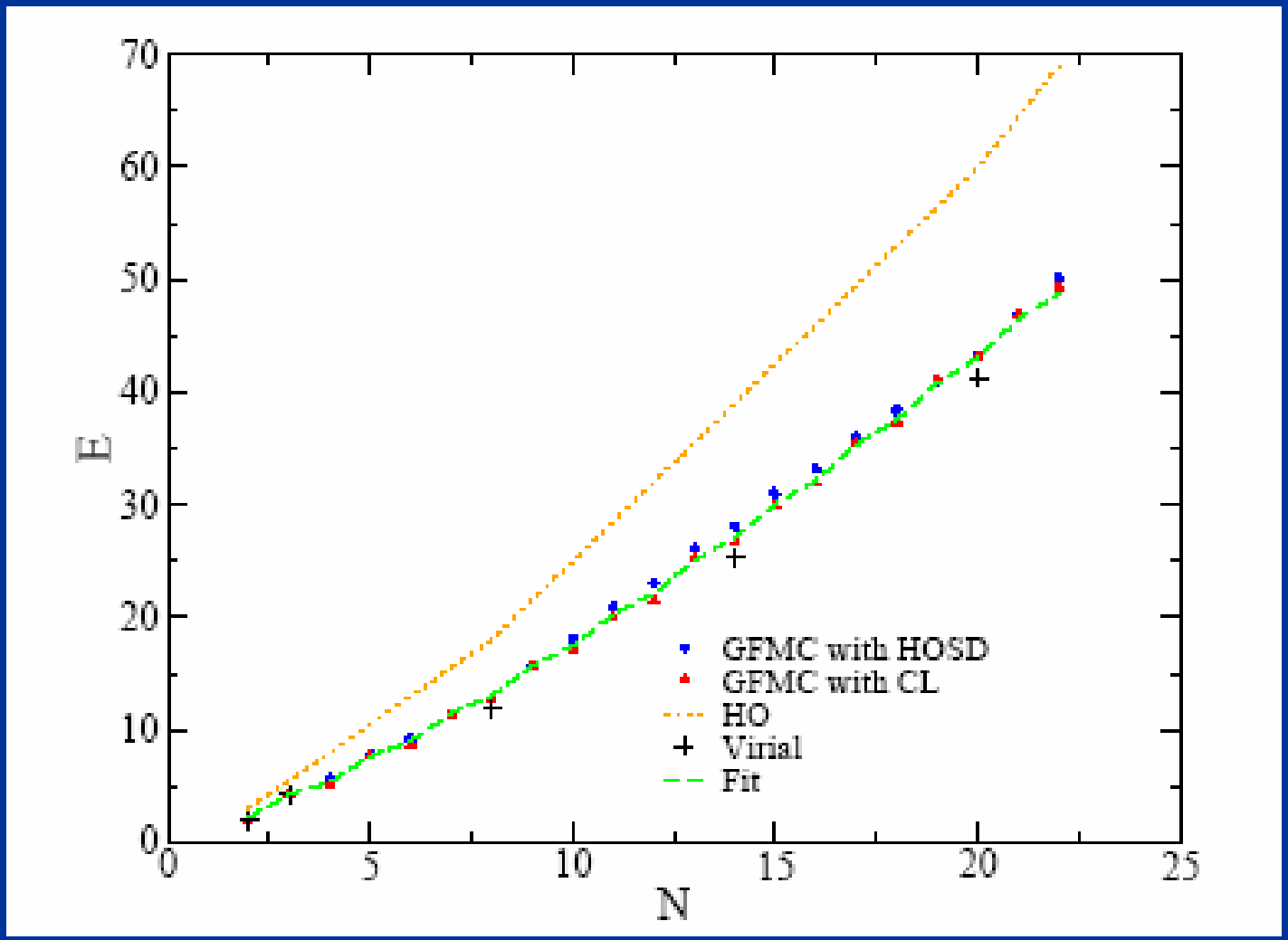
Local Density Functional Theory for Superfluid Fermionic Systems

The Unitary Fermi Gas

Unitary Fermi gas in a harmonic trap

Chang and Bertsch, physics/0703190



Outline:

- **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**

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

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)

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

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

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

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

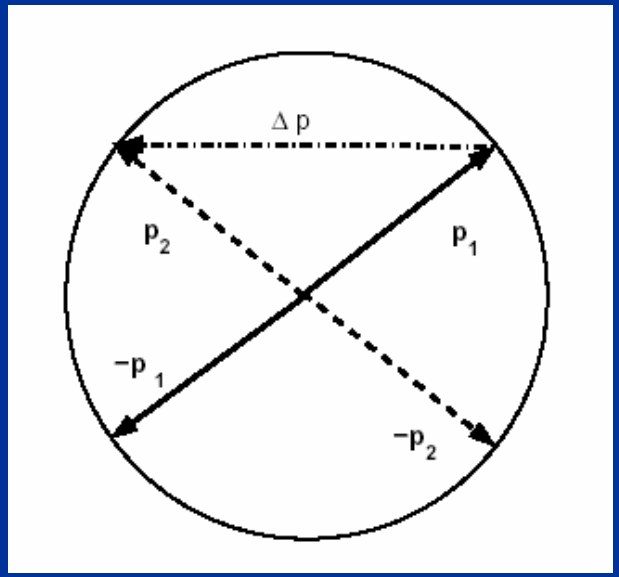
$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} \mathrm{u}_k(\vec{r}) \\ \mathrm{v}_k(\vec{r}) \end{pmatrix}$$

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.



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

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)

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

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

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

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

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

The SLDA (renormalized) equations

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

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

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

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

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

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

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

Position and momentum dependent running coupling constant

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

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 renormalized SLDA energy density functional

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

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

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

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

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

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

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

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

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

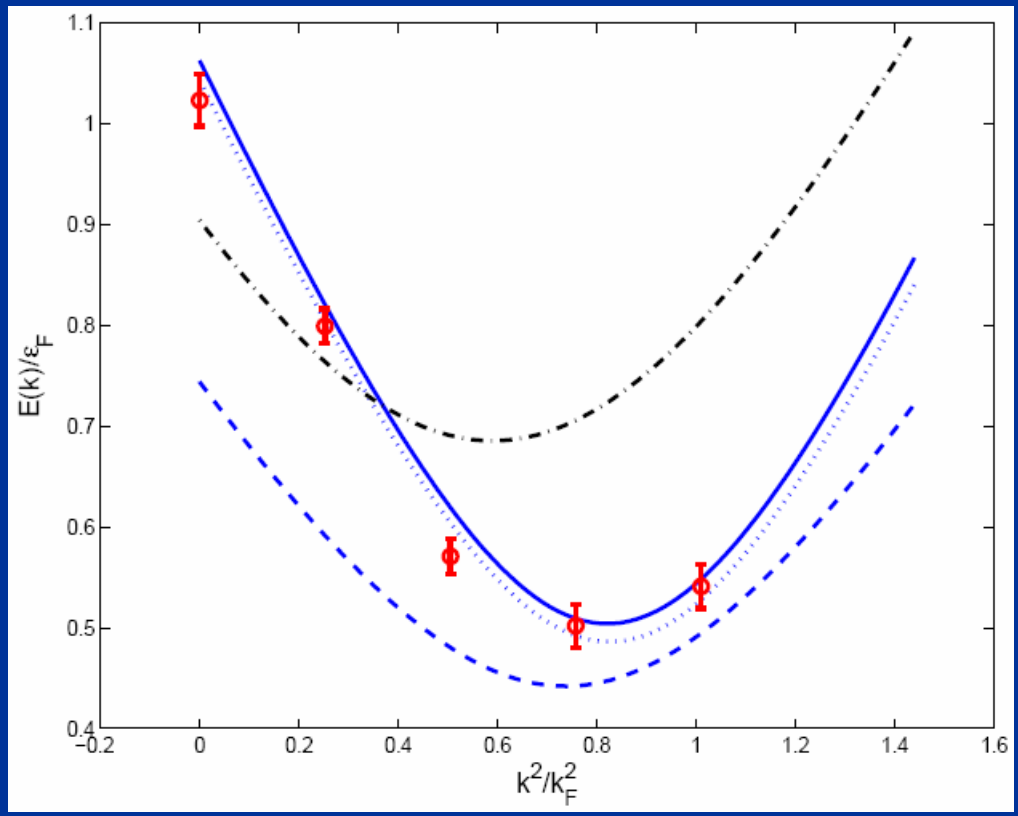
$$\frac{3}{5}\varepsilon_F n \xi_S = \frac{3}{5}\varepsilon_F n \beta + \int \frac{d^3k}{(2\pi)^3}\left[\alpha \frac{k^2}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right) - \frac{\Delta^2}{2E_k}\right]$$

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

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/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

One more universal parameter characterizing the unitary Fermi gas and its excitation spectrum: *effective mass*

Extra Bonus!

The normal state has been also determined in GFMC

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

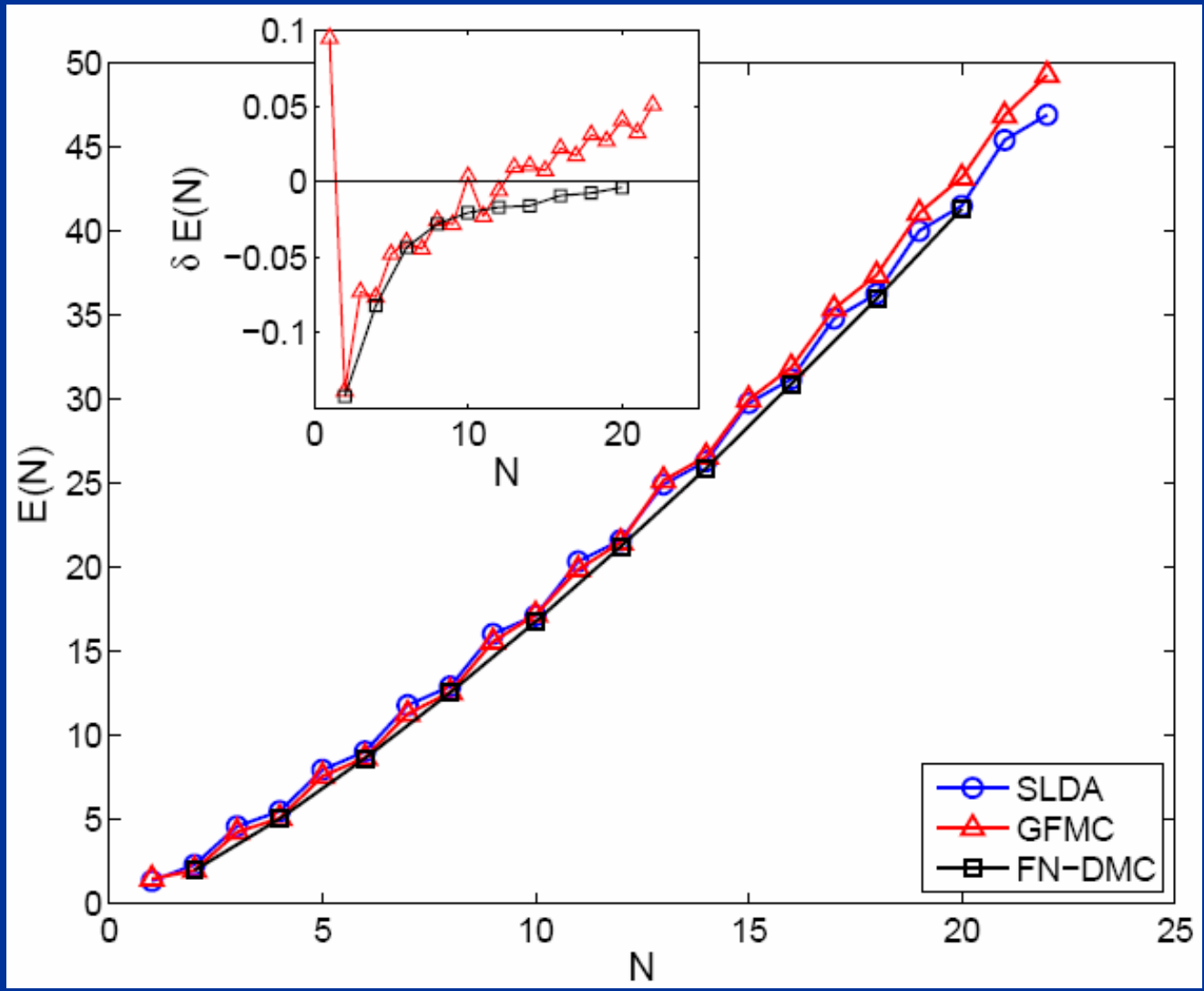
SLDA functional predicts

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

Fermions at unitarity in a harmonic trap

GFMC - Chang and Bertsch, arXiv:physics/0703190
FN-DMC - von Stecher, Greene and Blume, arXiv:0705.0671

Fermions at unitarity in a harmonic trap

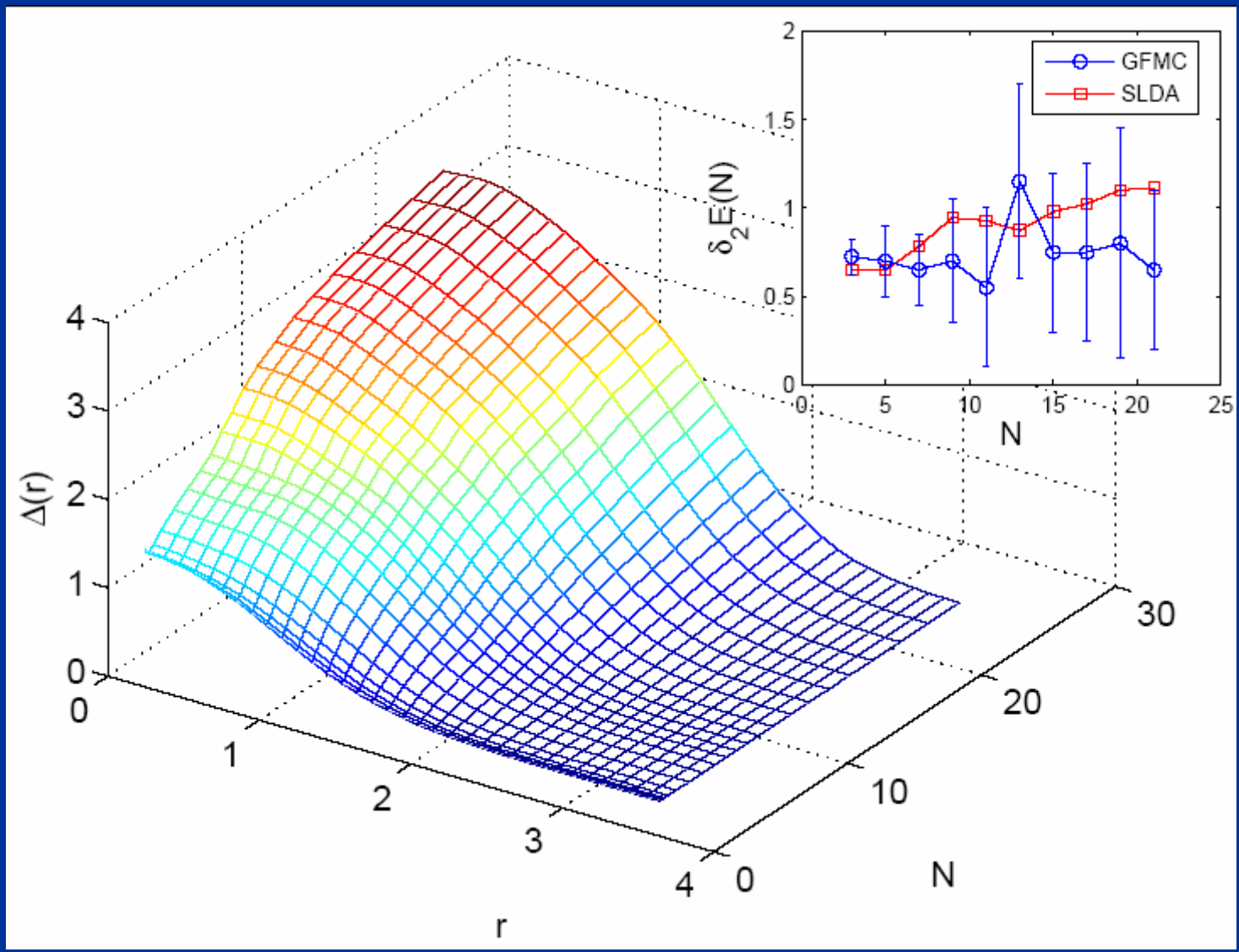


GFMC - Chang and Bertsch, arXiv:physics/0703190

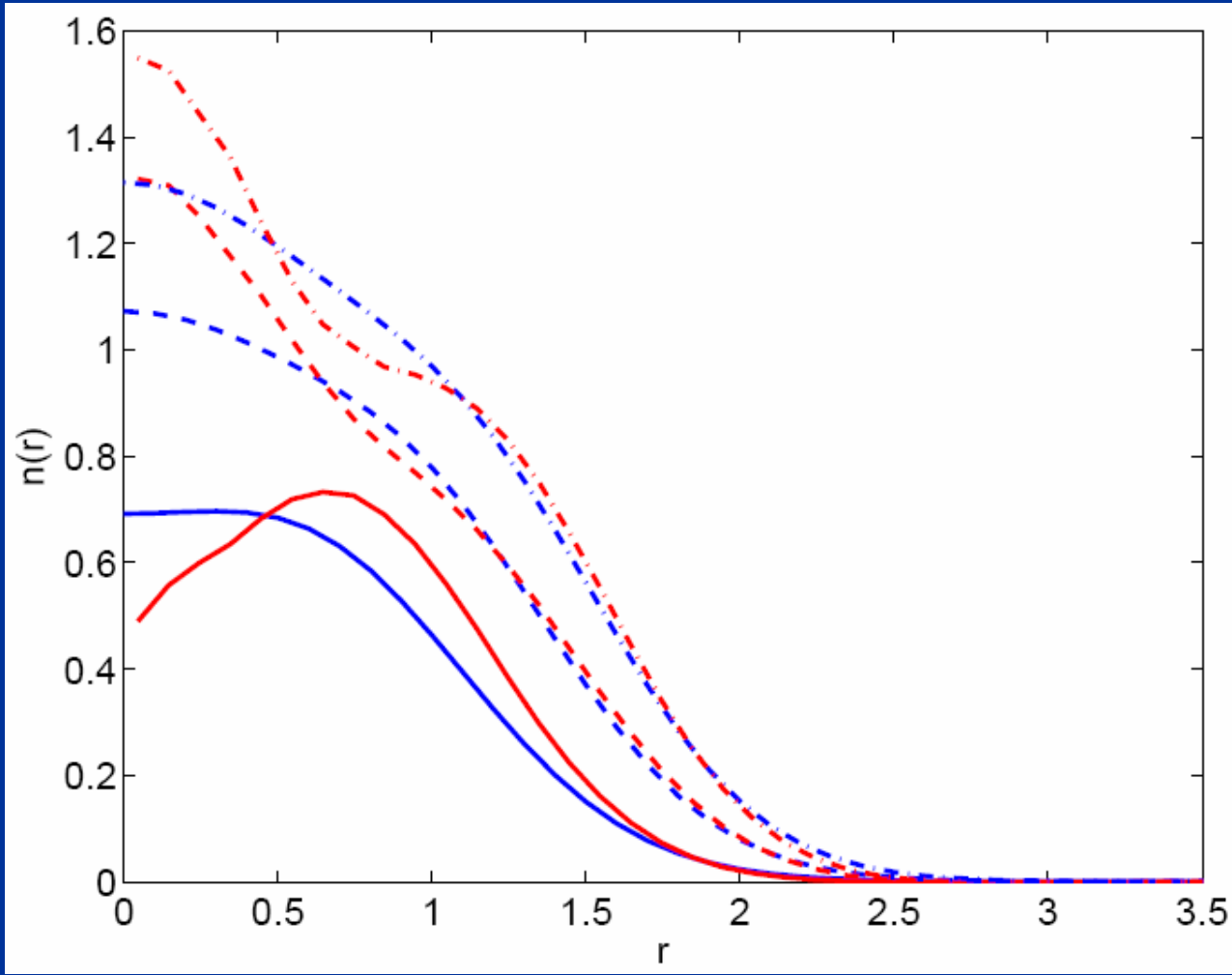
FN-DMC - von Stecher, Greene and Blume, arXiv:0705.0671

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 $E(N) = m\omega^2 \int d^3 r n(\mathbf{r}) r^2$ [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



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



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

- **Agreement between GFMC/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**

Outlook

Extension away from unitarity - trivial

Extension to excited states - easy

Extension to time dependent problems - easy

Extension to finite temperatures - easy, but one more parameter is needed, the pairing gap dependence as a function of T

Extension to asymmetric systems straightforward (at unitarity quite a bit is already know about the equation of state)