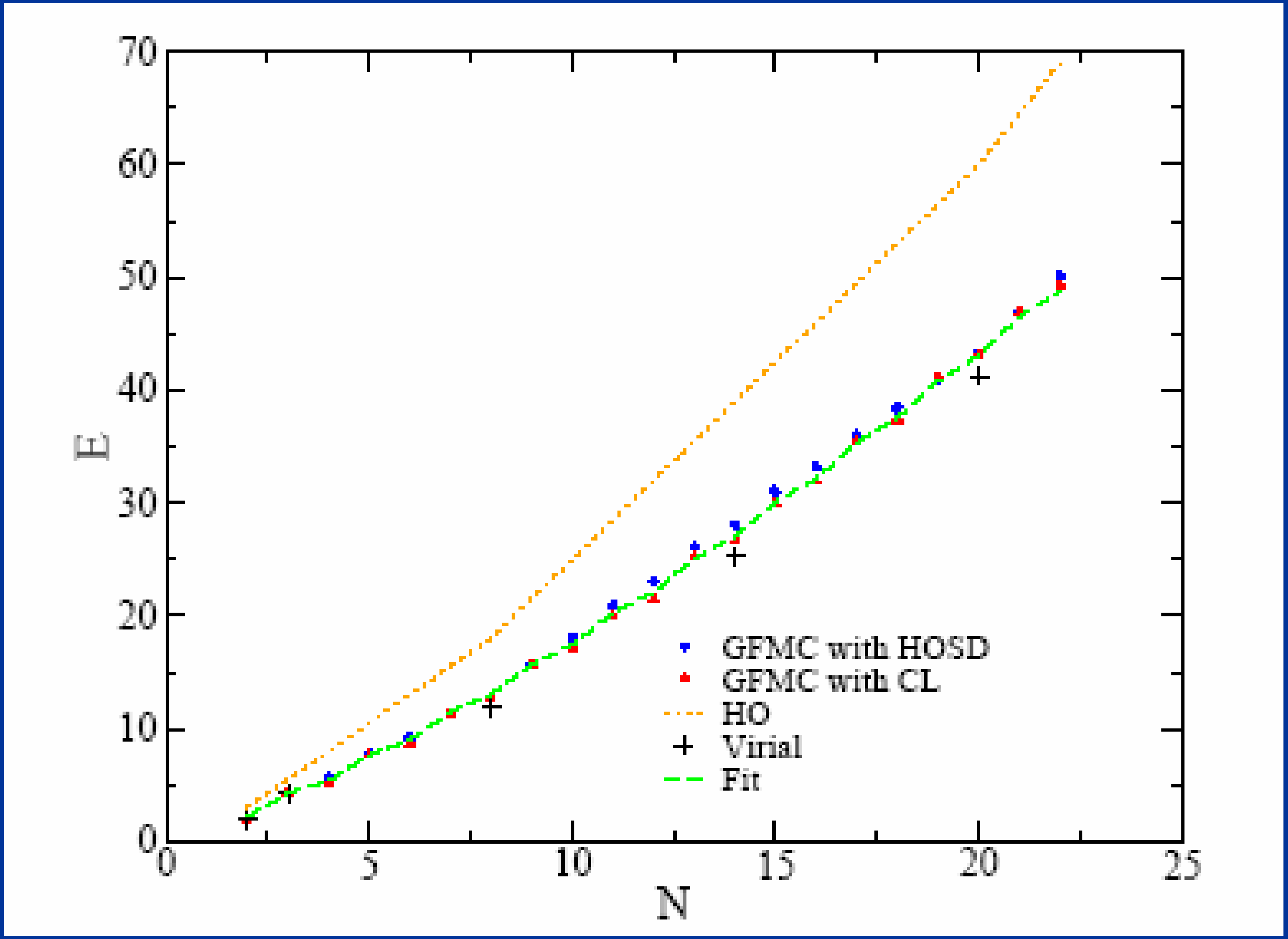
Local Density Functional Theory for Superfluid Fermionic Systems

The Unitary Fermi Gas

Unitary Fermi gas in a harmonic trap

Chang and Bertsch, physics/0703190



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**

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

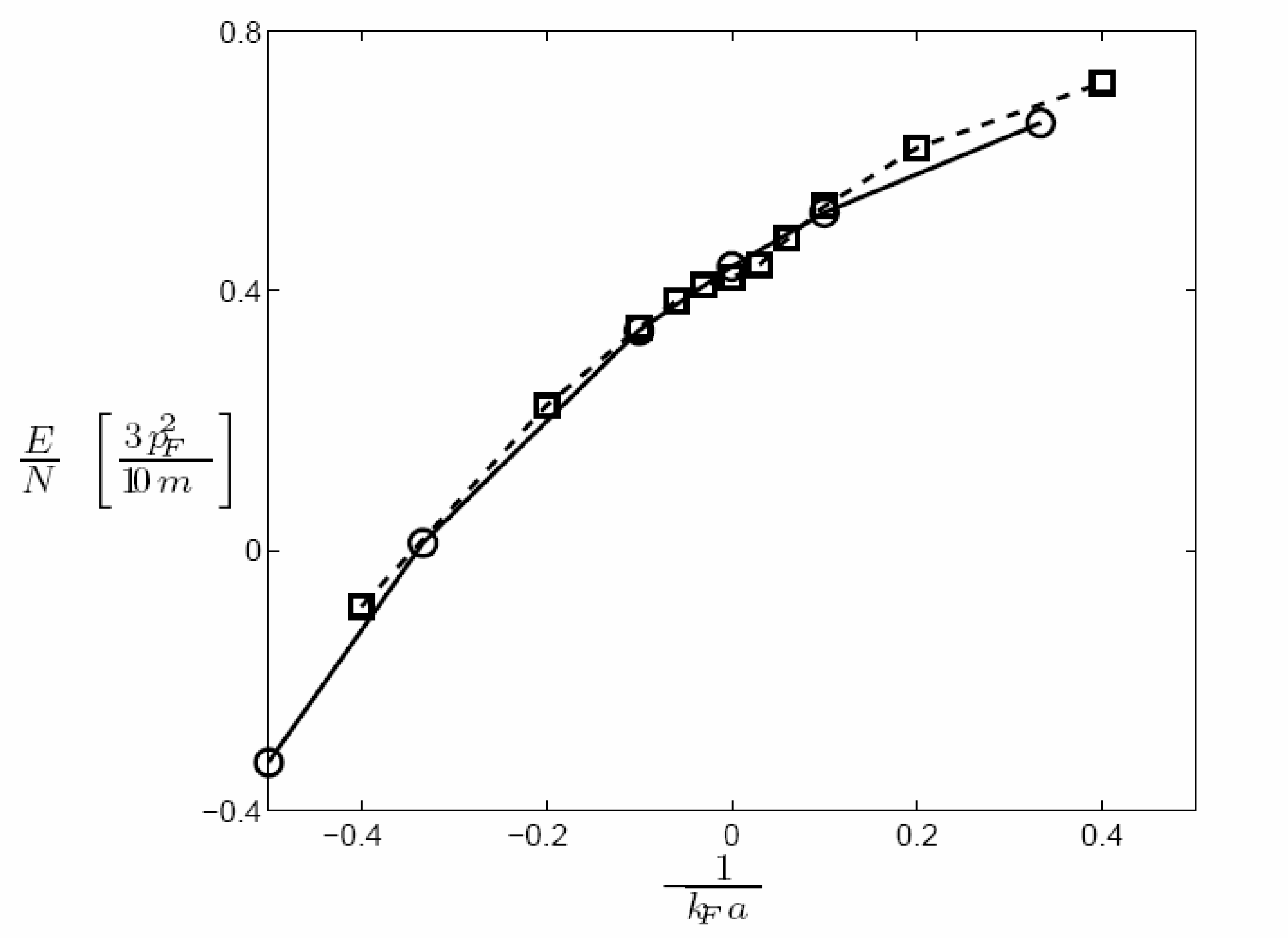
- Carlson, Chang, Pandharipande and Schmidt, PRL 91, 050401 (2003), with GFMC

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

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.

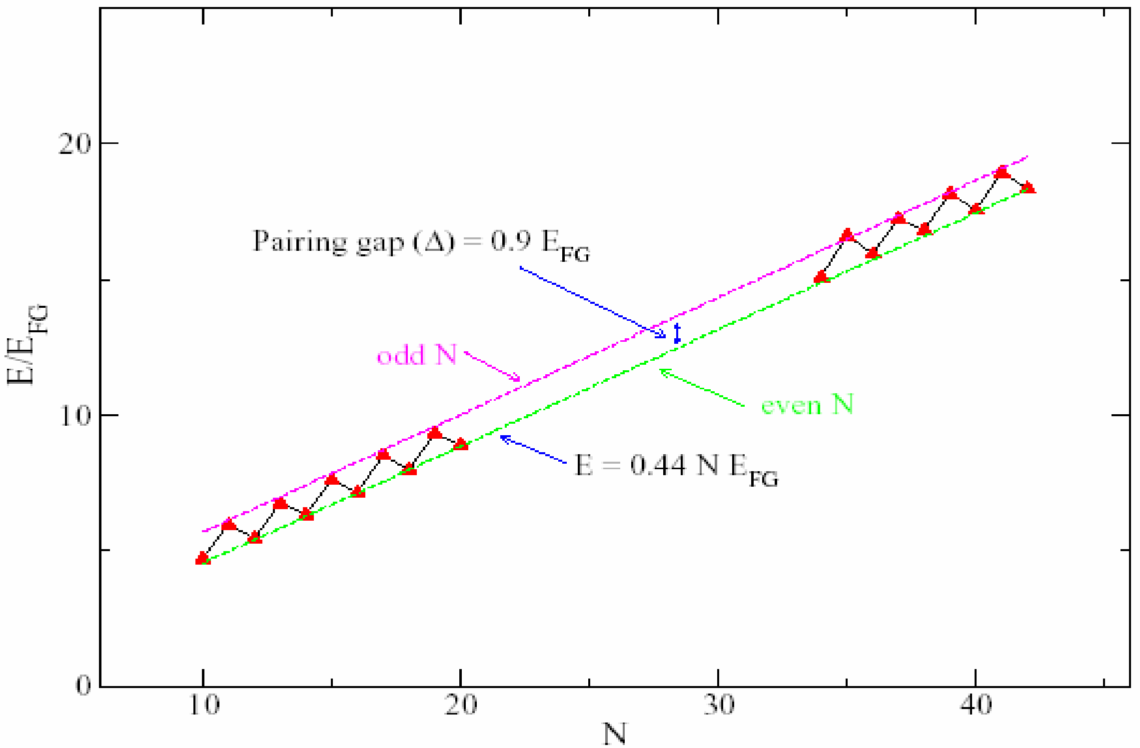
BEC side **BCS side**



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

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

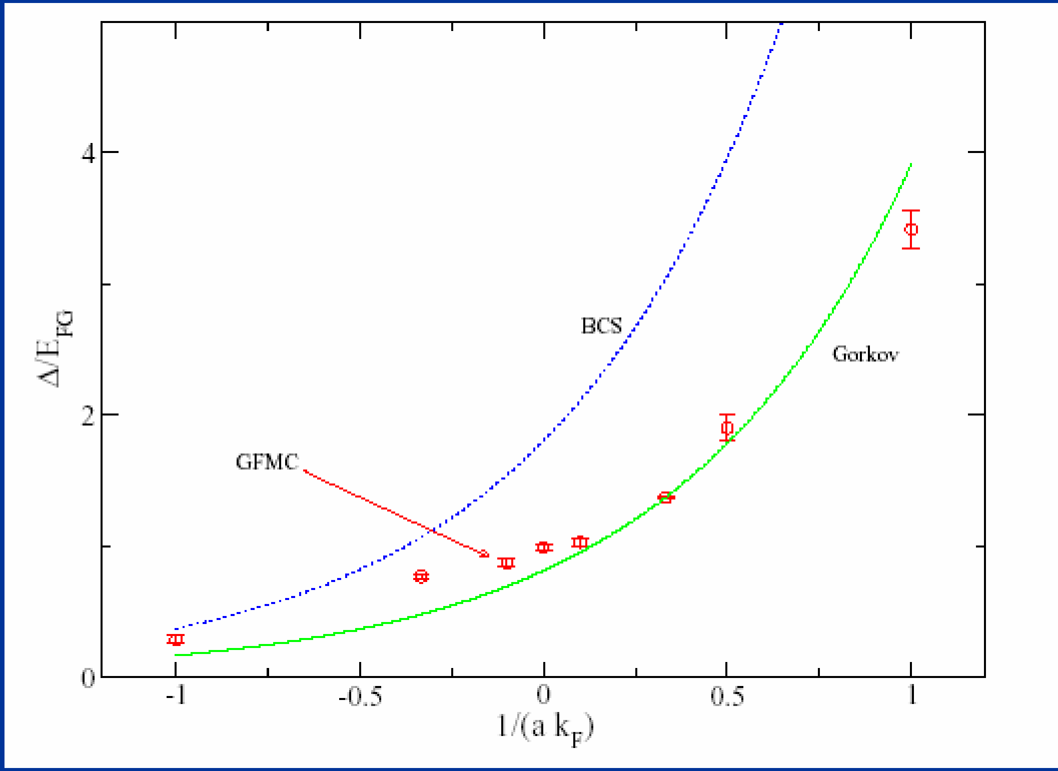
$$\Delta(2n+1) = E(2n+1) - \frac{1}{2}(E(2n) + E(2n+2))$$



Result for $ak_F = -\infty$

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

Green Function Monte Carlo with Fixed Nodes
S.-Y. Chang, J. Carlson, V. Pandharipande and K. Schmidt
physics/0403041



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

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

Fixed node GFMC results, S.-Y. Chang *et al.* (2003)

BCS $\rightarrow$BEC crossover

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

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

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

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

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

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

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

Very brief/skewed summary of DFT

Density Functional Theory (DFT)
Hohenberg and Kohn, 1964

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

particle density only!

Local Density Approximation (LDA)
Kohn and Sham, 1965

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

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

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

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

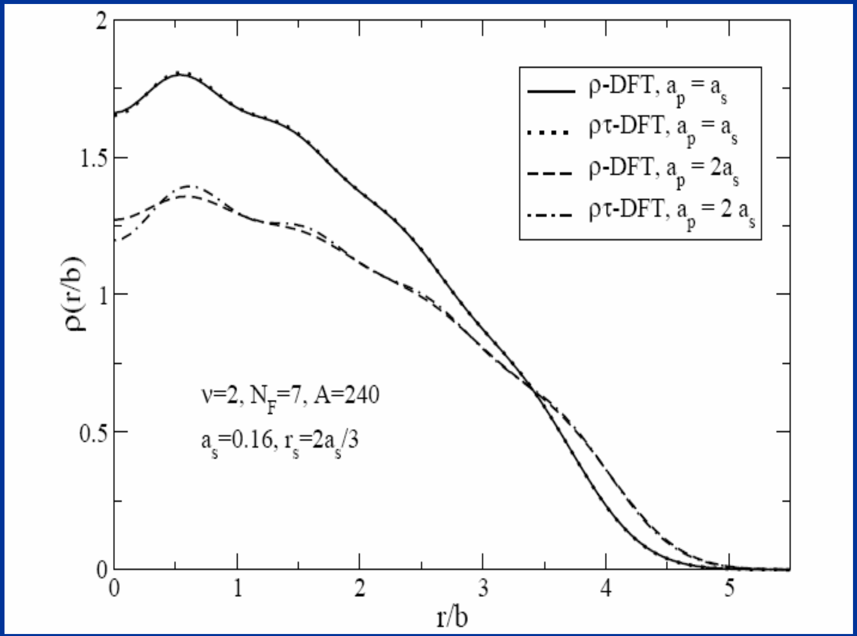
Kohn-Sham equations

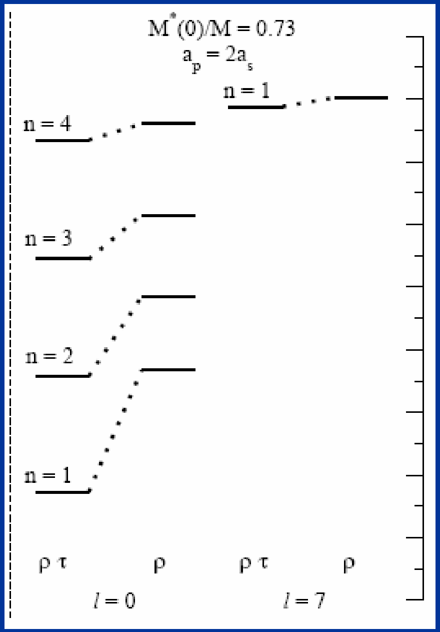
One can construct however an EDF which depends both on particle density and kinetic energy density and use it in a extended Kohn-Sham approach (perturbative result)

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

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/0408014





The single-particle spectrum of usual Kohn-Sham approach is unphysical, with the exception of the Fermi level.

The single-particle spectrum of extended Kohn-Sham approach has physical meaning.

TABLE I: Energies per particle, averages of the local Fermi momentum k_F, and rms radii for sample parameters and particle numbers for a dilute Fermi gas in a harmonic trap. See the text for a description of units. The scattering length is fixed at $a_s = 0.16$ and the effective range is set to $r_s = 2a_s/3$ when $a_p \neq 0$. Results with the DFT functional including τ are marked "τ–NNLO."

ν	N_F	A	a_p	E/A	$\langle k_F \rangle$	$\sqrt{\langle r^2 \rangle}$	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

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

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

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

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

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

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

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

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

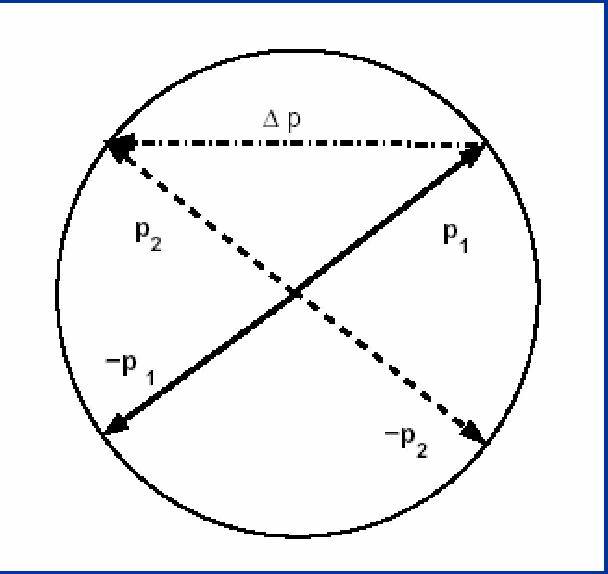
Mean-field and pairing field are both local fields!

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

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

Why would one consider a local pairing field?

- ✓ Because it makes sense physically!
- ✓ The treatment is so much simpler!
- ✓ Our intuition is so much better also.



$$r_0 \cong \frac{\hbar}{p_F} = k_F^{-1}$$

radius of interaction **inter-particle separation**

$$\Delta = \omega_D Exp\left(-\frac{1}{|V|N}\right) << \varepsilon_F$$

$$\xi \approx \frac{1}{k_F}\frac{\varepsilon_F}{\Delta} >> r_0$$

coherence length
size of the Cooper pair

Nature of the problem

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

at small separations

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

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

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

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

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

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)

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

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

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

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

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

The SLDA (renormalized) equations

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

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

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

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

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

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

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

Position and momentum dependent running coupling constant

Observables are (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

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

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

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

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

The renormalized SLDA energy density functional

$$\varepsilon(\vec{r}) = \alpha\frac{\tau_c(\vec{r})}{2} + \beta\frac{3(3\pi^2)^{2/3}n^{5/3}(\vec{r})}{5} + g_{eff}(\vec{r})\left|\nu_c(\vec{r})\right|^2$$

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

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

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

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

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

How to determine the dimensionless parameters α, β and γ ?

$$n = \frac{k_F^3}{3\pi^2} = \int \frac{d^3k}{(2\pi)^3}\left(1 - \frac{\alpha k^2/2 + \bar{\beta} k_F^2/2 - \mu}{\sqrt{\left(\alpha k^2/2 + \bar{\beta} k_F^2/2 - \mu\right)^2 + \Delta^2}}\right)$$

$$= \int \frac{d^3k}{(2\pi)^3}\left(1 - \frac{\varepsilon_k}{E_k}\right)$$

$$\frac{3}{5}\varepsilon_F n \xi_S = \frac{3}{5}\varepsilon_F n \beta + \int \frac{d^3k}{(2\pi)^3}\left[\alpha \frac{k^2}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right) - \frac{\Delta^2}{2E_k}\right]$$

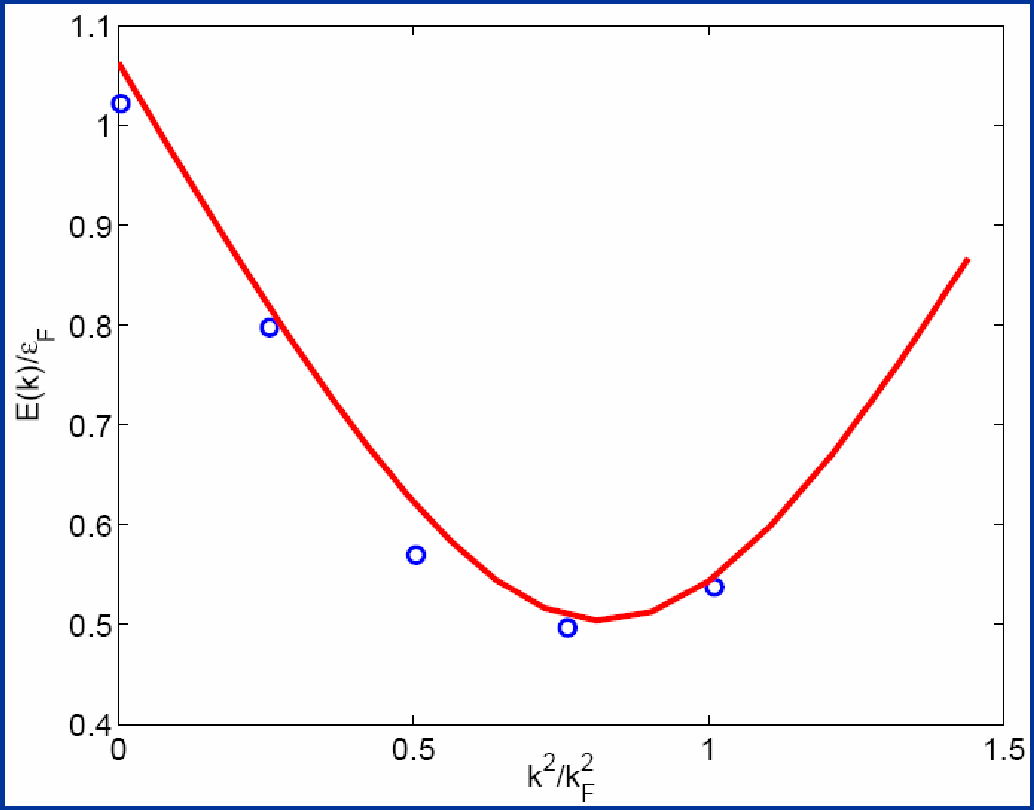
$$\frac{n^{1/3}}{\gamma} = \int \frac{d^3k}{(2\pi)^3}\left(\frac{1}{\alpha k^2} - \frac{1}{2E_k}\right)$$

One thus obtains:

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

Bonus!

Quasiparticle spectrum in homogeneous matter



solid line - SLDA

circles - GFMC due to Carlson and Reddy

Extra Bonus!

The normal state has been also determined in GFMC

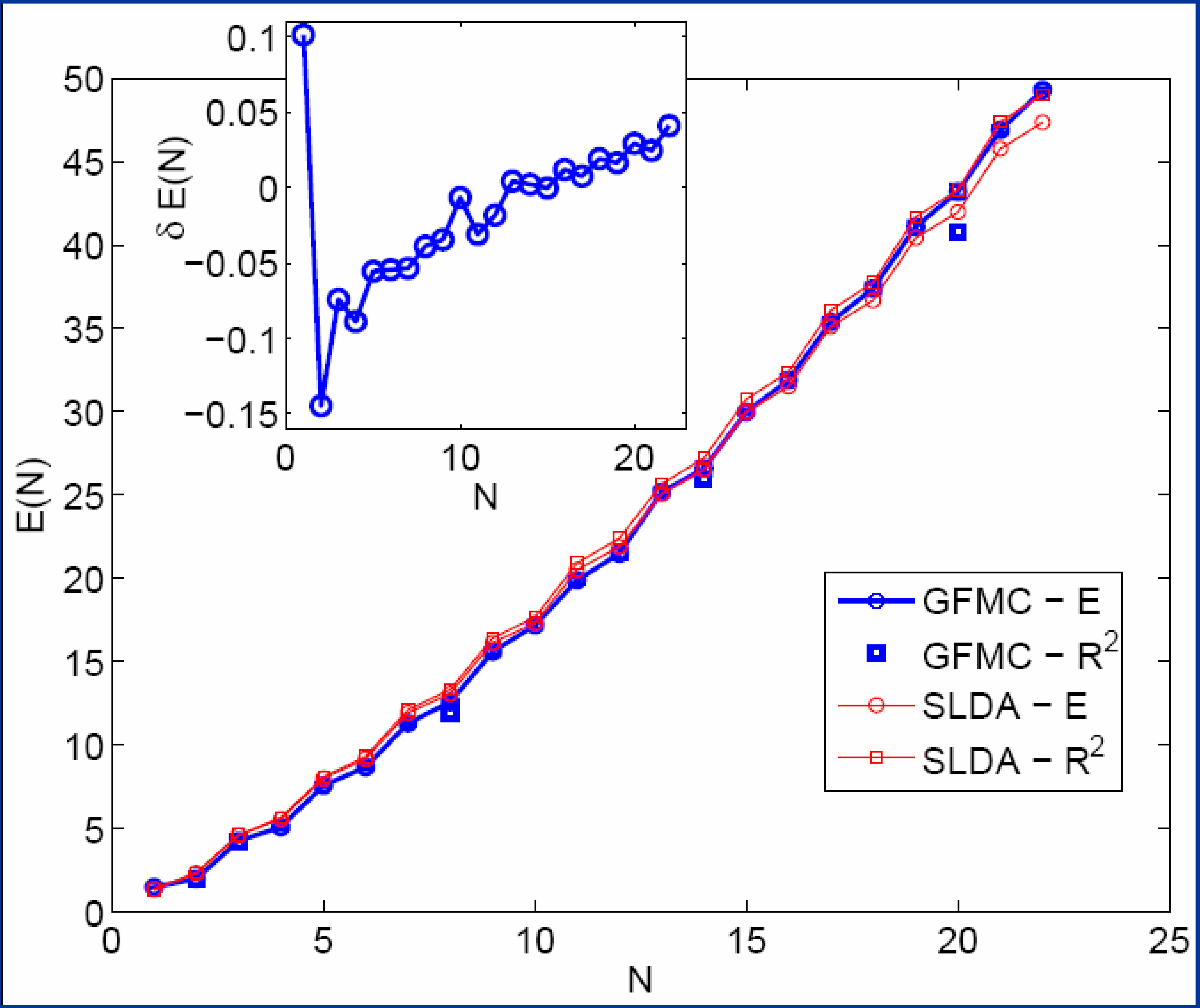
$$\xi_N = \frac{5E}{3N\varepsilon_F} = 0.55(2)$$

SLDA functional predicts

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

Fermions at unitarity in a harmonic trap

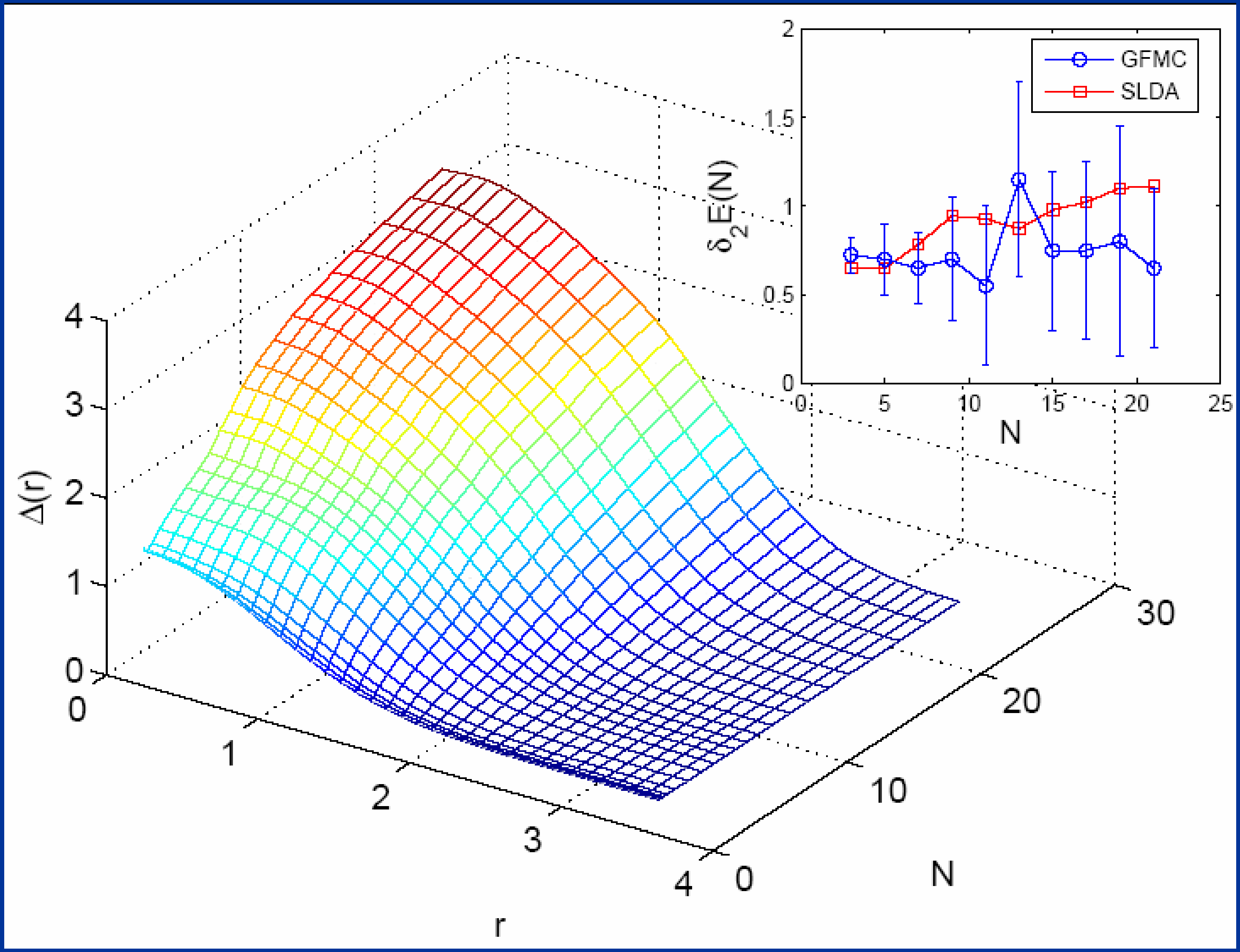
GFMC calculations of Chang and Bertsch



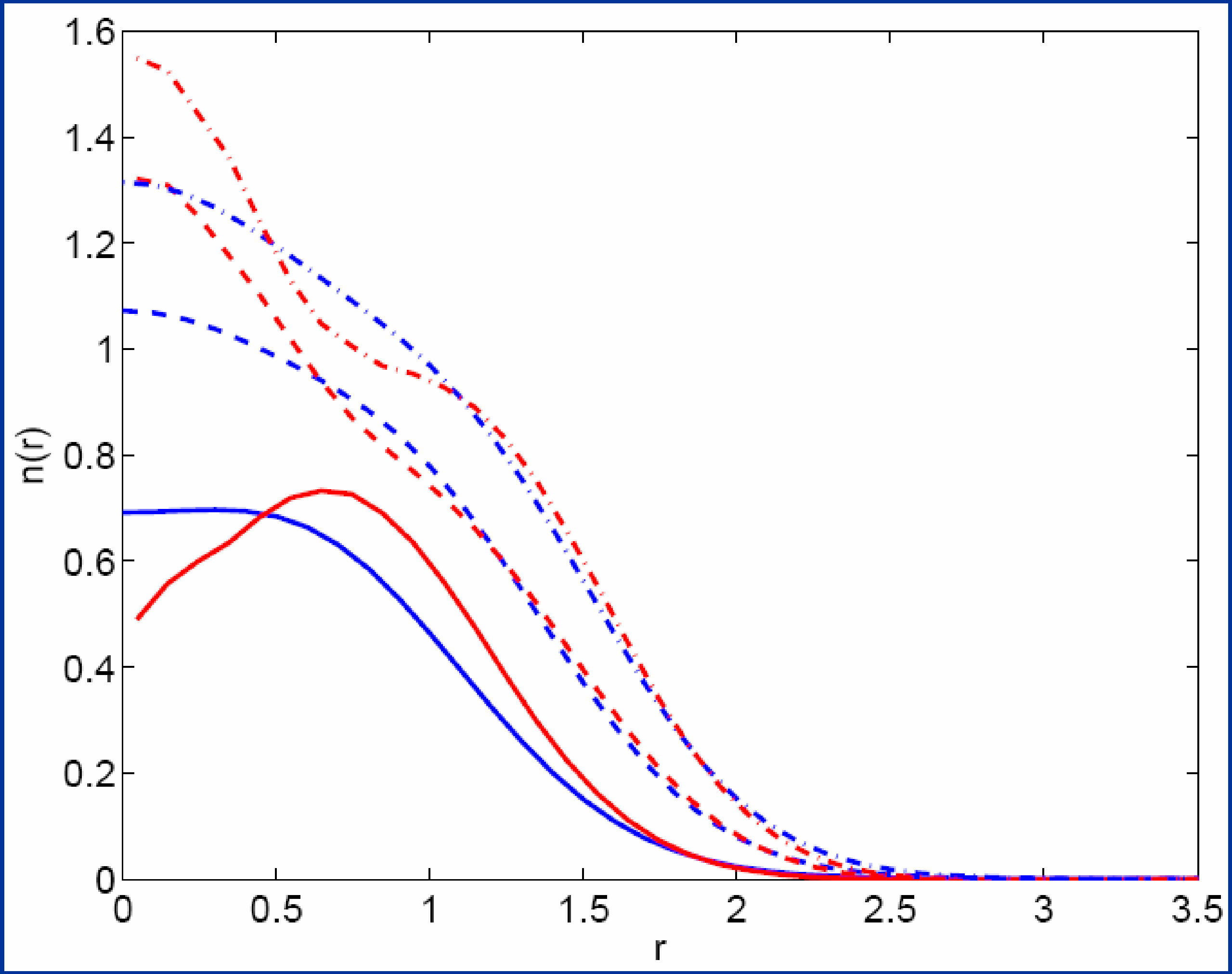
GFMC - Chang and Bertsch

TABLE I: Table 1. The energies $E(N)$ calculated within the GFMC [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 [20].

N	E_{GFMC}	E_{SLDA}	N	E_{GFMC}	E_{SLDA}
1	1.5	1.36	12	21.5	21.9/22.4
2	2.01/1.95	2.35/2.36	13	25.2	25.1/25.7
3	4.28/4.19	4.62/4.63	14	26.6/26.0	26.5/27.2
4	5.10	5.60/5.66	15	30.0	30.0/30.8
5	7.60	8.04/8.12	16	31.9	31.5/32.4
6	8.70	9.20/9.34	17	35.4	35.1/36.1
7	11.3	11.9/12.1	18	37.4	36.7/37.8
8	12.6/11.9	13.1/13.3	19	41.1	40.4/41.7
9	15.6	16.2/16.4	20	43.2/40.8	42.0/43.3
10	17.2	17.3/17.7	21	46.9	45.8/47.4
11	19.9	20.5/20.9	22	49.3	47.4/49.0



$$\delta_2 E(N) = E(N) - \frac{1}{2}\left[E(N+1) + E(N-1)\right]$$



Densities for N=8 (solid), N=14 (dashed) and N=20 (dot-dashed) GFMC (red), SLDA (blue)

- **Agreement between GFMC and SLDA very good (a few percent 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**