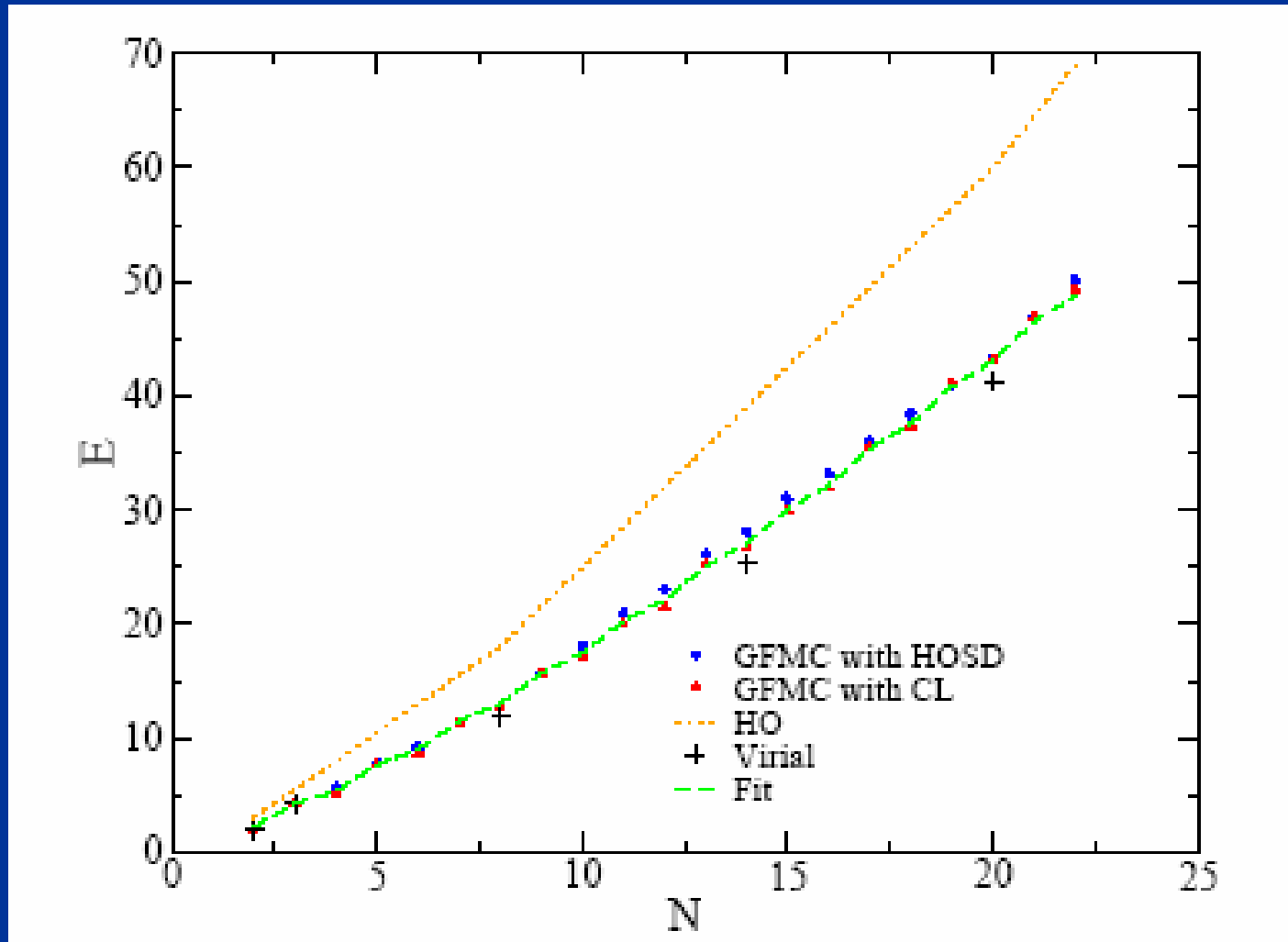# Local Density Functional Theory for Superfluid Fermionic Systems

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)

$$\frac{E_N}{N} = \alpha_N \frac{3}{5} \varepsilon_F, \quad \alpha_N = 0.54$$

normal state

➢ Carlson, Chang, Pandharipande and Schmidt, PRL 91, 050401 (2003), with GFMC
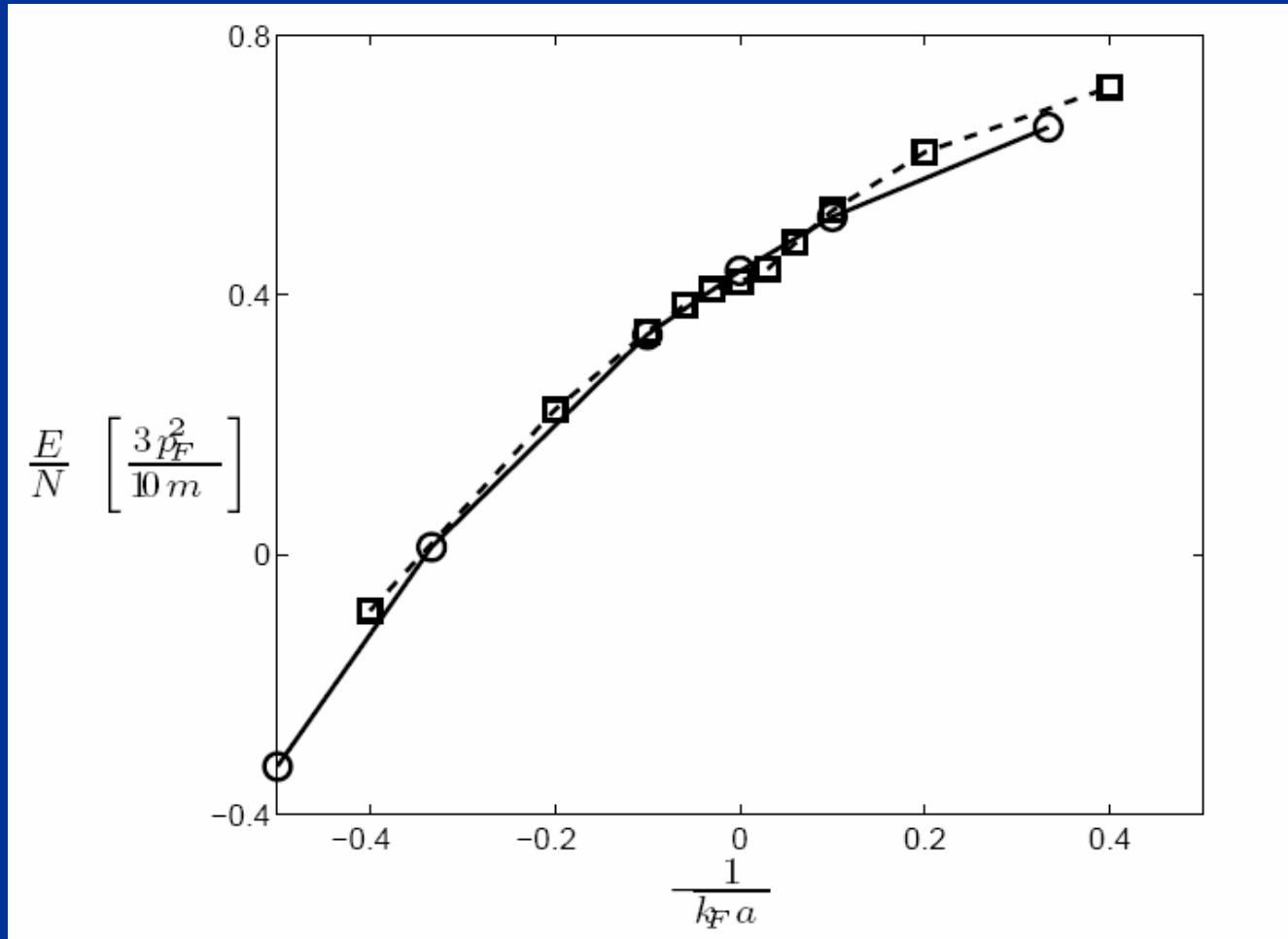
$$\frac{E_S}{N} = \alpha_S \frac{3}{5} \varepsilon_F, \quad \alpha_S = 0.44$$

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.
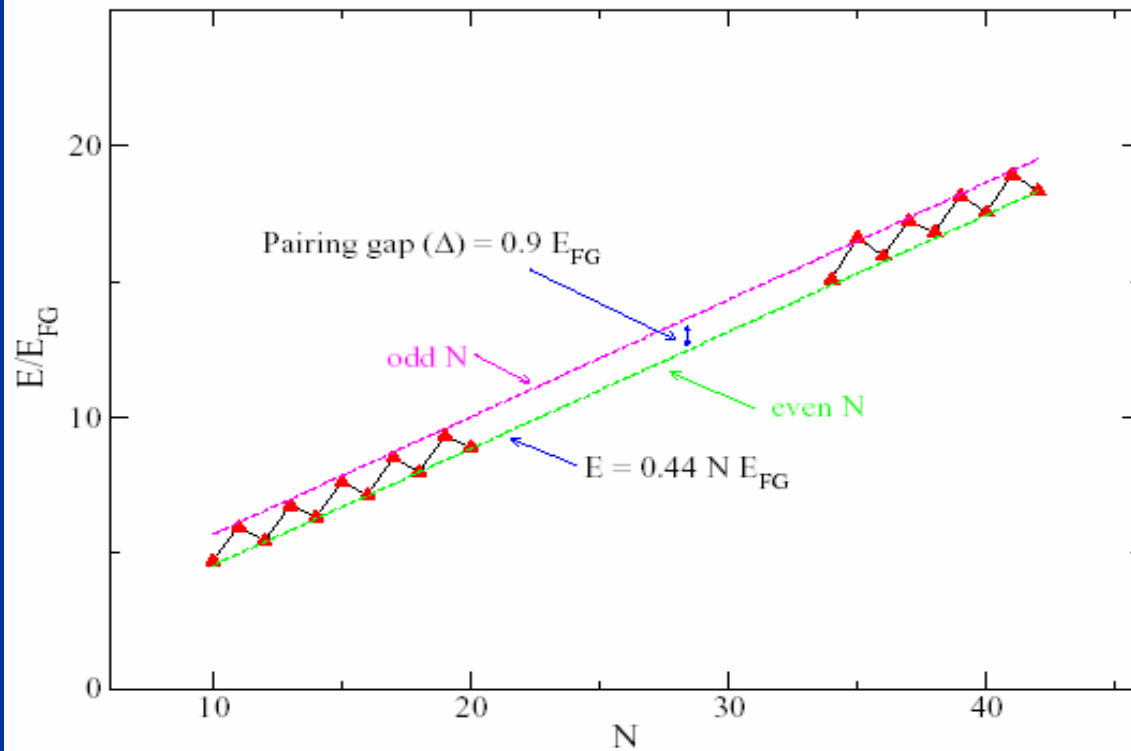
BEC side **BCS side**

Solid line with open circles – Chang *et al.* physics/0404115
Dashed line with squares - Astrakharchik *et al.* cond-mat/0406113

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

Pairing gap (Δ) = 0.9 E_{FG}

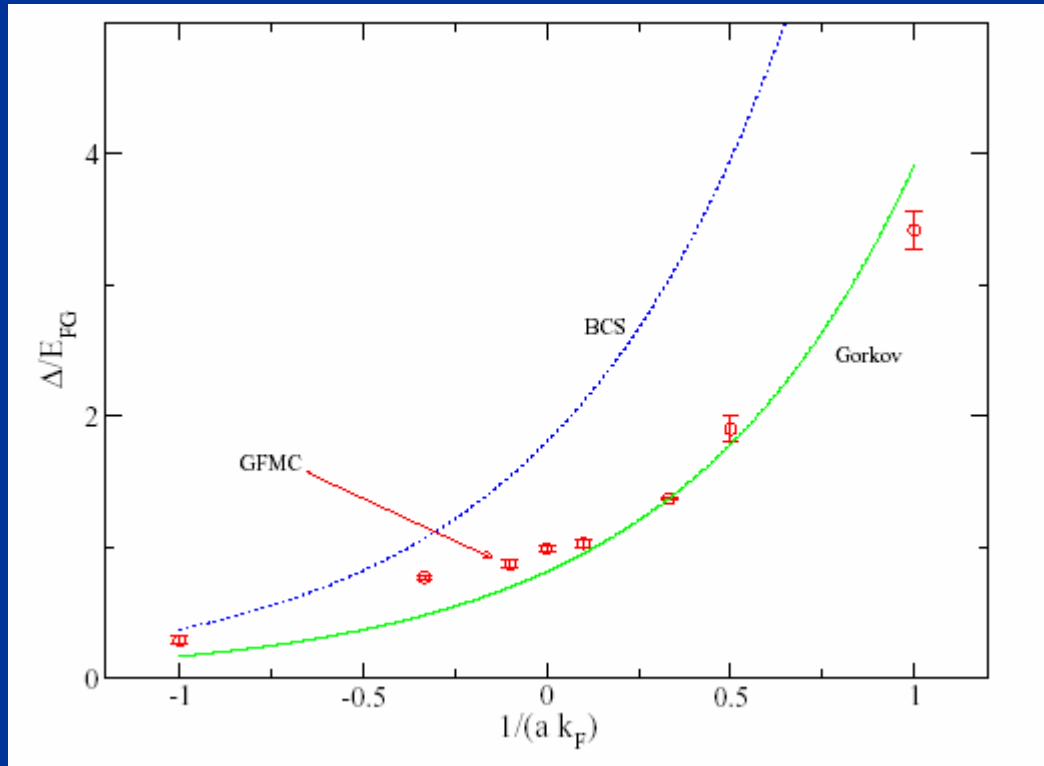odd N

even N

$E = 0.44 \ N \ E_{FG}$

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

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

If a>0 (a≫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

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

← **particle density only!**

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

Local Density Approximation (LDA)
Kohn and Sham, 1965

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

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

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

← **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)

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

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

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 ^{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)

Bogoliubov-de Gennes equations and renormalization

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

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

$$\rho(\vec{r}) = 2\sum_k |v_k(\vec{r})|^2, \quad \tau(\vec{r}) = 2\sum_k |\vec{\nabla} v_k(\vec{r})|^2$$

$$\nu(\vec{r}) = \sum_k u_k(\vec{r}) v_k^*(\vec{r})$$

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

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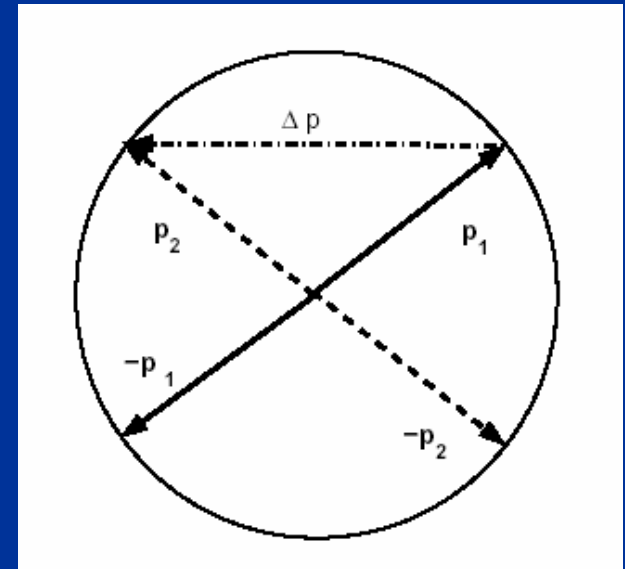
$$r_0 \cong \frac{\hbar}{p_F} = k_F^{-1}$$

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

$$\nu(\vec{r}_1, \vec{r}_2) = \sum_{E_k > 0} v_k^*(\vec{r}_1) u_k(\vec{r}_2) \propto \frac{1}{|\vec{r}_1 - \vec{r}_2|} \quad \longleftarrow \text{ at small separations}$$

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

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

$$v_k(\vec{r}_1) = v_k \exp(i\vec{k} \cdot \vec{r}_1), \quad u_k(\vec{r}_2) = u_k \exp(i\vec{k} \cdot \vec{r}_2)$$

$$v_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k - \mu}{\sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}}\right), \quad u_k^2 + v_k^2 = 1, \quad \varepsilon_k = \frac{\hbar^2 \vec{k}^2}{2m} + U, \quad \Delta = \frac{\hbar^2 \delta}{2m}$$

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

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)

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

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

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

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

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

The SLDA (renormalized) equations

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

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

$$\begin{cases} [h(\vec{r}) - \mu] u_i(\vec{r}) + \Delta(\vec{r}) v_i(\vec{r}) = E_i u_i(\vec{r}) \\ \Delta^*(\vec{r}) u_i(\vec{r}) - [h(\vec{r}) - \mu] v_i(\vec{r}) = E_i v_i(\vec{r}) \end{cases} \qquad \begin{cases} h(\vec{r}) = -\vec{\nabla} \dfrac{\hbar^2}{2m(\vec{r})} \vec{\nabla} + U(\vec{r}) \\[2mm] \Delta(\vec{r}) = -g_{eff}(\vec{r}) v_c(\vec{r}) \end{cases}$$

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

$$\rho_c(\vec{r}) = 2 \sum_{E_i \geq 0}^{E_c} \left| v_i(\vec{r}) \right|^2, \qquad v_c(\vec{r}) = \sum_{E_i \geq 0}^{E_c} v_i^*(\vec{r}) u_i(\vec{r})$$

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

Position and momentum dependent running coupling constant
Observables are (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

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

$$n(\vec{r}) = 2\sum_k \left| v_k(\vec{r}) \right|^2$$

$$\tau(\vec{r}) = 2\sum_k \left| \vec{\nabla} v_k(\vec{r}) \right|^2$$

$$\nu(\vec{r}) = \sum_k u_k(\vec{r}) v_k^*(\vec{r})$$

The renormalized SLDA energy density functional

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

$$\tau_c(\vec{r}) = 2 \sum_{E<E_c} \left|\vec{\nabla} v_k(\vec{r})\right|^2, \qquad \nu_c(\vec{r}) = \sum_{E<E_c} u_k(\vec{r}) v_k^*(\vec{r})$$

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

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

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

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

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

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

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

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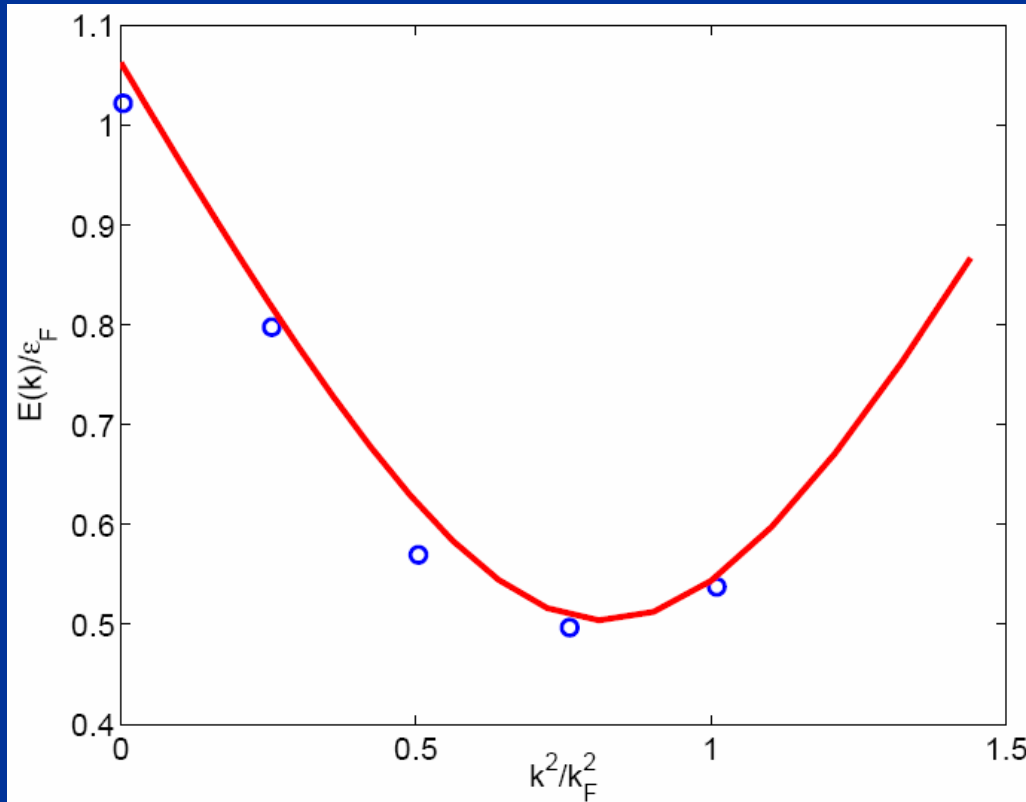
$$\frac{n^{1/3}}{\gamma} = \int \frac{d^3k}{(2\pi)^3}\left(\frac{1}{\alpha k^2} - \frac{1}{2E_k}\right)$$

One thus obtains:

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

Bonus!

Quasiparticle spectrum in homogeneous matter

solid line   - SLDA
circles   - GFMC due to Carlson and Reddy

Extra Bonus!

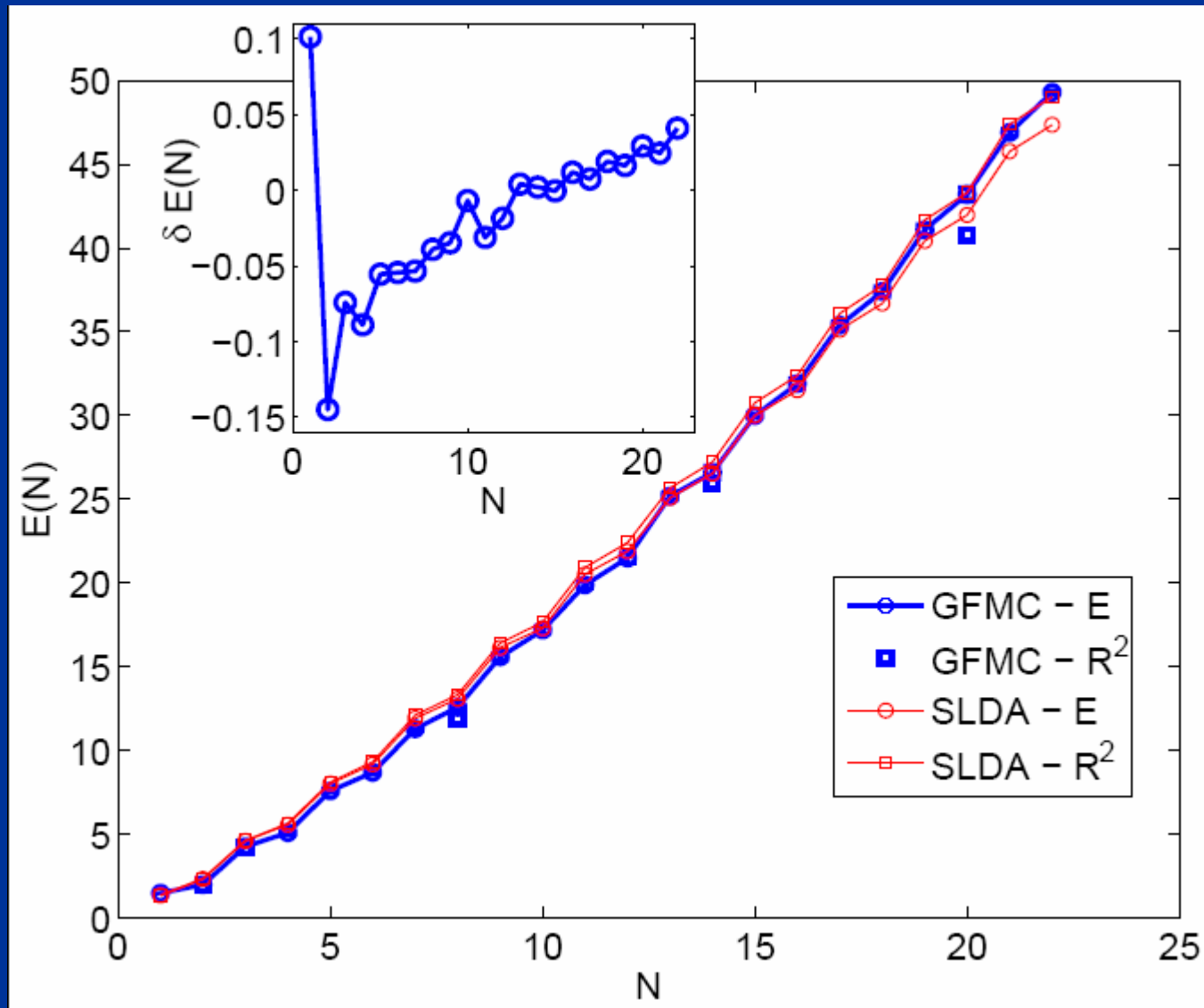**The normal state has been also determined in GFMC**

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

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
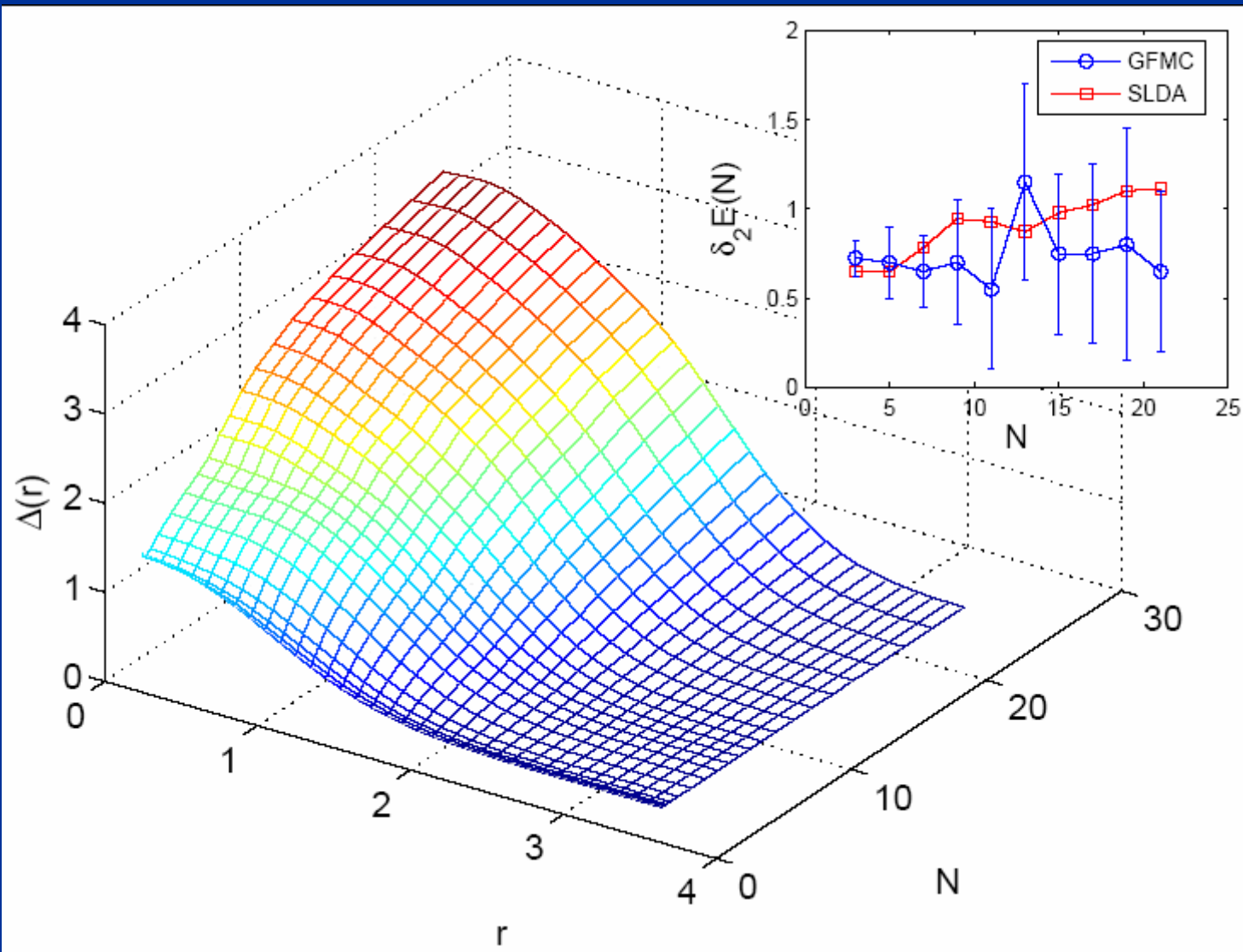
$$\delta_2 E(N) = E(N) - \frac{1}{2}\left[E(N+1) + E(N-1)\right]$$
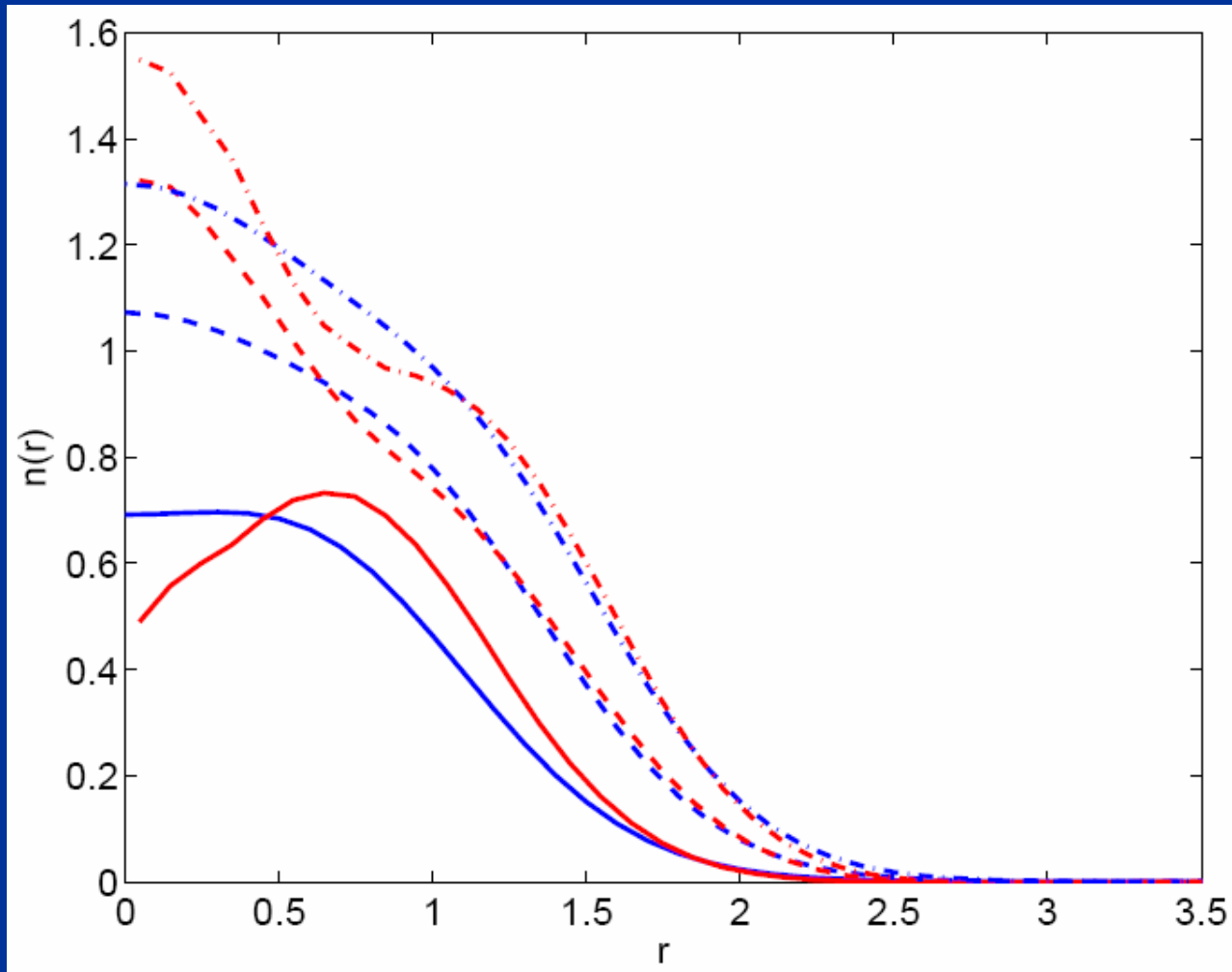
Densities for N=8 (solid), N=14 (dashed) and N=20 (dot-dashed) GFMC (red), SLDA (blue)

- **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**