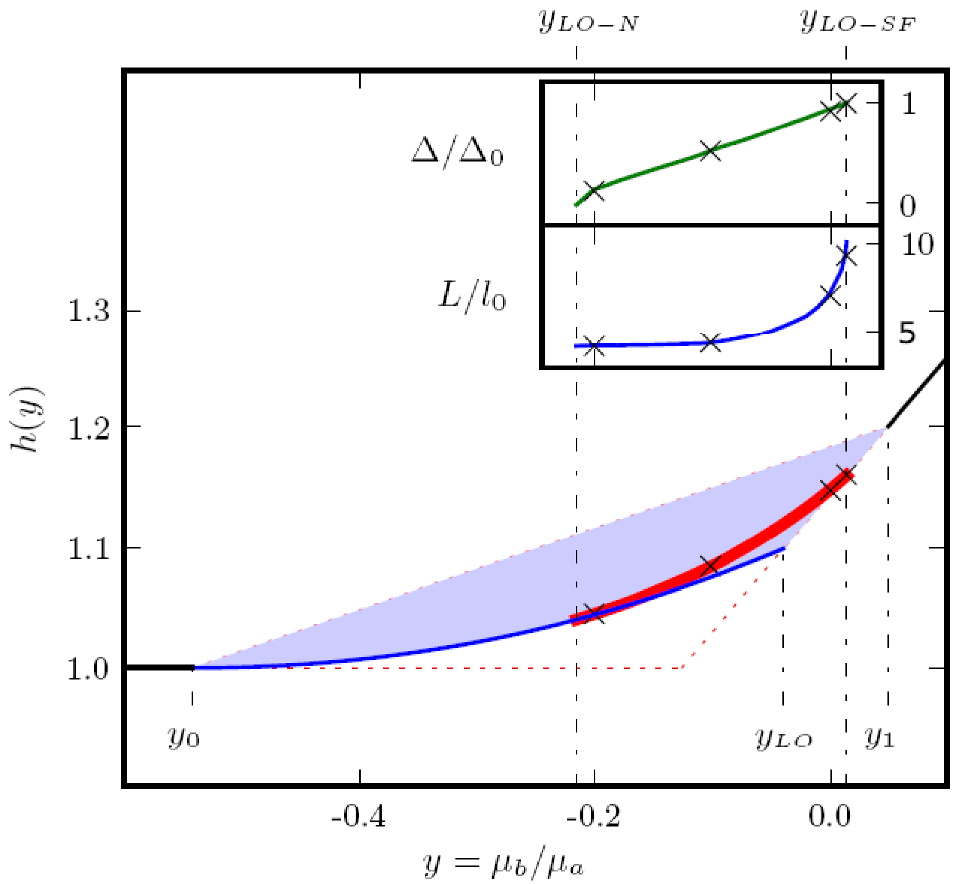
$$\alpha_a(\vec{r}) = \alpha\left[x(\vec{r})\right], \qquad \alpha_b(\vec{r}) = \alpha\left[1/x(\vec{r})\right], \qquad x(\vec{r}) = n_b(\vec{r})/n_a(\vec{r}),$$

$$\Omega = -\int d^3\vec{r}\ \mathrm{P}(\vec{r}) = \int d^3\vec{r}\ \left[\mathrm{E}(\vec{r}) - \mu_a n_a(\vec{r}) - \mu_b n_b(\vec{r})\right]$$

Bulgac and Forbes, arXiv:0804:3364

A Unitary Fermi Supersolid: the Larkin-Ovchinnikov phase





Bulgac and Forbes
PRL 101, 215301 (2008)

$$P[\mu_a, \mu_b] = \frac{2}{30\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left[\mu_a h\left(\frac{\mu_b}{\mu_a}\right)\right]^{5/2}$$

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

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

where $\varepsilon_{\mathrm{kin}}$ 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

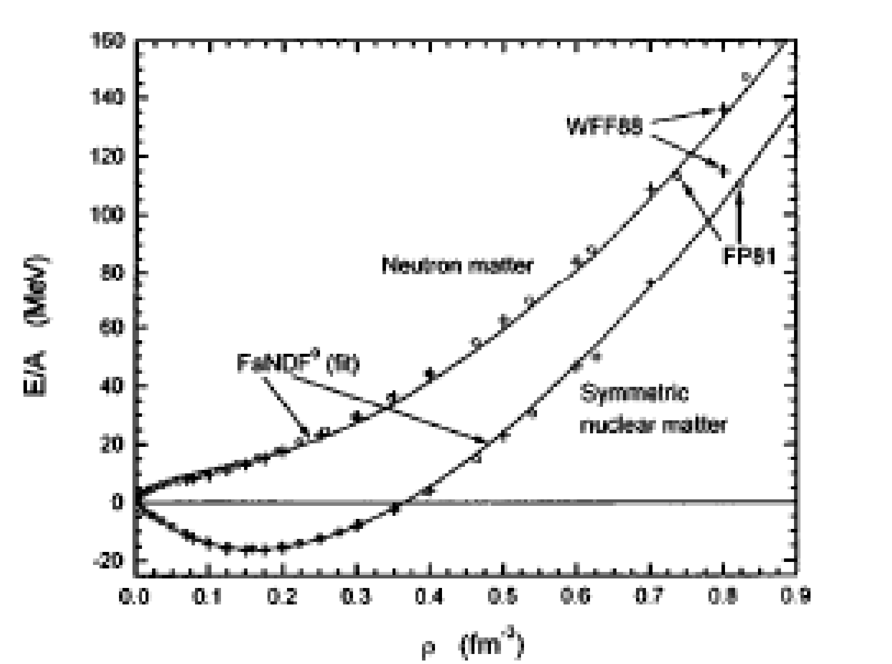
$$\varepsilon_v = \frac{2}{3}\epsilon_F^0\rho_0\left[a_+^v \frac{1-h_{1+}^v x_+^\sigma}{1+h_{2+}^v x_+^\sigma} x_+^2 + a_-^v \frac{1-h_{1-}^v x_+}{1+h_{2-}^v x_+} x_-^2\right].$$

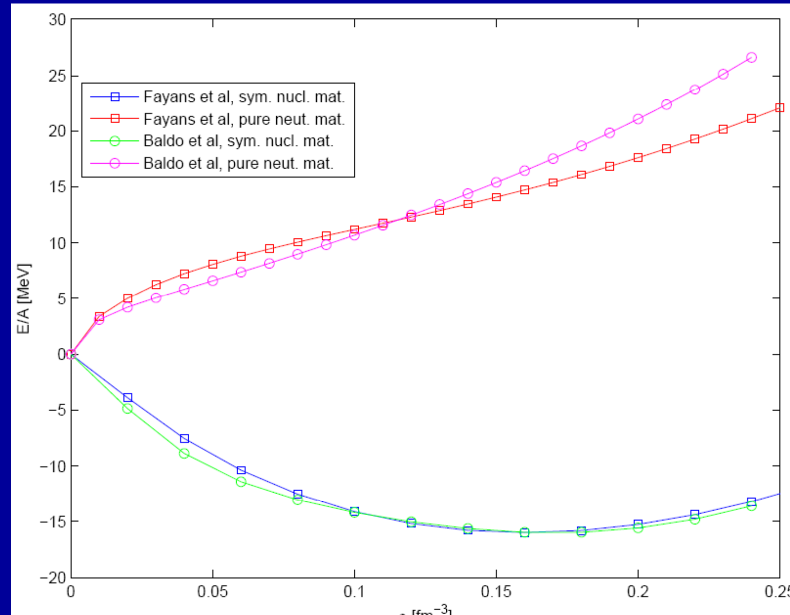
Here and in the following $x_\pm = (\rho_n \pm \rho_p)/2\rho_0$, $\rho_{n(p)}$ is the neutron (
$2\rho_0$ is the equilibrium density of symmetric nuclear matter wit

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:

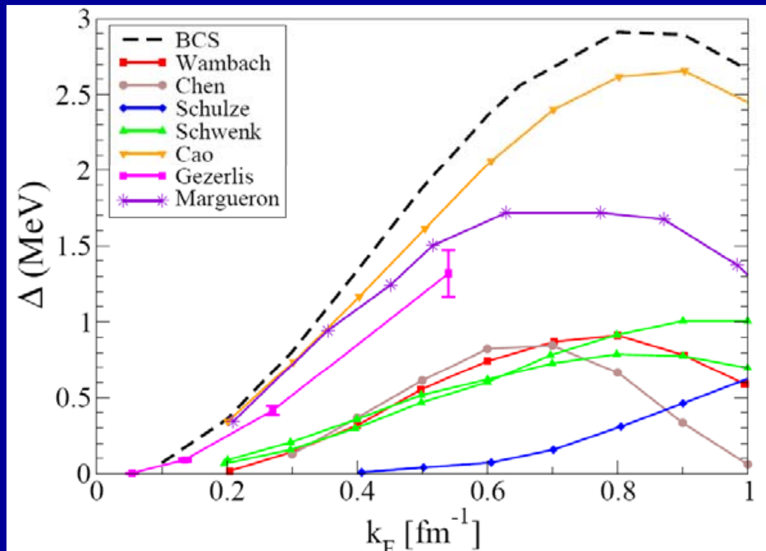
$$\varepsilon_s = \frac{2}{3}\epsilon_F^0\rho_0 \frac{a_+^s r_0^2(\nabla x_+)^2}{1+h_+^s x_+^\sigma + h_\nabla^s r_0^2(\nabla x_+)^2}, \qquad (3)$$

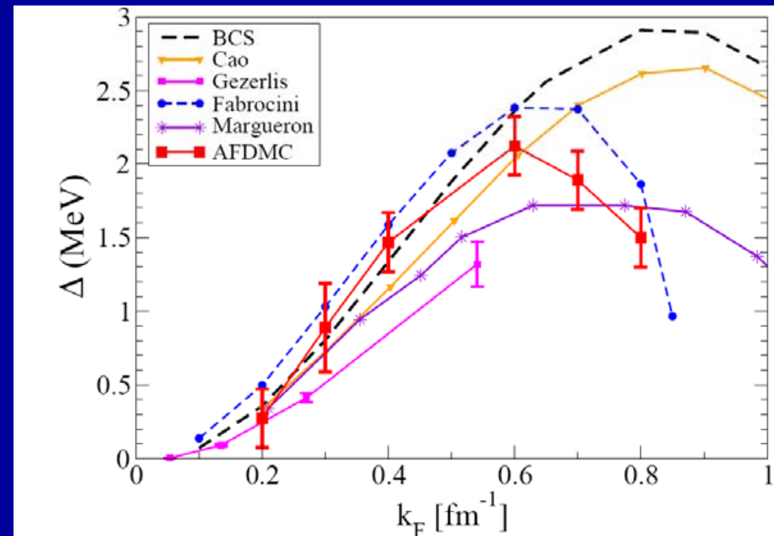
with $h_+^s = h_{2+}^v$, a_+^s and h_∇^s the two free parameters. Such a form is obtained by adding



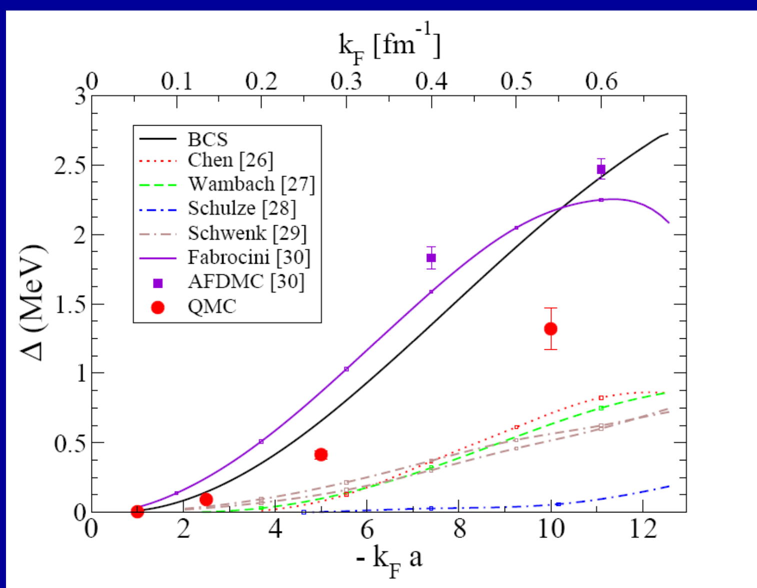


Baldo, Schuck, and Vinas, arXiv:0706.0658

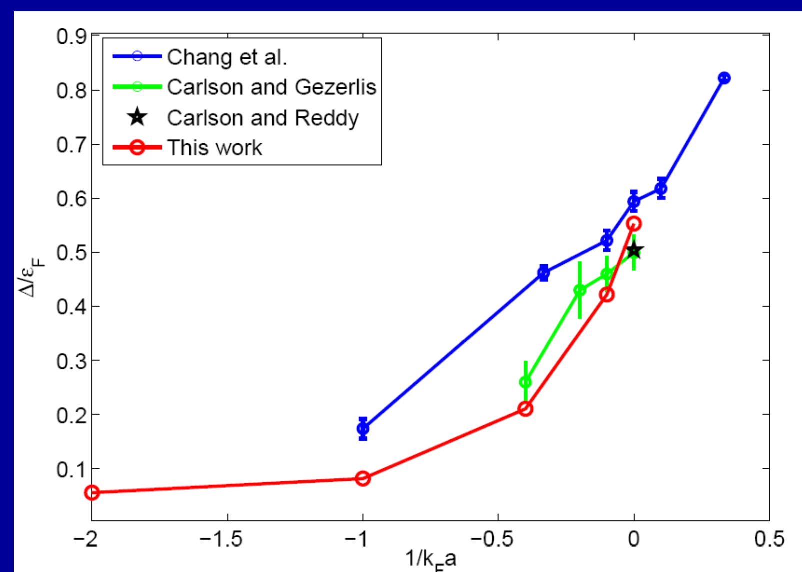




Gandolfi et al. arXiv:0805.2513



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

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

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

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 the anomalous 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.

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

Isospin symmetric

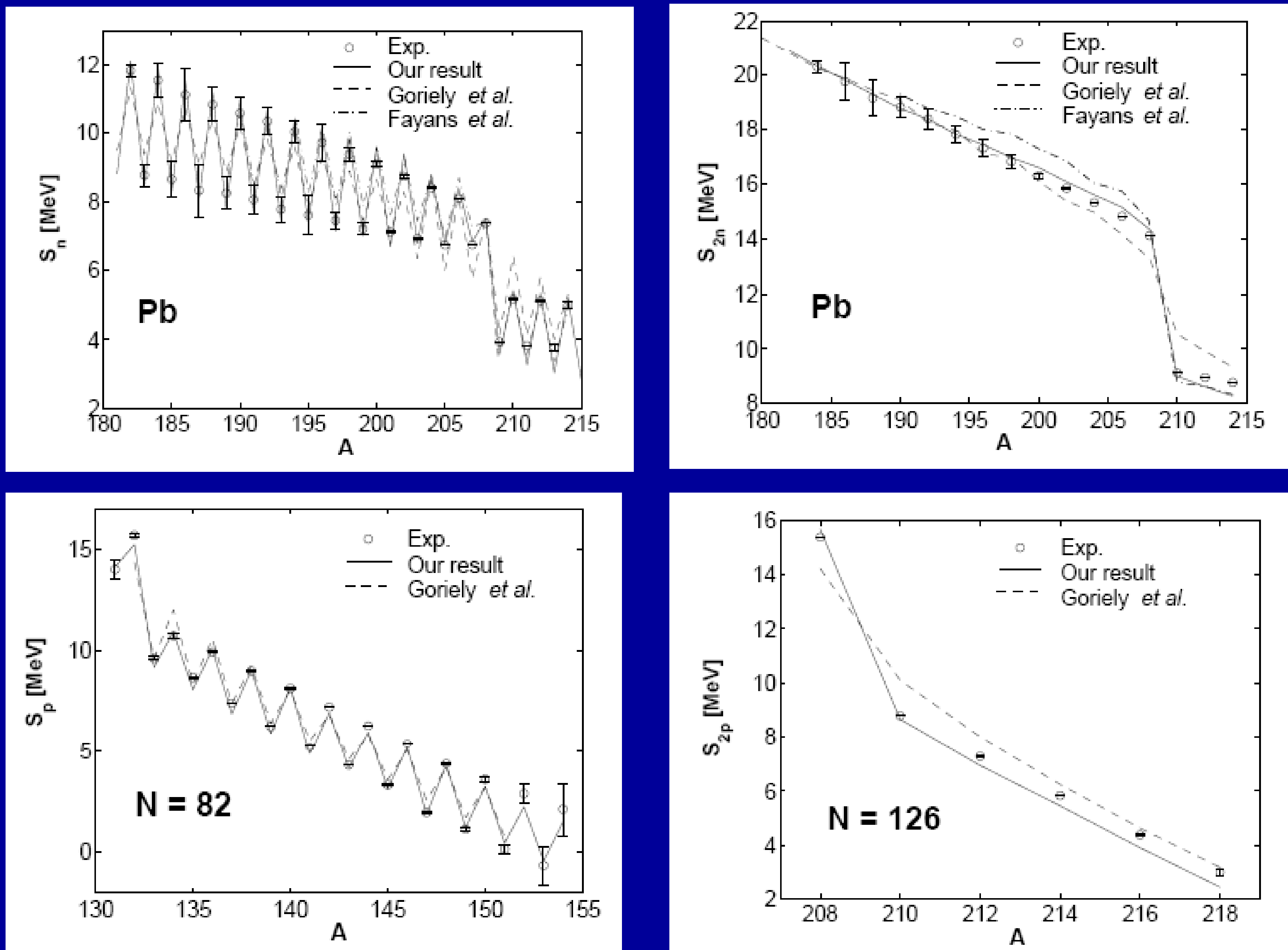
$$\varepsilon_S\left[\nu_p,\nu_n\right]=\overbrace{g(\rho_p,\rho_n)[|\nu_p|^2+|\nu_n|^2]}$$

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

$$\text{where}\quad g(\rho_p,\rho_n)=g(\rho_n,\rho_p)$$

$$\text{and}\quad f(\rho_p,\rho_n)=f(\rho_n,\rho_p)$$

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



A single universal parameter for pairing!

Intermission

Part II

Time Dependent Phenomena

The time-dependent density functional theory is viewed in general as a reformulation of the exact quantum mechanical time evolution of a many-body system when only single-particle properties are considered.

TDDFT for normal systems:

A.K. Rajagopal and J. Callaway, Phys. Rev. B 7, 1912 (1973)
V. Peuckert, J. Phys. C 11, 4945 (1978)
E. Runge and E.K.U. Gross, Phys. Rev. Lett. 52, 997 (1984)
http://www.tddft.org

TDSLDA

$$E(t) = \int d^3r \ \left[\ \varepsilon(n(\vec{r},t), \tau(\vec{r},t), \nu(\vec{r},t), \underline{\vec{j}(\vec{r},t)}) + V_{ext}(\vec{r},t)n(\vec{r},t) + \ldots \right]$$

$$\begin{cases} [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu]\mathrm{u}_\mathrm{i}(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)]\mathrm{v}_\mathrm{i}(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{u}_\mathrm{i}(\vec{r},t)}{\partial t} \\ [\Delta^*(\vec{r},t) + \Delta^*_{ext}(\vec{r},t)]\mathrm{u}_\mathrm{i}(\vec{r},t) - [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu]\mathrm{v}_\mathrm{i}(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{v}_\mathrm{i}(\vec{r},t)}{\partial t} \end{cases}$$

For time-dependent phenomena one has to add currents!

Mathematical formulation

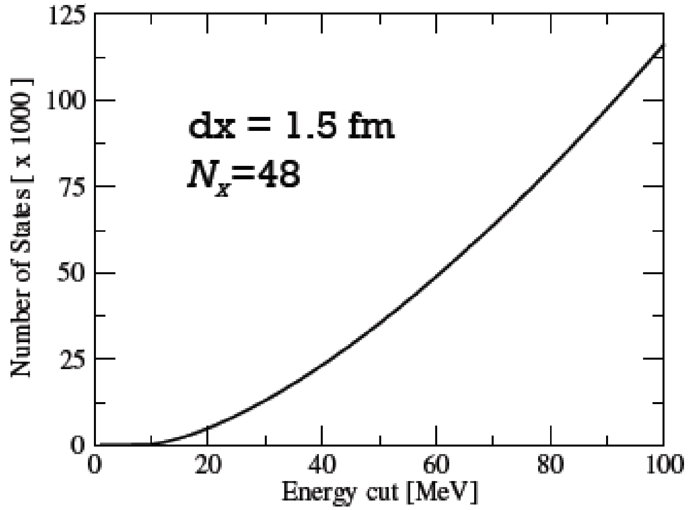
$$E_{g.s.} = \int d^3r \left(\frac{\hbar^2}{2m}\tau(r) + \mathcal{E}[\rho(\vec{r}), \tau(\vec{r}), \nu(\vec{r})] + V_{ext}(\vec{r})\rho(\vec{r}) \right)$$

$$\mathcal{E}[\rho(\vec{r}), \tau(\vec{r}), \nu(\vec{r})] = \mathcal{E}_N[\rho(\vec{r}), \tau(\vec{r})] + \mathcal{E}_S[\rho(\vec{r}), \nu(\vec{r})]$$

$$\begin{pmatrix} h(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(h^*(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix}$$

- Hermitian eigenvalue problem
- (Almost) all eigenvalues required

$$h(\vec{r}) = -\vec{\nabla}\frac{\hbar^2}{2m^*(\vec{r})}\vec{\nabla} + U(\vec{r})$$



From a talk given by I. Stetcu, UNEDF 2010

Normal Energy Functionals

Cold atoms:

$$\mathcal{E}(\vec{r}) = \frac{1}{2}\tau(\vec{r}) + \gamma\frac{|\nu(\vec{r})|^2}{\rho^{1/3}(\vec{r})} + \beta\frac{3(3\pi^2)^{2/3}\rho^{5/3}(\vec{r})}{10} + V_{ext}(\vec{r})\rho(\vec{r})$$

$$h(\vec{r}) = \frac{1}{2}\vec{\nabla}^2 + \beta\frac{3\pi^2\rho^{1/3}(\vec{r}))^{2/3}}{2} - \frac{|\Delta(\vec{r})|^2}{3\gamma\rho^{2/3}(\vec{r})} + V_{ext}(\vec{r})$$

Nuclear systems:

$$\mathcal{E}(\vec{r}) = \frac{1}{2M_n}\tau_n(\vec{r}) + \frac{1}{2M_p}\tau_p(\vec{r}) - \Delta(\vec{r})\nu_c(\vec{r})$$
$$+ \sum_{T=0,1}\Big(C_T^\rho\rho_T^2 + C_T^\Delta\rho_T\nabla^2\rho_T + C_\gamma\rho_0^\gamma\rho_T^2$$
$$+C_T^\tau(\rho_T\tau_T - \vec{j}_T^2) + C_T^{\nabla J}(\rho_T\vec{\nabla}\cdot\vec{J} + \vec{s}_T\times\vec{j}_T)\Big)$$

Galilean invariance

$$h(\vec{r}) = U(\vec{r}) + \vec{V}(\vec{r})\cdot\vec{\sigma} - i\vec{V}_1(\vec{r})\cdot\vec{\nabla} - i\vec{W}(\vec{r})\cdot(\vec{\sigma}\times\vec{\nabla})$$

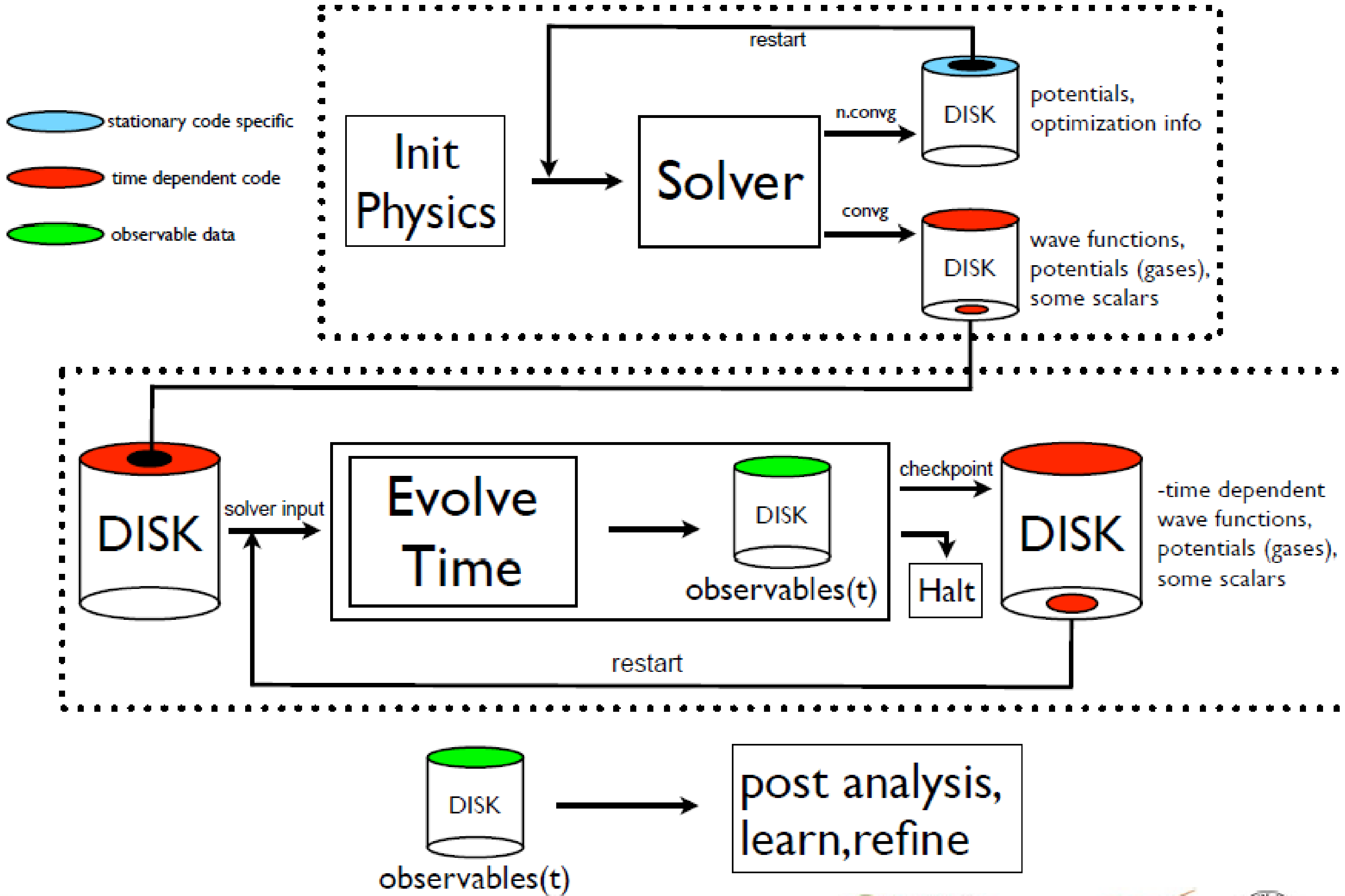
From a talk given by I. Stetcu, UNEDF 2010

Lattice representation

- quasiparticle wavefunctions represented on a lattice
- periodic boundary conditions
- N_x, N_y, N_z spatial points
- derivatives computed with FFT
- good description of the relevant DOF for E>0
- <u>(almost) unique ability to describe correctly all components of the quasiparticle wavefunctions</u>

From a talk given by I. Stetcu, UNEDF 2010

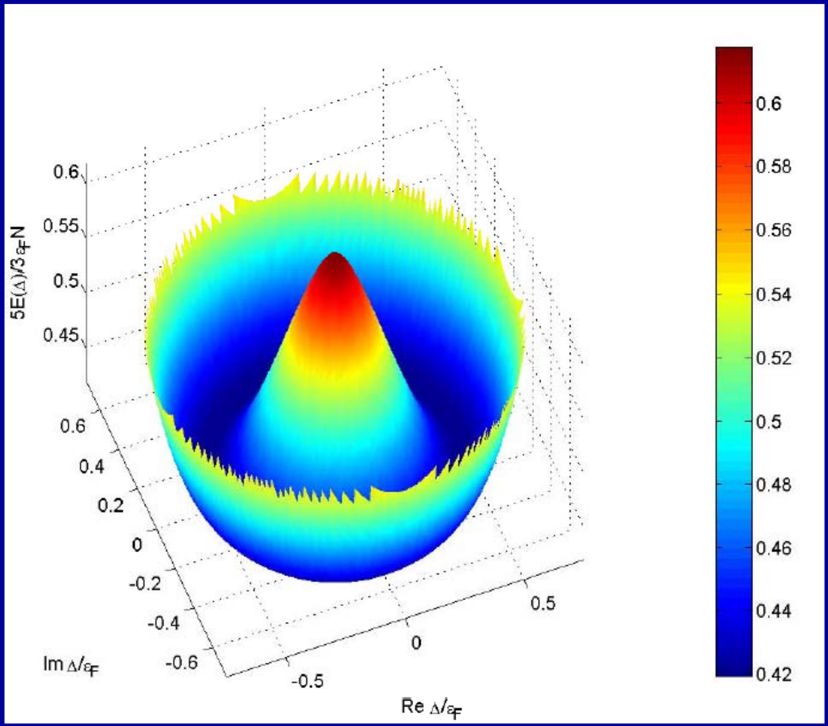
Structure of the SLDA Production Software



From a talk given by K.J. Roche, UNEDF 2010

A very rare excitation mode: the Higgs pairing mode.

Energy of a Fermi system as a function of the pairing gap



$$\dot{n} + \vec{\nabla} \cdot \left[\vec{v} n \right] = 0$$

$$m\dot{\vec{v}} + \vec{\nabla} \left\{ \frac{m\vec{v}^2}{2} + \mu\left[n \right] \right\} = 0$$

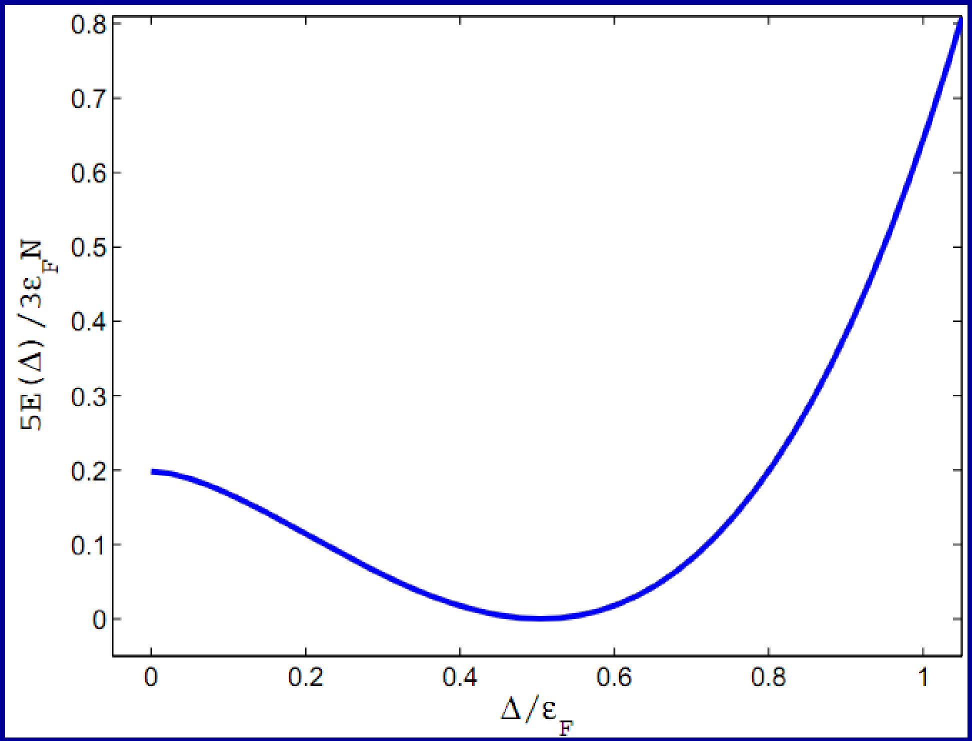
$$i\hbar\dot{\Psi}(\vec{r},t) = -\frac{\hbar^2 \Delta}{4m}\Psi(\vec{r},t) + U\left(\left| \Psi(\vec{r},t) \right|^2 \right)\Psi(\vec{r},t)$$

Quantum hydrodynamics

"Landau-Ginzburg" equation

Higgs mode

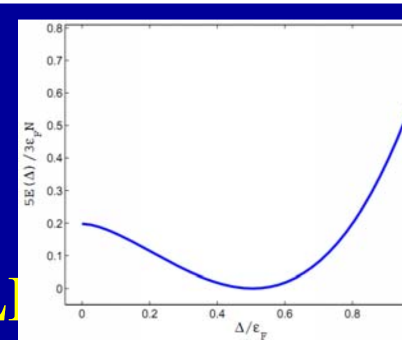
Small amplitude oscillations of the modulus of the order parameter (pairing gap)



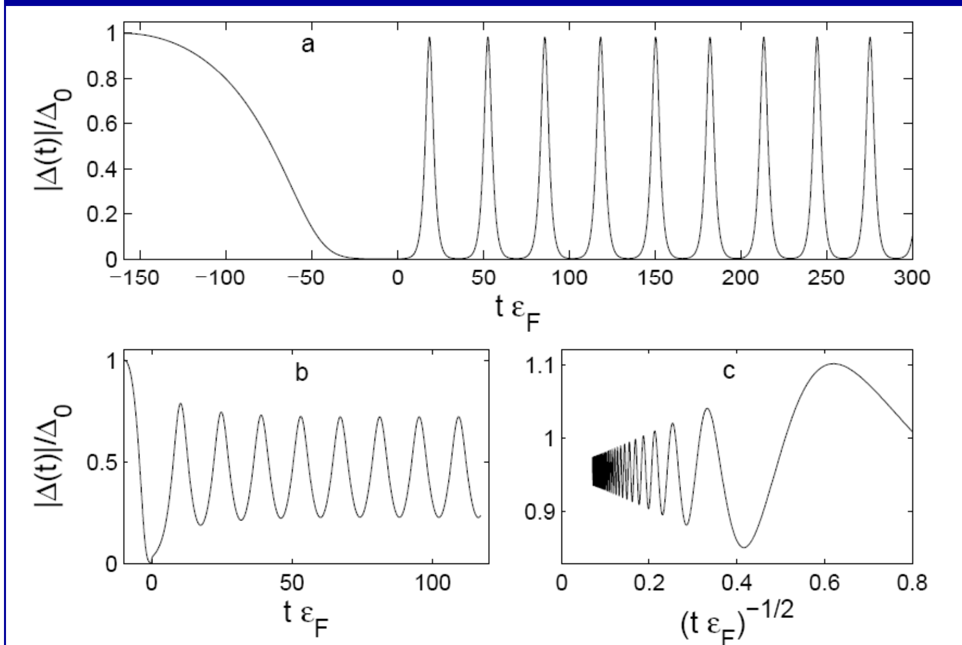
$$\hbar\Omega_H = 2\Delta_0$$

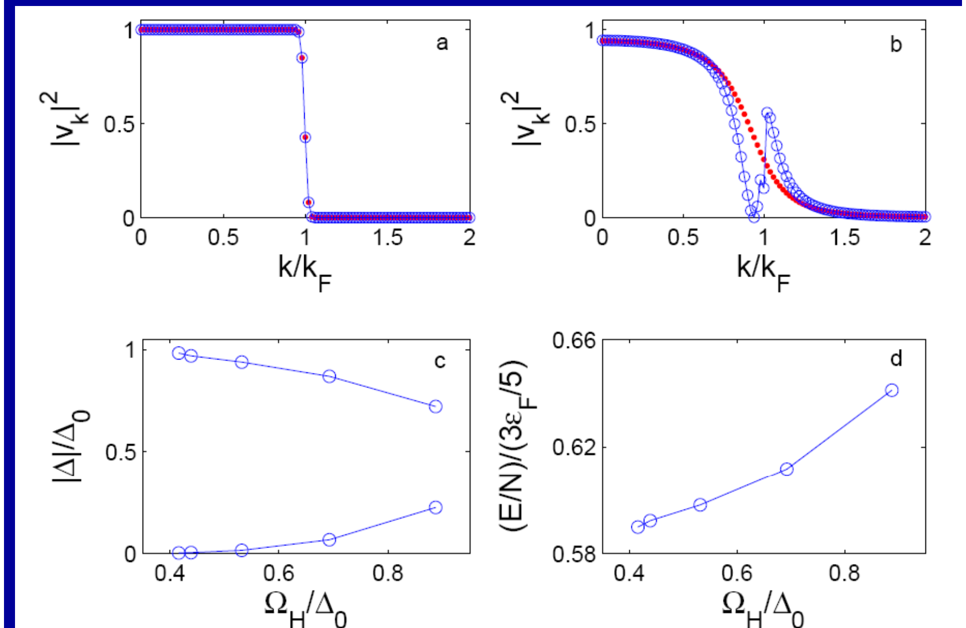
This mode has a bit more complex character
cf. **Volkov and Kogan (1972)**

Response of a unitary Fermi system to changing the scattering length with time



Tool: TD DFT extension to superfluid systems (TD-SL





- All these modes have a very low frequency below the pairing gap and a very large amplitude and excitation energy as well

- None of these modes can be described either within Quantum Hydrodynamics or Landau-Ginzburg like approaches

Bulgac and Yoon, Phys. Rev. Lett. 102, 085302 (2009)

TDSLDA
(equations TDHFB/TDBdG like)

$$
i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{h}_{\uparrow\uparrow}(\vec{r},t)-\mu & \hat{h}_{\uparrow\downarrow}(\vec{r},t) & 0 & \Delta(\vec{r},t) \\ \hat{h}_{\downarrow\uparrow}(\vec{r},t) & \hat{h}_{\downarrow\downarrow}(\vec{r},t)-\mu & -\Delta(\vec{r},t) & 0 \\ 0 & -\Delta^{*}(\vec{r},t) & -\hat{h}^{*}_{\uparrow\uparrow}(\vec{r},t)+\mu & -\hat{h}^{*}_{\uparrow\downarrow}(\vec{r},t) \\ \Delta^{*}(\vec{r},t) & 0 & -\hat{h}^{*}_{\downarrow\uparrow}(\vec{r},t) & -\hat{h}^{*}_{\downarrow\downarrow}(\vec{r},t)+\mu \end{pmatrix}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix}
$$

- **The system is placed on a 3D spatial lattice**
- **Derivatives are computed with FFTW**
- **Fully self-consistent treatment with Galilean invariance**
- **No symmetry restrictions**
- **Number of quasiparticle wave functions is of the order of the number of spatial lattice points**
- **Initial state is the ground state of the SLDA (formally like HFB/BdG)**
- **The code was implementation on JaguarPf**

I will present a few short movies, illustrating the complex time-dependent dynamics in 3D of a unitary Fermi superfluid and of ^{280}Cf excited with various external probes.

In each case we solved on JaguarPf the TDSLDA equations for a 32^3 spatial lattice (approximately 30k to 40k quasiparticle wavefunctions) for about 10k to 100k time steps using from about 30K to approximately 40K PEs

Fully unrestricted calculations!

The size of the problem we solve here is <u>several orders of magnitude</u> larger than any other similar problem studied by other groups (and we plan to further increase the size significantly).

The movies will be eventually posted at

http://www.phys.washington.edu/groups/qmbnt/index.html

Summary

• ***<u>Created a set of accurate and efficient tools for the petaflop regime</u>***

Successfully implementated on leadership class computers (Franklin, JaguarPF)

• Currently capable of treating nuclear volumes as large as 50^3 fm^3 , for up to 10,000-20,000 fermions , and for times up to a fraction of an attosecond fully self-consistently and with no symmetry restrictions and under the action of complex spatio-temporal external probes

• Capable of treating similarly large systems of cold atoms

• The suites of codes can handle systems and phenomena ranging from:

ground states properties
excited states in the linear response regime,
large amplitude collective motion,
response to various electromagnetic and nuclear probes,

• There is a clear path towards exascale applications and implementation of the Stochastic TD(A)SLDA