Static and TD (A)SLDA for cold atoms and nuclei

Aurel Bulgac

UNEDF collaborators: Piotr Magierski, Kenny Roche, Sukjin Yoon
Non-UNEDF collaborators: Joaquin E. Drut, Michael M. Forbes, Yongle Yu
Likely future collaborators: Mihai Horoi, Ionel Stetcu

We are facing two types of challenges in UNEDF:

- **Conceptual challenge: How to relate *ab initio* calculations to a nuclear DFT?**

- **Computational challenge: How to implement nuclear DFT on petascale (and beyond) on computers?**

Some of these aspects have been covered in talks given by Piotr Magierski (static ASLDA) and by Kenny Roche (TD ASLDA).

Static ASLDA awaits to be implemented on parallel architectures.

TD ASLDA awaits to be "married" to the static ASLDA and applied to a new physical problem, and used on a large scale.

Outline:

- SLDA and fermions in traps
- Pairing gap in cold atoms and neutron matter
- SLDA and pairing in nuclei
- ASLDA
- TD-SLDA, and a remarkable case of LACM
- the 3rd year plan and the 4th and 5th year projections

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**

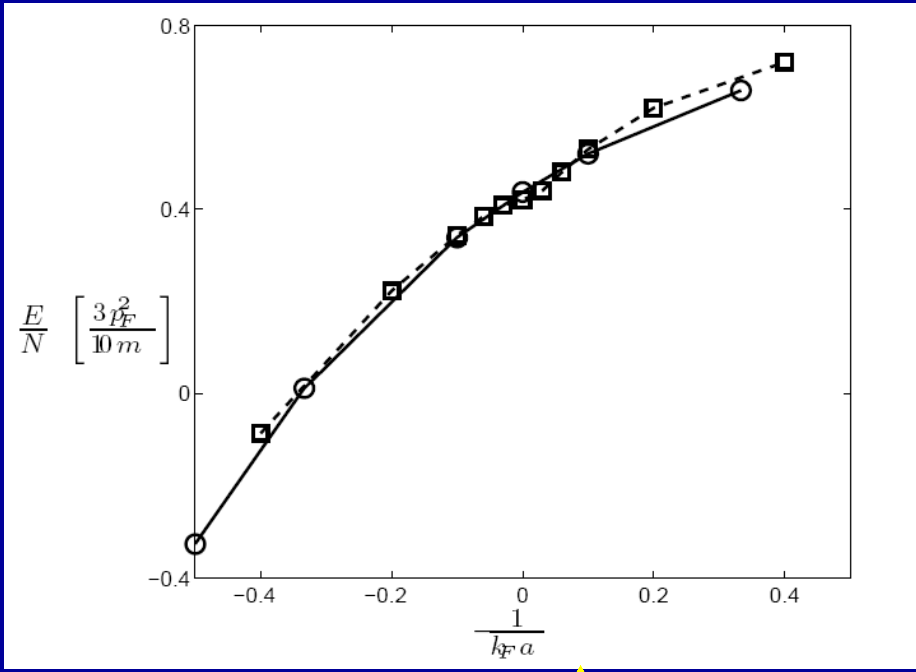
- ❑ **Extract the energy density functional (EDF)**

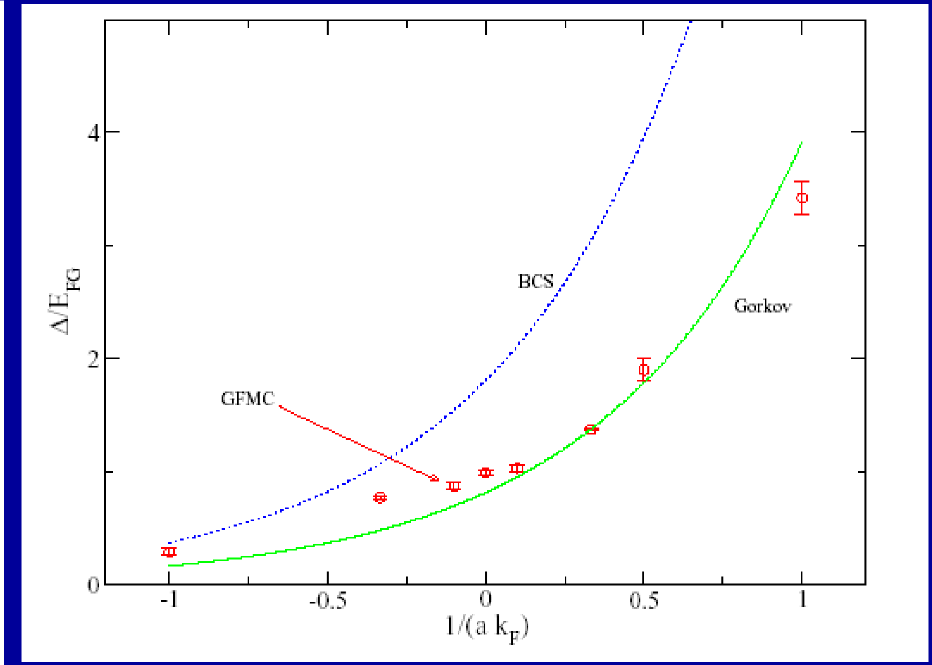
- ❑ **Add gradient corrections, if needed or known how (?)**

- ❑ **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!**

BEC side **BCS side**





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)

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

Only this combination is cutoff independent

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

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

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

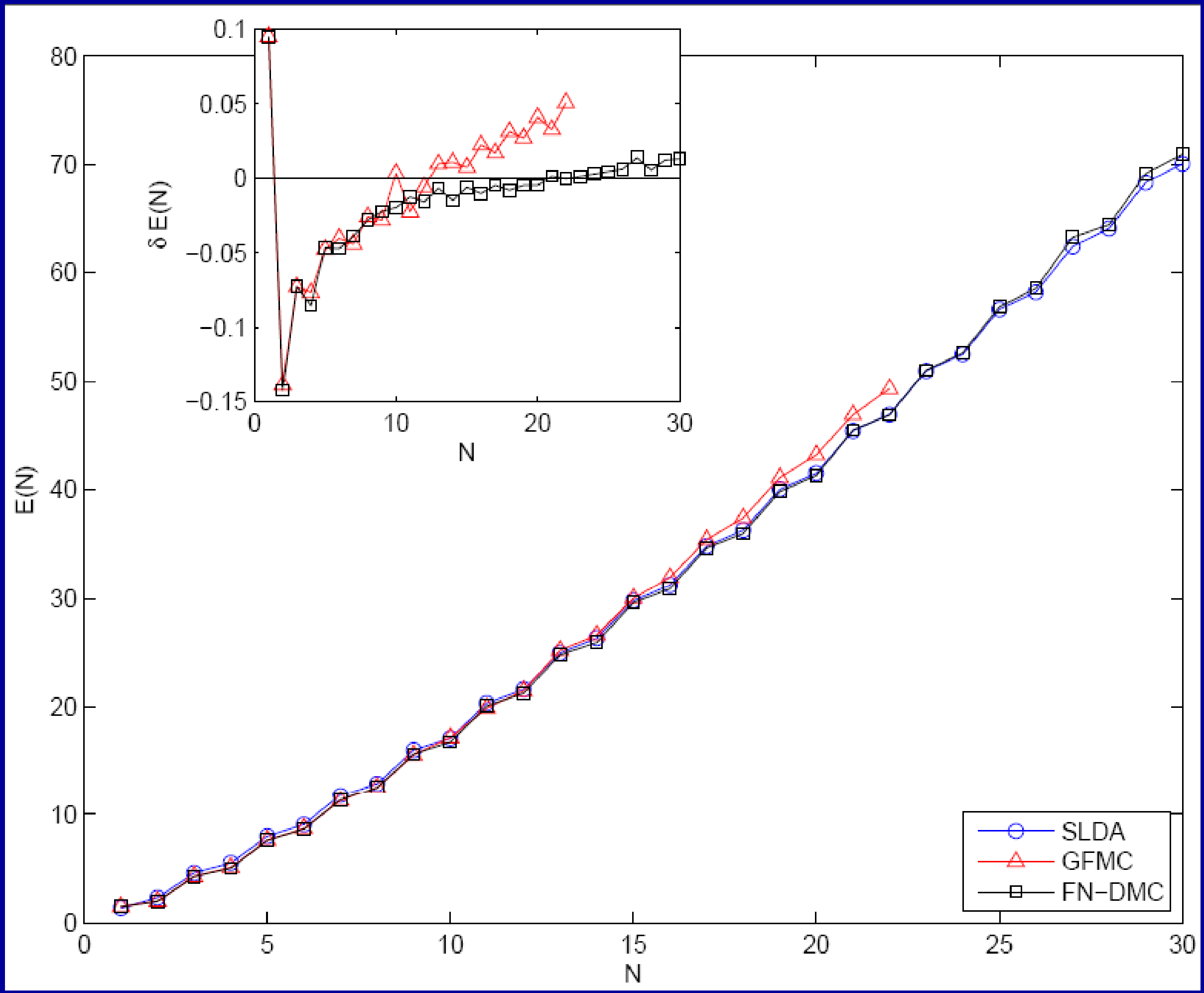
$$U(\vec{r}) = \beta \frac{(3\pi^2)^{2/3} n^{2/3}(\vec{r})}{2} - \frac{\left|\Delta(\vec{r})\right|^2}{3\gamma n^{2/3}(\vec{r})} + V_{ext}(\vec{r}) + \text{small correction}$$

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

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

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

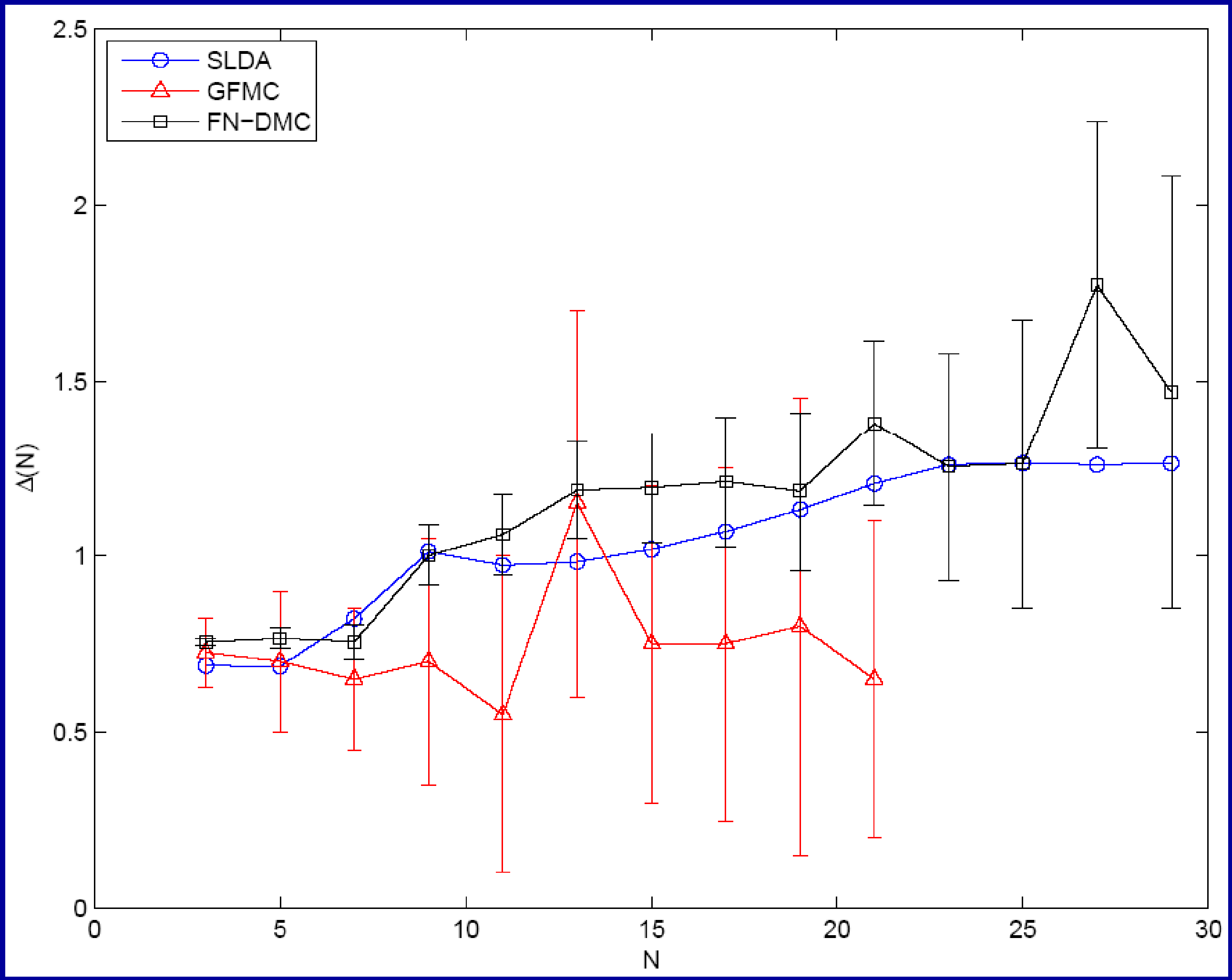


GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)

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

PRA 76, 053613 (2007)

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



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**

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

- **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, … <u>but very likely small</u>!!!**

How to make SLDA work in case of nuclei?

JETP LETTERS VOLUME 68, NUMBER 3 10 AUGUST 1998

Towards a universal nuclear density functional

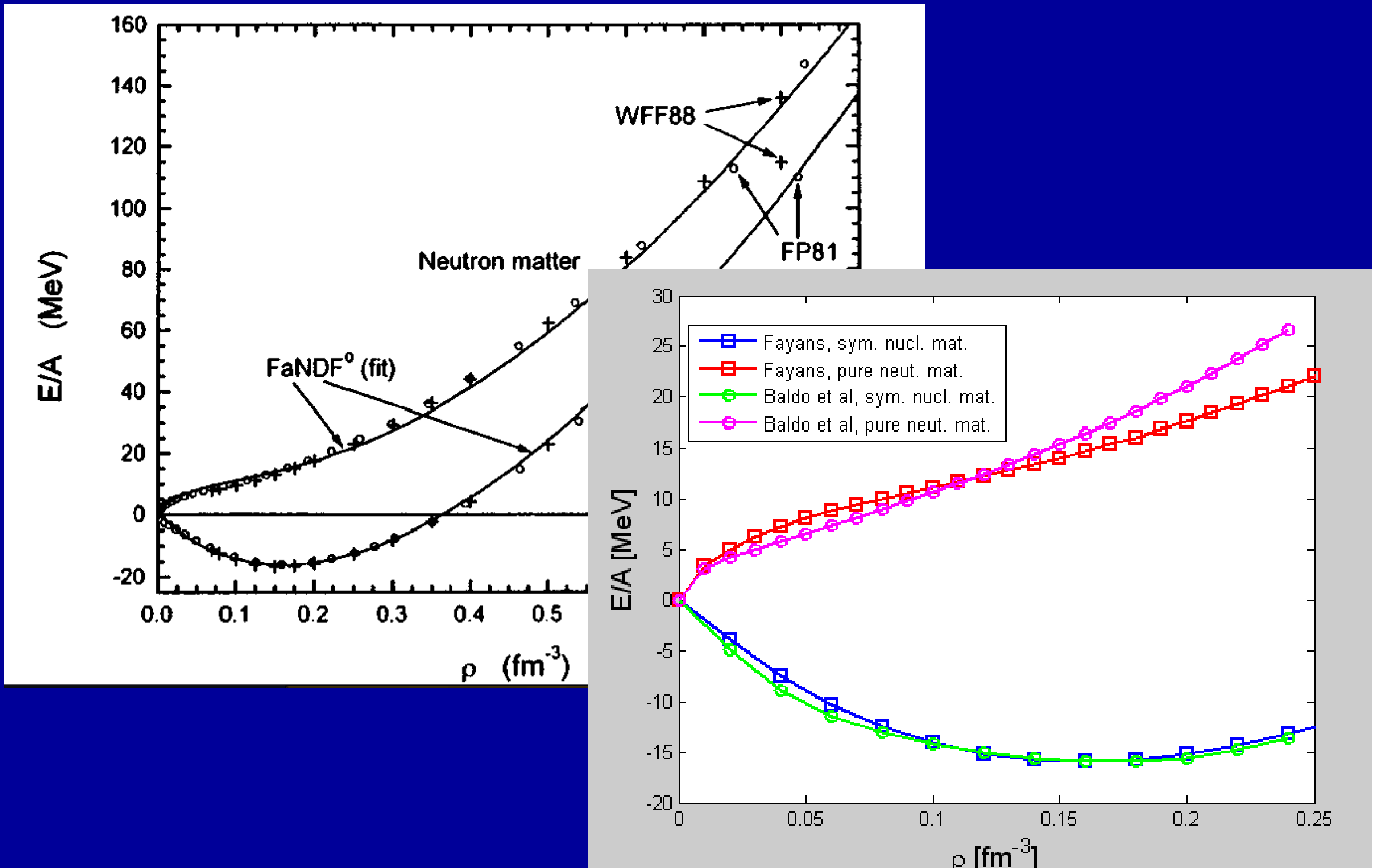
S. A. Fayans
Kurchatov Institute Russian Science Center, 123182 Moscow, Russia

$$\mathcal{E} = \mathcal{E}_{\text{kin}} + \mathcal{E}_{\text{vol}} + \mathcal{E}_{\text{surf}} + \mathcal{E}_{\text{Coul}} + \mathcal{E}_{\text{so}} + \mathcal{E}_{\text{pair}}, \qquad \mathcal{E}_{\text{kin}} = \left\langle \frac{\vec{p}^{\,2}}{2m} \right\rangle$$

$$\mathcal{E}_{\text{surf}} = \frac{2}{3}\varepsilon_F^0 \rho_0 \frac{a_+^s r_0^2 \left(\vec{\nabla} x_+\right)^2}{1 + h_+^s x_+^\sigma + h_\nabla^s r_0^2 \left(\vec{\nabla} x_+\right)^2}, \quad \mathrm{x}_\pm = \frac{\rho_n \pm \rho_p}{2\rho_0}$$

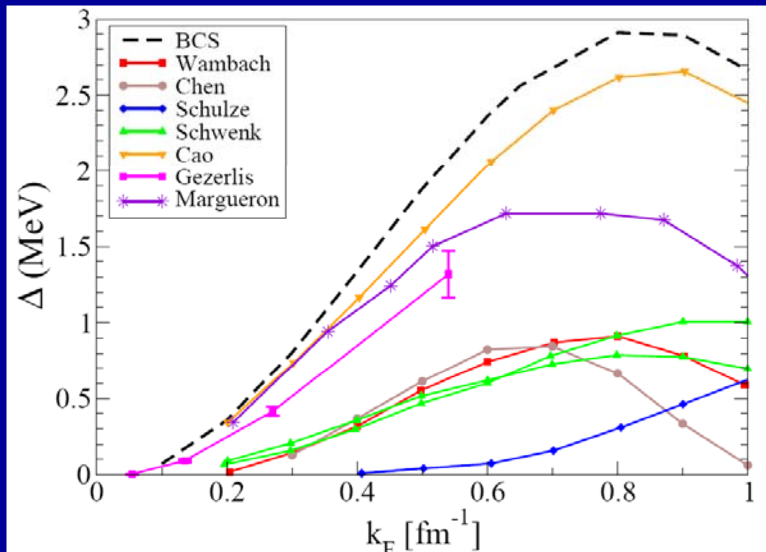
This is likely the first implementation of Kohn-Sham (DFT) methodology to nuclei.

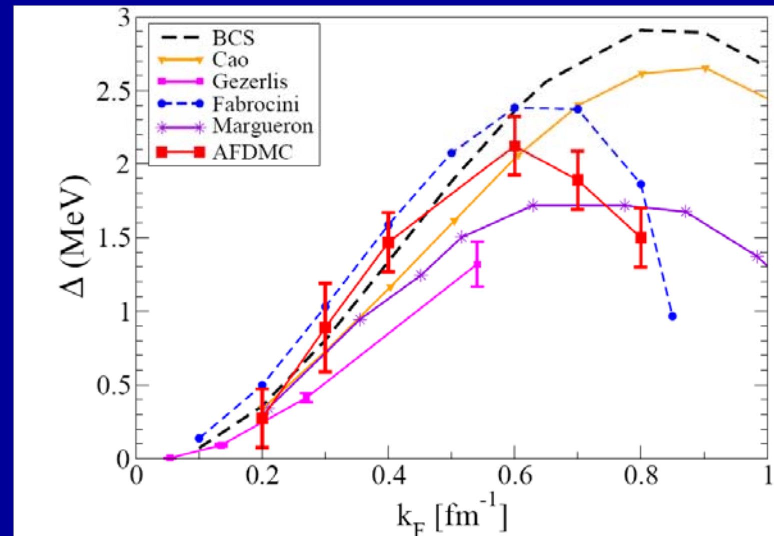
NB The term DFT is very much misused and abused in nuclear physics literature.



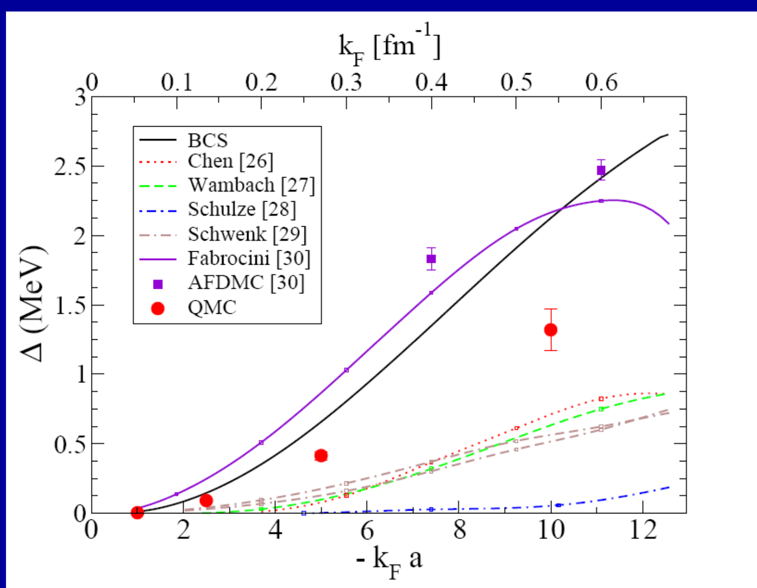
Baldo, Schuck, and Vinas, arXiv:0706.0658

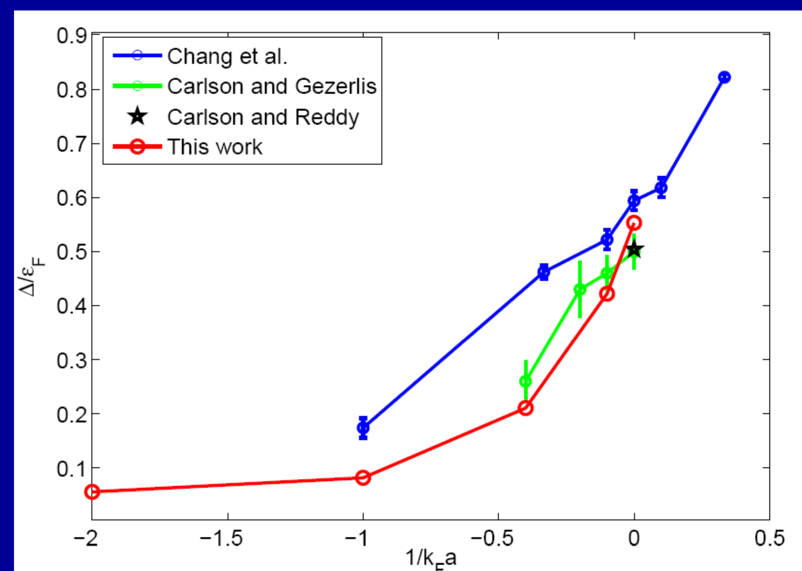
$$\mathcal{E} = \mathcal{E}_{\text{kin}} + \mathcal{E}_{\text{vol}} + \mathcal{E}_{\text{surf}} + \mathcal{E}_{\text{Coul}} + \mathcal{E}_{\text{so}} + \mathcal{E}_{\text{pair}}$$





Gandolfi et al. arXiv:0805.2513





Gezerlis and Carlson
PRC 77, 032801 (2008)

Bulgac, Drut and Magierski,
arXiv:0801.1504, arXiv:0803.3238

So far we seem to have (at last) a good handle <u>only</u> on the pure neutron/proton pairing in pure neutron/proton matter only at low densities!

It would be nice if one could improve on numerical accuracy.

In symmetric/non-pure matter the pairing is very likely stronger!

There is no compelling/phenomenological evidence for the presence of gradient terms for pairing.

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 Here s-wave pairing only (S=0 and T=1)!

The last term could not arise from a two-body bare interaction.

Are these the only terms compatible with isospin symmetry?

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

Isospin symmetric

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

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

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

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

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

Structure of nuclear (A)SLDA equations:

$$\begin{pmatrix} \hat{h}(\vec{r}) & \hat{\Delta}(\vec{r}) \\ \hat{\Delta}^\dagger(\vec{r}) & -\hat{h}(\vec{r}) \end{pmatrix} \begin{pmatrix} \mathrm{u}_\mathrm{n}(\vec{r}) \\ \mathrm{v}_\mathrm{n}(\vec{r}) \end{pmatrix} = E_n \begin{pmatrix} \mathrm{u}_\mathrm{n}(\vec{r}) \\ \mathrm{v}_\mathrm{n}(\vec{r}) \end{pmatrix},$$

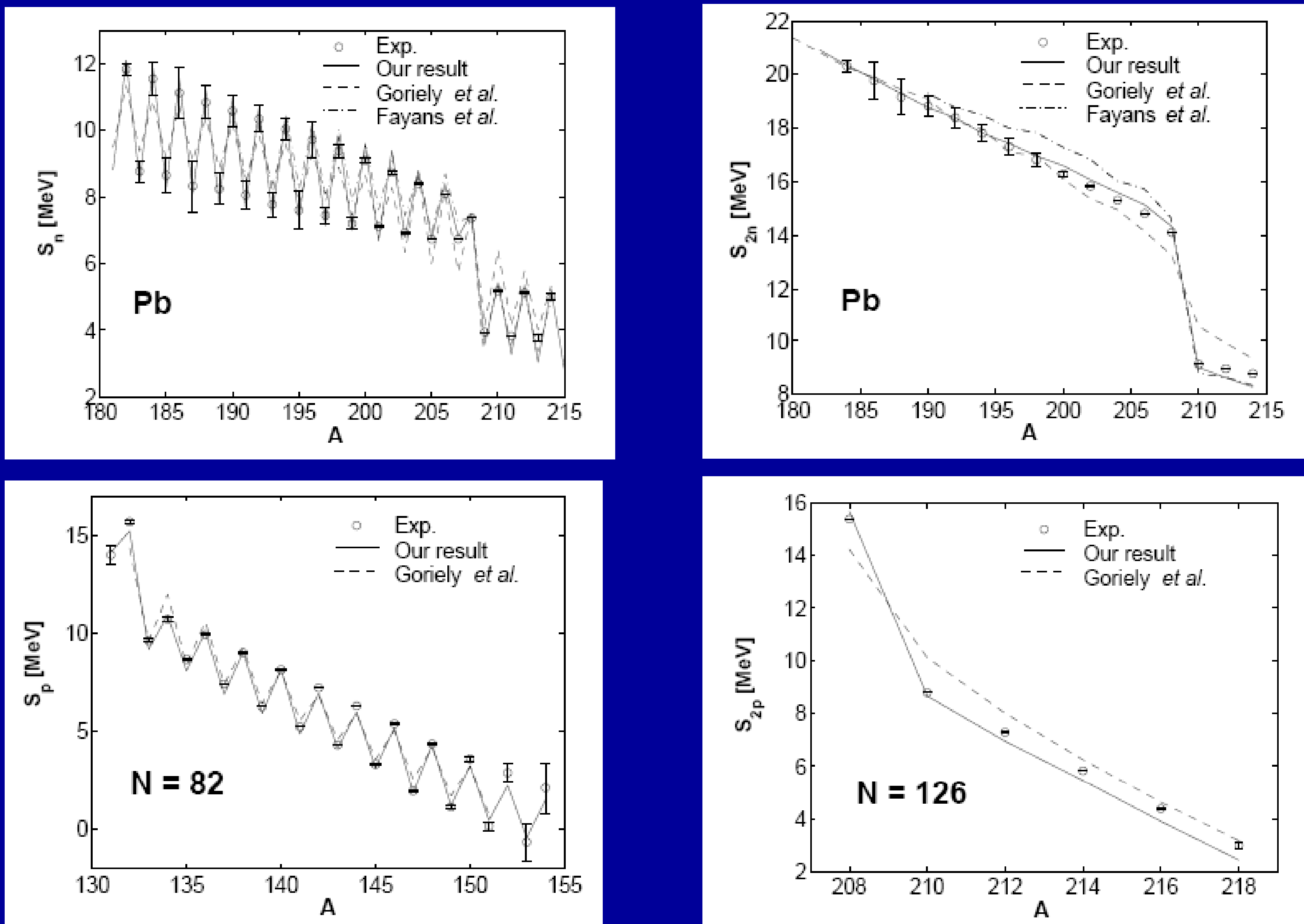
where both $\hat{h}(\vec{r})$ and $\hat{\Delta}(\vec{r})$ are 2×2 matrices and $\mathrm{u}_\mathrm{n}(\vec{r})$ and $\mathrm{v}_\mathrm{n}(\vec{r})$ are $2-$vectors

$$\mathrm{u}_\mathrm{n}(\vec{r}) = \begin{pmatrix} \mathrm{u}_{\mathrm{n}\uparrow}(\vec{r}) \\ \mathrm{u}_{\mathrm{n}\downarrow}(\vec{r}) \end{pmatrix}, \text{ and } \mathrm{v}_\mathrm{n}(\vec{r}) = \begin{pmatrix} \mathrm{v}_{\mathrm{n}\uparrow}(\vec{r}) \\ \mathrm{v}_{\mathrm{n}\downarrow}(\vec{r}) \end{pmatrix}, \text{ and}$$

$$\hat{h}(\vec{r}) = \begin{pmatrix} -\vec{\nabla}\cdot\left(\dfrac{\hbar^2}{2m_\uparrow(r)}\vec{\nabla}\right) + U_\uparrow(\vec{r}) - \mu_\uparrow & 0 \\ 0 & -\vec{\nabla}\cdot\left(\dfrac{\hbar^2}{2m_\downarrow(r)}\vec{\nabla}\right) + U_\downarrow(\vec{r}) - \mu_\downarrow \end{pmatrix} - i\hbar[\vec{\sigma}\times\vec{W}(\vec{r})]\cdot\vec{\nabla},$$

$$\hat{\Delta}(\vec{r}) = \begin{pmatrix} 0 & \Delta(\vec{r}) \\ -\Delta(\vec{r}) & 0 \end{pmatrix}.$$

NB Different effective masses, potentials and chemical potentials for spin-up and spin-down!



A single universal parameter for pairing!

Yu and Bulgac, Phys. Rev. Lett. 90, 222501 (2003)

Asymmetric SLDA (ASLDA), Bulgac and Forbes, arXiv:0804:3364

For spin polarized systems

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

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

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

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

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

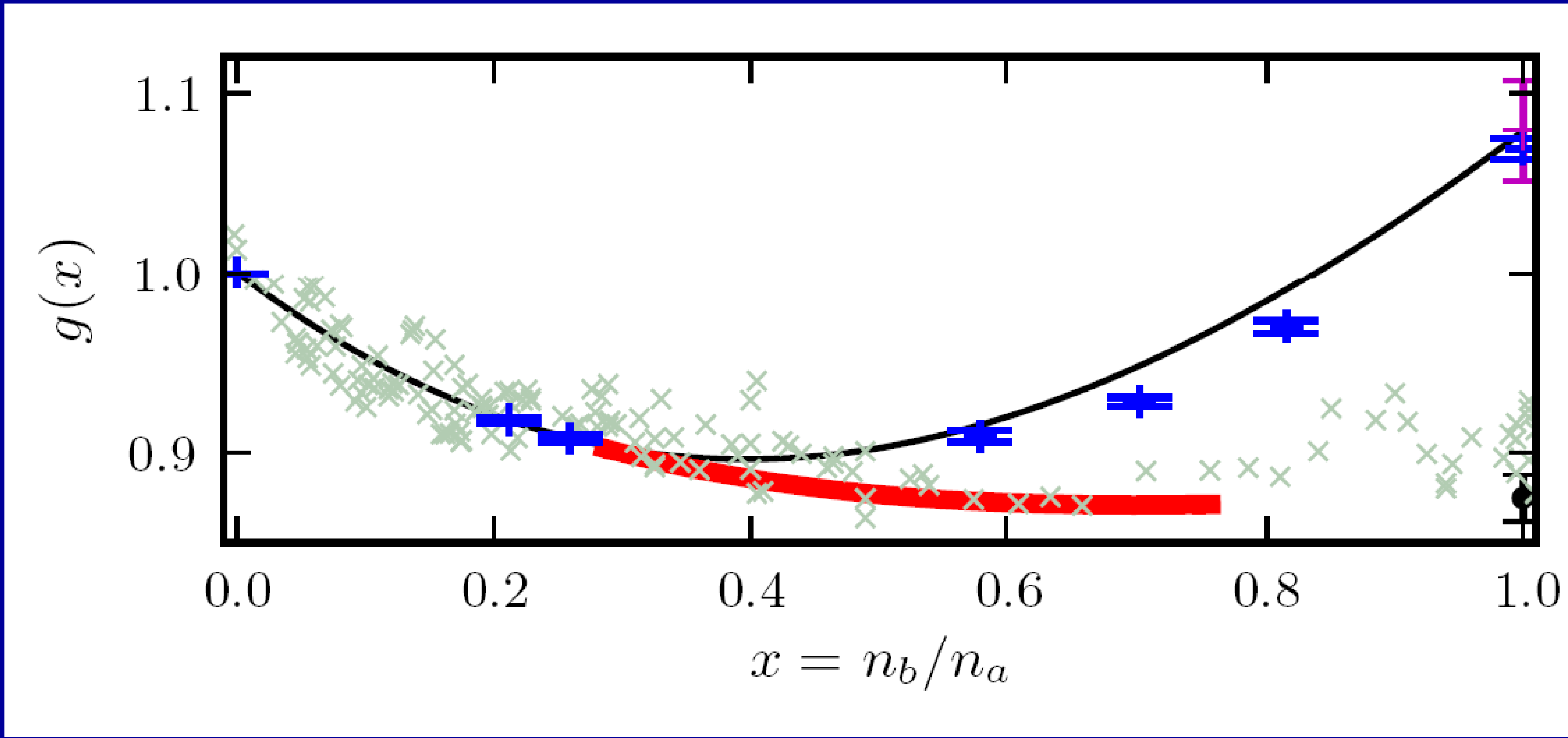
$$\alpha_a(\vec{r}) = \alpha\left[x(\vec{r})\right], \qquad \alpha_b(\vec{r}) = \alpha\left[1/x(\vec{r})\right], \qquad x(\vec{r}) = n_b(\vec{r})/n_a(\vec{r}),$$

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

Unitary spin polarized Fermi system

Bulgac and Forbes
PRA 75, 031605(R) (2007)
arXiv:0804:3364

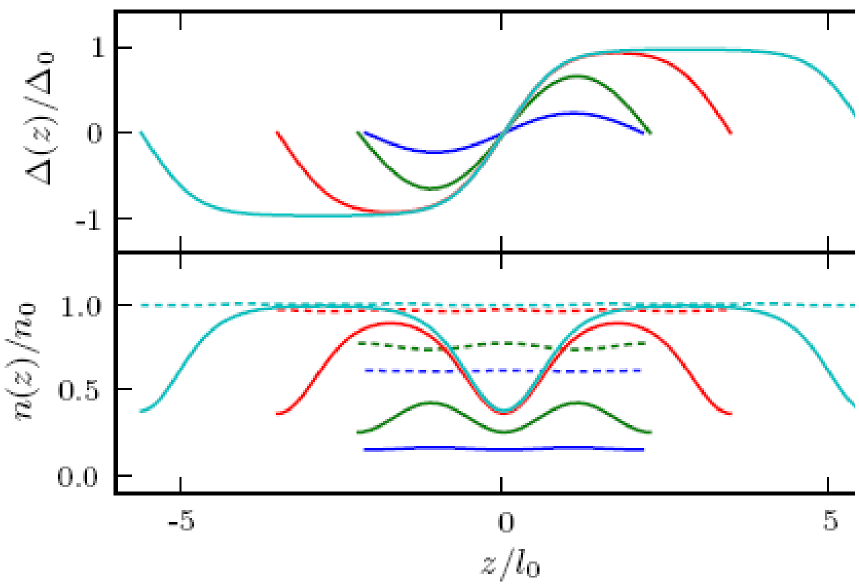
$$E[x] = \frac{3\left(3\pi^2\right)^{2/3}\hbar^2}{10m}\left[n_a g(x)\right]^{5/3}$$

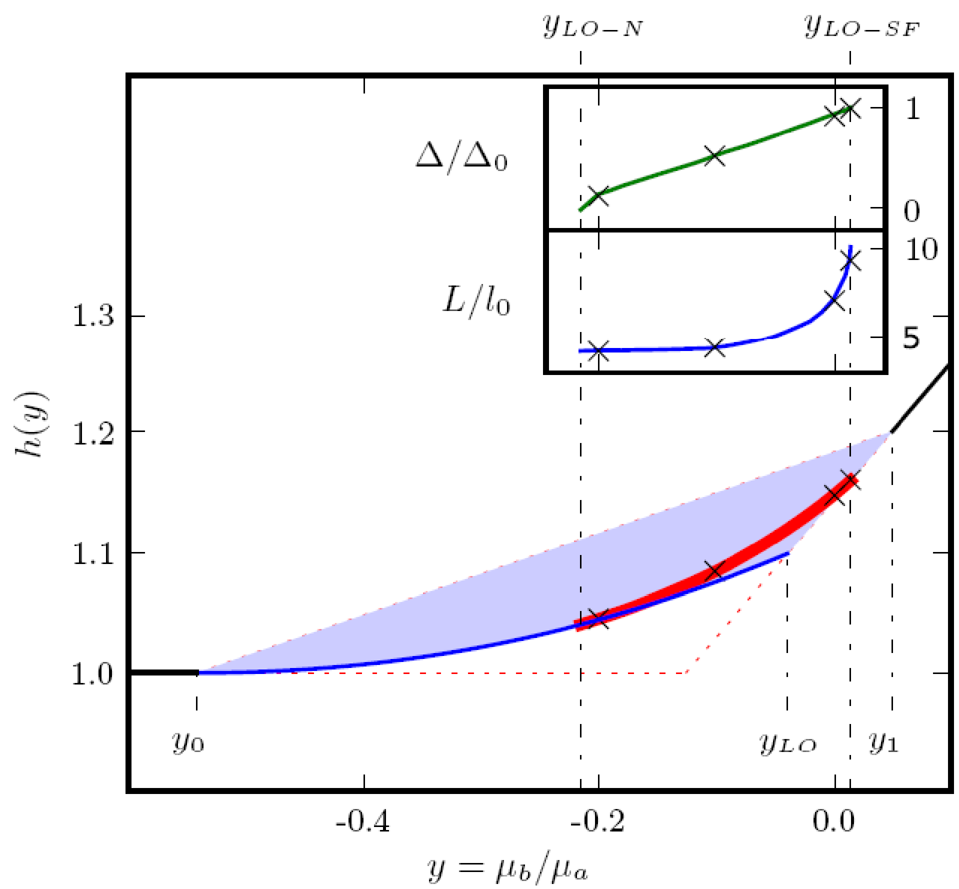


Crosses- MIT experiment 2007
Blue dots with error bars - MC for normal state 2007
Black dot with error bar s - MC for superfluid symmetric state 2003, 2004
Solid black line – normal part of EDF
Red solid line - Larkin-Ovchinnikov (B&F 2008)

Unitary Fermi Supersolid

Bulgac and Forbes, arXiv:0804:3364





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

TD ASLDA

Bulgac, Roche, Yoon

Future collaborators: Horoi(?) , Magierski, Stetcu(?)

$$i\hbar \frac{\partial}{\partial t}\begin{pmatrix} \mathrm{u}_\mathrm{n}(\vec{r},t) \\ \mathrm{v}_\mathrm{n}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{h}(\vec{r},t)+\hat{V}_\mathrm{ext}(\vec{r},t) & \hat{\Delta}(\vec{r},t)+\hat{\Delta}_\mathrm{ext}(\vec{r},t) \\ \hat{\Delta}^\dagger(\vec{r},t)+\hat{\Delta}^\dagger_\mathrm{ext}(\vec{r},t) & -\hat{h}(\vec{r},t)-\hat{V}_\mathrm{ext}(\vec{r},t) \end{pmatrix}\begin{pmatrix} \mathrm{u}_\mathrm{n}(\vec{r},t) \\ \mathrm{v}_\mathrm{n}(\vec{r},t) \end{pmatrix}$$

$$Q(\omega) = \sum_\sigma \int d^3 r dt Q(\vec{r},\sigma,t)\rho(\vec{r},\sigma,t)\exp(i\omega t)$$

$$N_x^3 \times N_t, \quad N_x \approx 50...100, \quad N_t \approx 10^4...10^5$$

$$\text{number of } \psi_n(\vec{r},\sigma,t) \approx O(N_x^3 \times 40)$$

Space-time lattice, use of FFTW for spatial derivative

No matrix operations (unlike (Q)RPA)

All nuclei (odd, even, spherical, deformed)

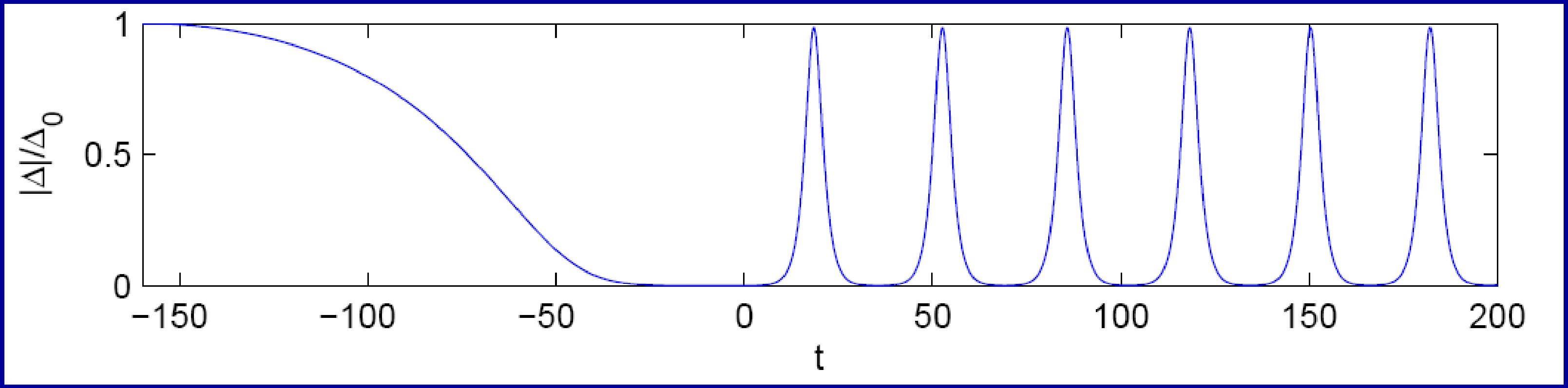
Any quantum numbers of QRPA modes

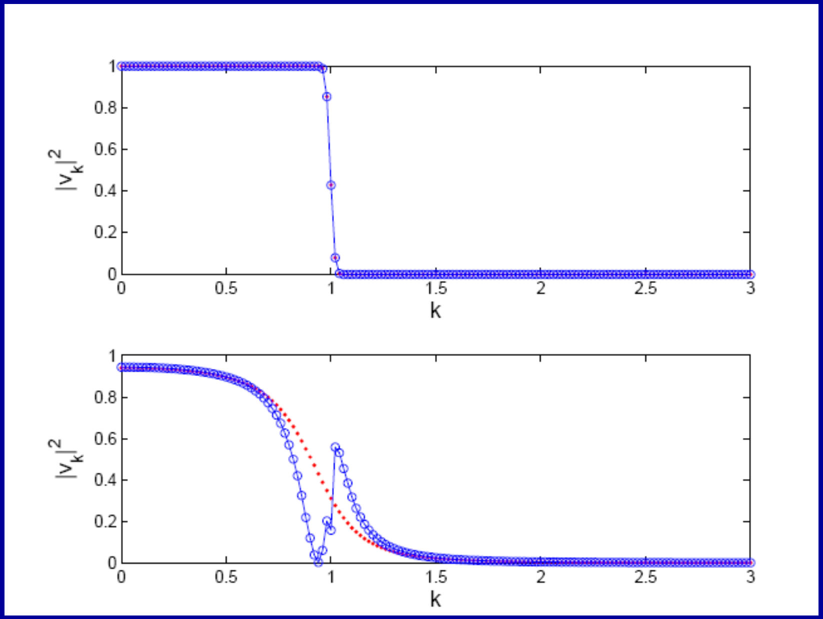
Fully selfconsistent, no self-consistent symmetries imposed

Higgs mode of the pairing field in a homogeneous unitary Fermi gas

Bulgac and Yoon, (2008, in preparation)

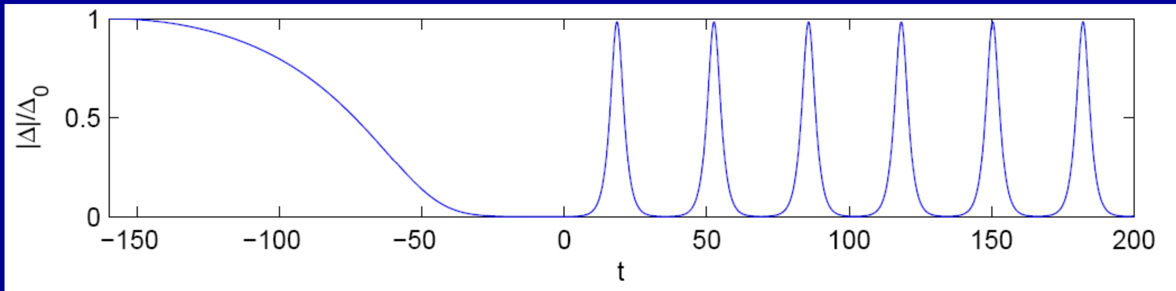
A remarkable example of extreme LACM

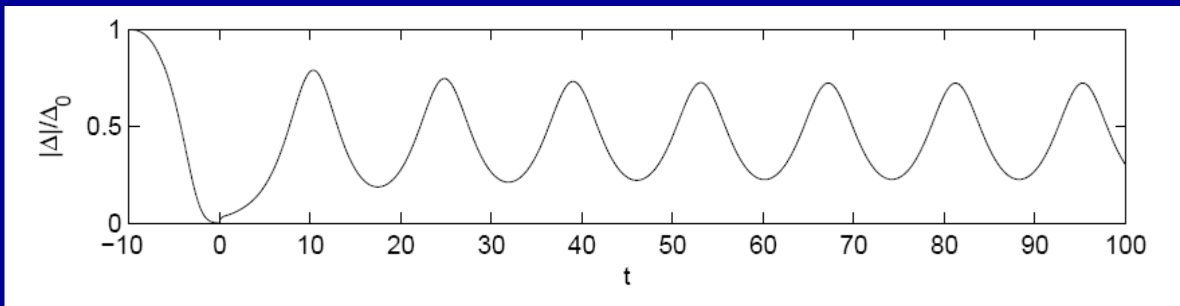


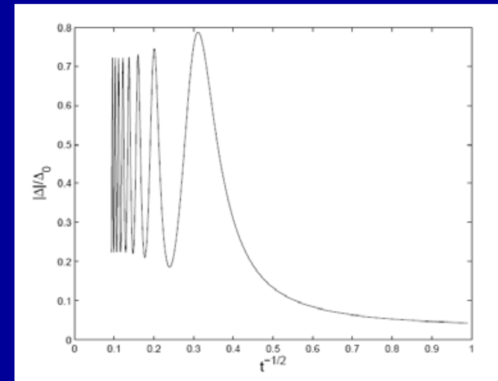


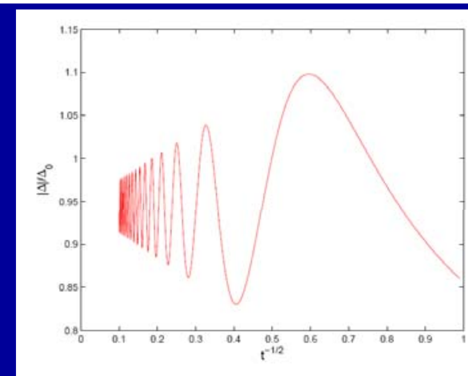
Energy and density constant!

Circa 30k-40k nonlinear coupled equations evolved for up to 250k time steps.



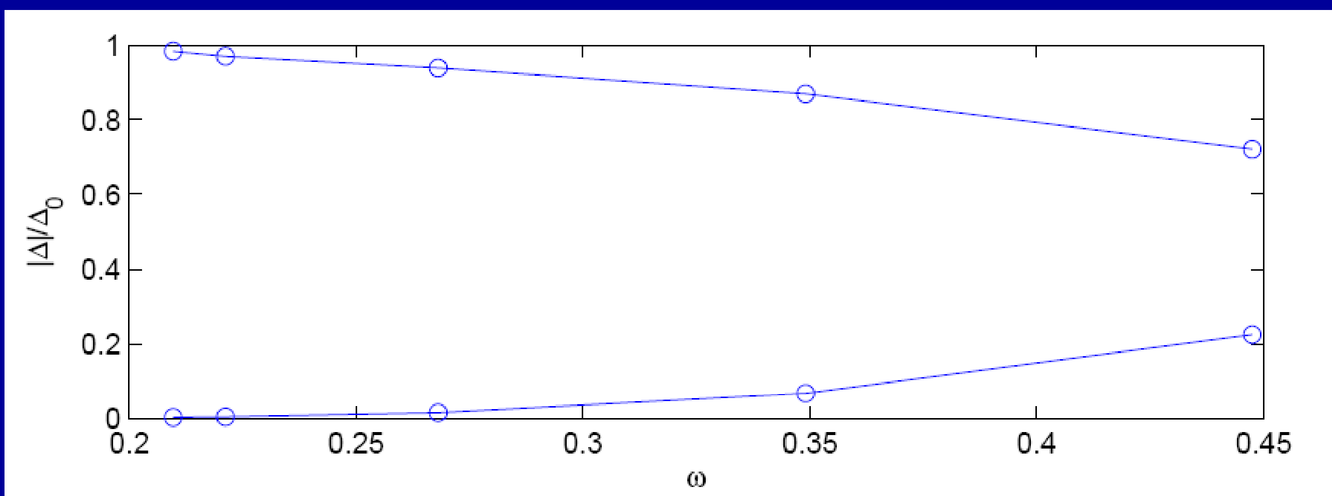






A zoo of Higgs-like pairing modes

The frequency of all these modes is below the 2-qp gap



Maximum and minimum oscillation amplitudes versus frequency

3rd year plan

- Validate the static 3D DFT solver and produce a parallel version (Bulgac, Magierski, Roche)
- Perform extensive tests and improve efficiency of the 3D DFT solver (Bulgac, Magierski, Roche)
- Investigate the potential implementation of a different type of 3D DFT solver
- Perform extensive testing of the nuclear TD ASLDA and produce a beta version (Bulgac, Roche, Stetcu(?))
- "Marry" the static ASLDA to TD ASLDA (Bulgac, Horoi (?), Magierski, Roche, Stetcu(?))
- Apply the nuclear TD ASLDA to an "interesting" problem (Bulgac, Horoi(?) Magierski, Roche, Stetcu(?))
- Investigate the spatio-temporal 1D dynamics of the Higgs mode (Bulgac, Yoon)
- Apply SLDA to neutron drops with the use of available *ab initio* results (Bulgac)

4th and 5th years projections

- Make both the static and the TD ASLDA available

- Use these codes for the refining of the Universal Nuclear Energy Density Functional and eventually for producing mass tables and properties of the excited states and pass on the results to for the use in nuclear reactions

- Start to use these codes for problems outside the nuclear physics in nuclear astrophysics , cold atom and condensed matter physics