

Local Density Functional Theory for Superfluid Fermionic Systems

The Unitary Fermi Gas

A. Bulgac, [arXiv:cond-mat/0703526](https://arxiv.org/abs/cond-mat/0703526)

Kohn-Sham theorem

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

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

$$n(\vec{r}) = \langle \Psi_0 | \sum_i^N \delta(\vec{r} - \vec{r}_i) | \Psi_0 \rangle$$

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

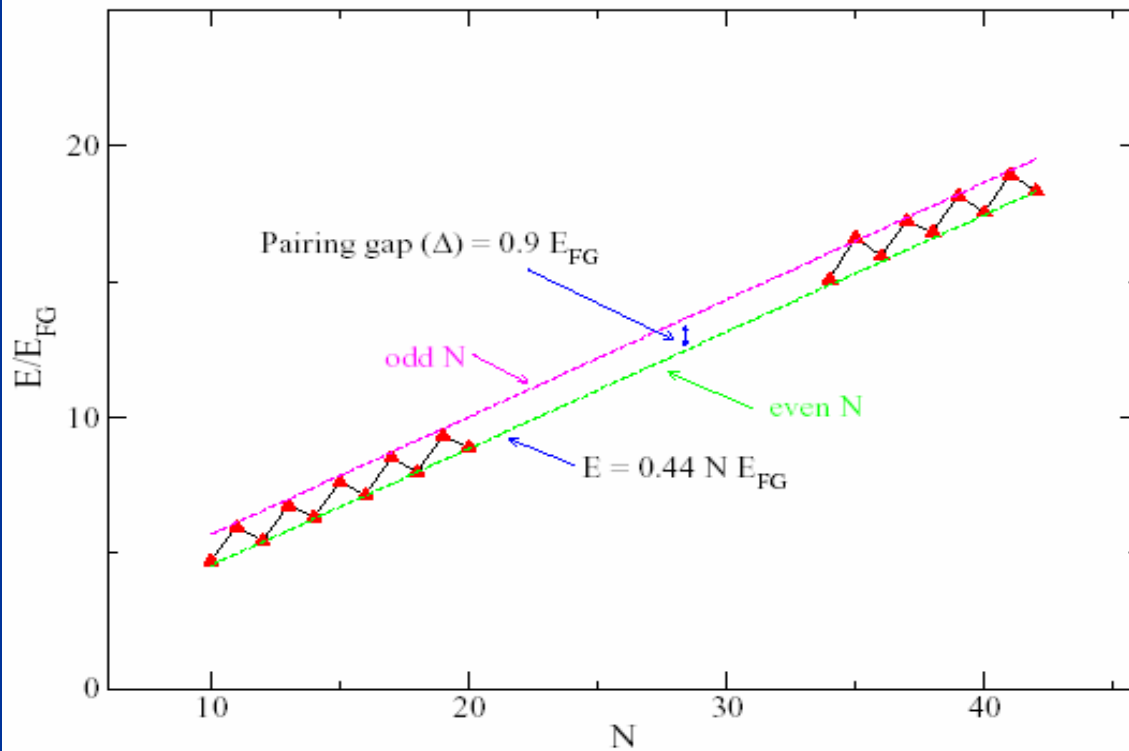
$$n(\vec{r}) = \sum_i^N |\varphi_i(\vec{r})|^2, \quad \tau(\vec{r}) = \sum_i^N |\vec{\nabla} \varphi_i(\vec{r})|^2$$


**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!

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



Result for $ak_F = -\infty$

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

Green Function Monte Carlo with Fixed Nodes

S.-Y. Chang, J. Carlson, V. Pandharipande and K. Schmidt
 Phys. Rev. Lett. 91, 050401 (2003).

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

$$E_{gs} = \int d^3r \left\{ \varepsilon(n(\vec{r}), \tau(\vec{r}), \nu(\vec{r})) + \leftarrow \text{universal functional} \right. \\ \left. (\text{independent of external potential}) \right. \\ \left. V_{ext}(\vec{r})n(\vec{r}) + \Delta_{ext}(\vec{r})\nu(\vec{r}) + \Delta_{ext}^*(\vec{r})\nu^*(\vec{r}) \right\}$$

$$n(\vec{r}) = 2 \sum_k |\mathbf{v}_k(\vec{r})|^2, \quad \tau(\vec{r}) = 2 \sum_k |\vec{\nabla} \mathbf{v}_k(\vec{r})|^2$$

$$\nu(\vec{r}) = \sum_k \mathbf{u}_k(\vec{r}) \mathbf{v}_k^*(\vec{r})$$

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

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.

Nature of the problem

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

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

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)

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

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

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

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

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

The SLDA (renormalized) equations

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

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

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

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

$$n_c(\vec{r}) = 2 \sum_{E_i \geq 0}^{E_c} |v_i(\vec{r})|^2, \quad \nu_c(\vec{r}) = \sum_{E_i \geq 0}^{E_c} v_i^*(\vec{r})u_i(\vec{r})$$

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

The naïve SLDA energy density functional for the unitary gas suggested by dimensional arguments

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

$$n(\vec{r}) = 2 \sum_k |\psi_k(\vec{r})|^2$$

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

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

The renormalized SLDA energy density functional for the unitary gas

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

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

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

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

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

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

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

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

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

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

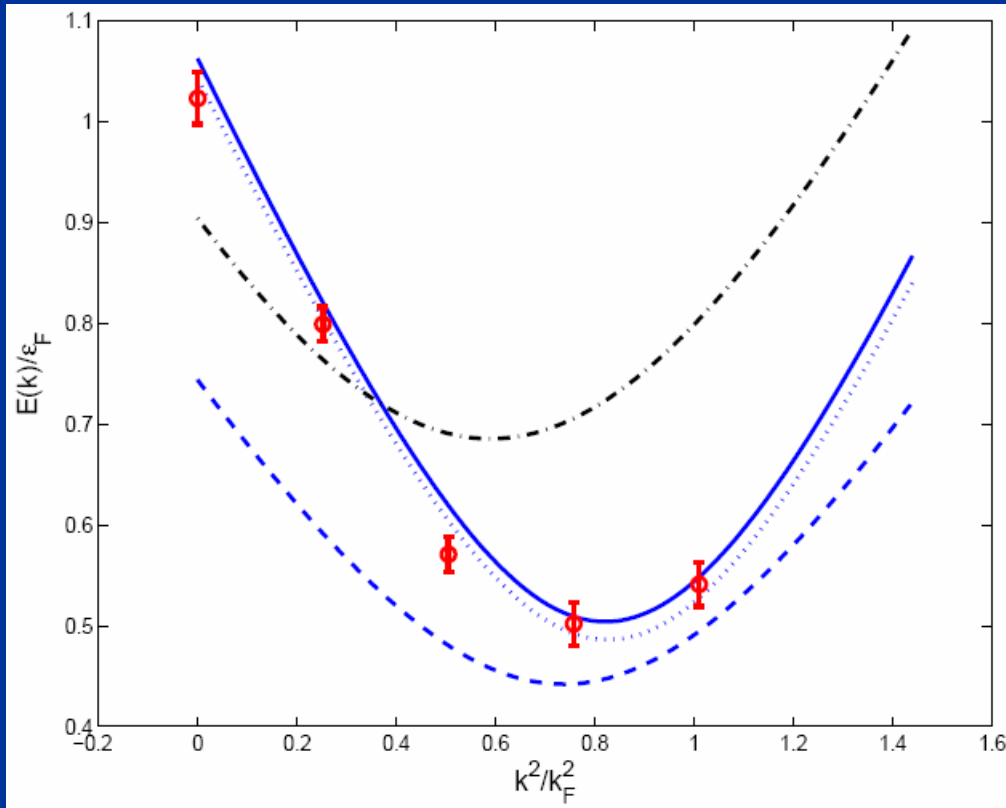
$$\frac{n^{1/3}}{\gamma} = \int \frac{d^3k}{(2\pi)^3} \left(\frac{1}{\alpha k^2} - \frac{1}{2E_k} \right)$$

One thus obtains:

$$\left\{ \begin{array}{l} \xi_s = \frac{5E}{3N \varepsilon_F} = 0.42(2) \\ \eta = \frac{\Delta}{\varepsilon_F} = 0.504(24) \\ \zeta = \frac{\mu}{\varepsilon_F} = 0.42(2) \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \alpha = 1.14 \\ \beta = -0.553 \\ \frac{1}{\gamma} = -0.0906 \end{array} \right.$$

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

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

Extra Bonus!

The normal state has been also determined in GFMC

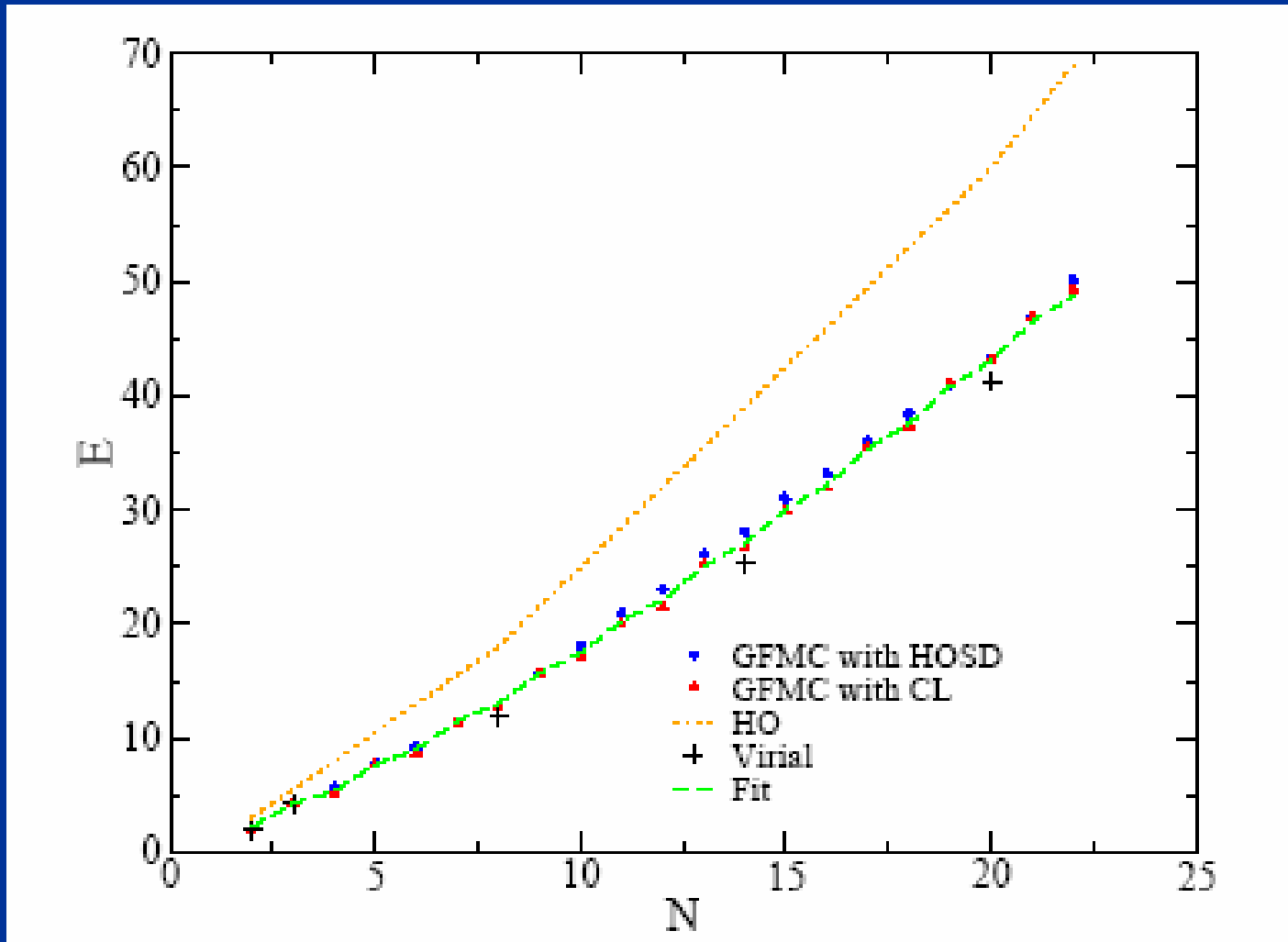
$$\xi_N = \frac{5E}{3N\varepsilon_F} = 0.55(2)$$

SLDA functional predicts

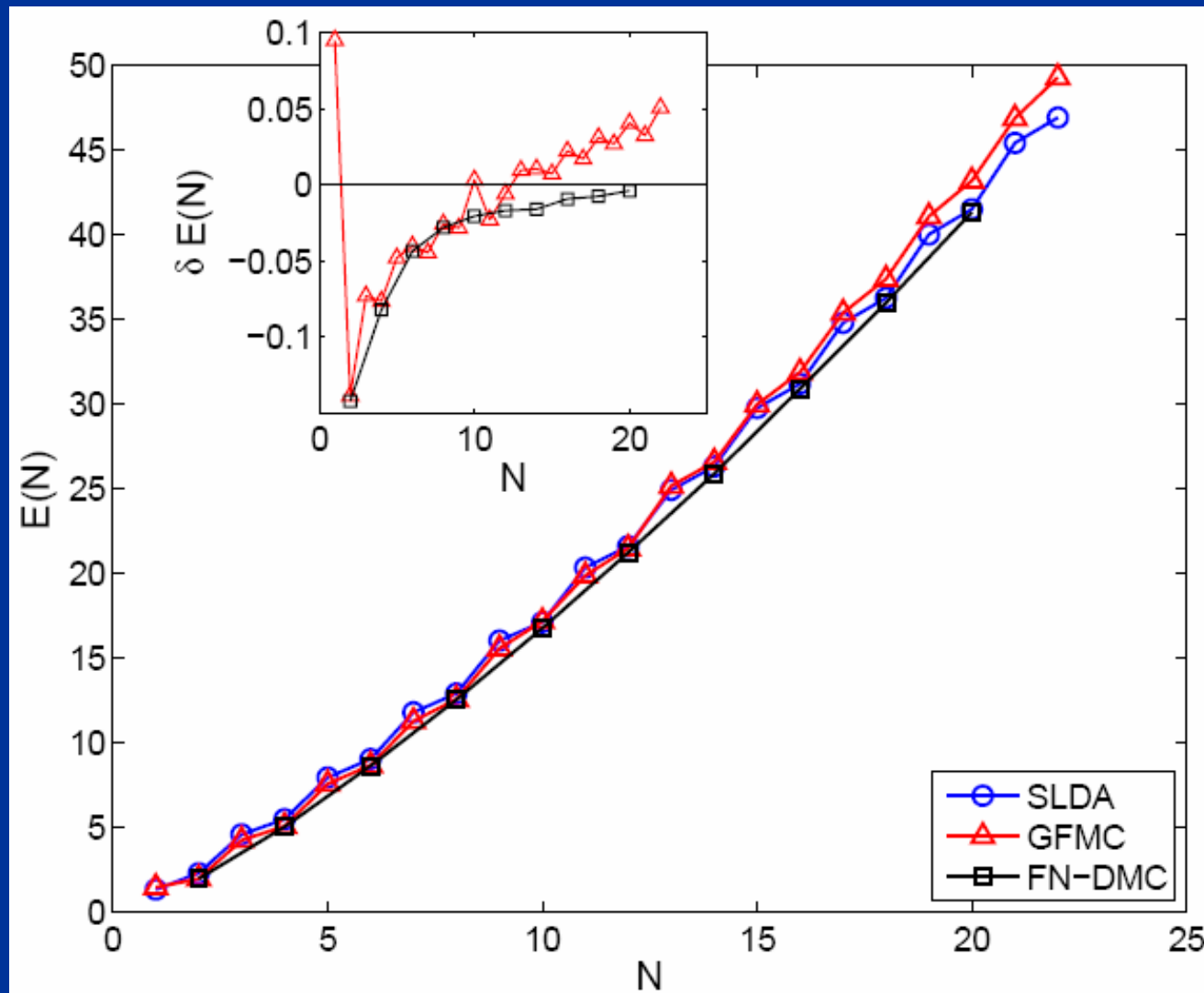
$$\xi_N = \alpha + \beta = 0.59$$

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

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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

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**NB Particle projection
neither required nor
needed in SLDA!!!**

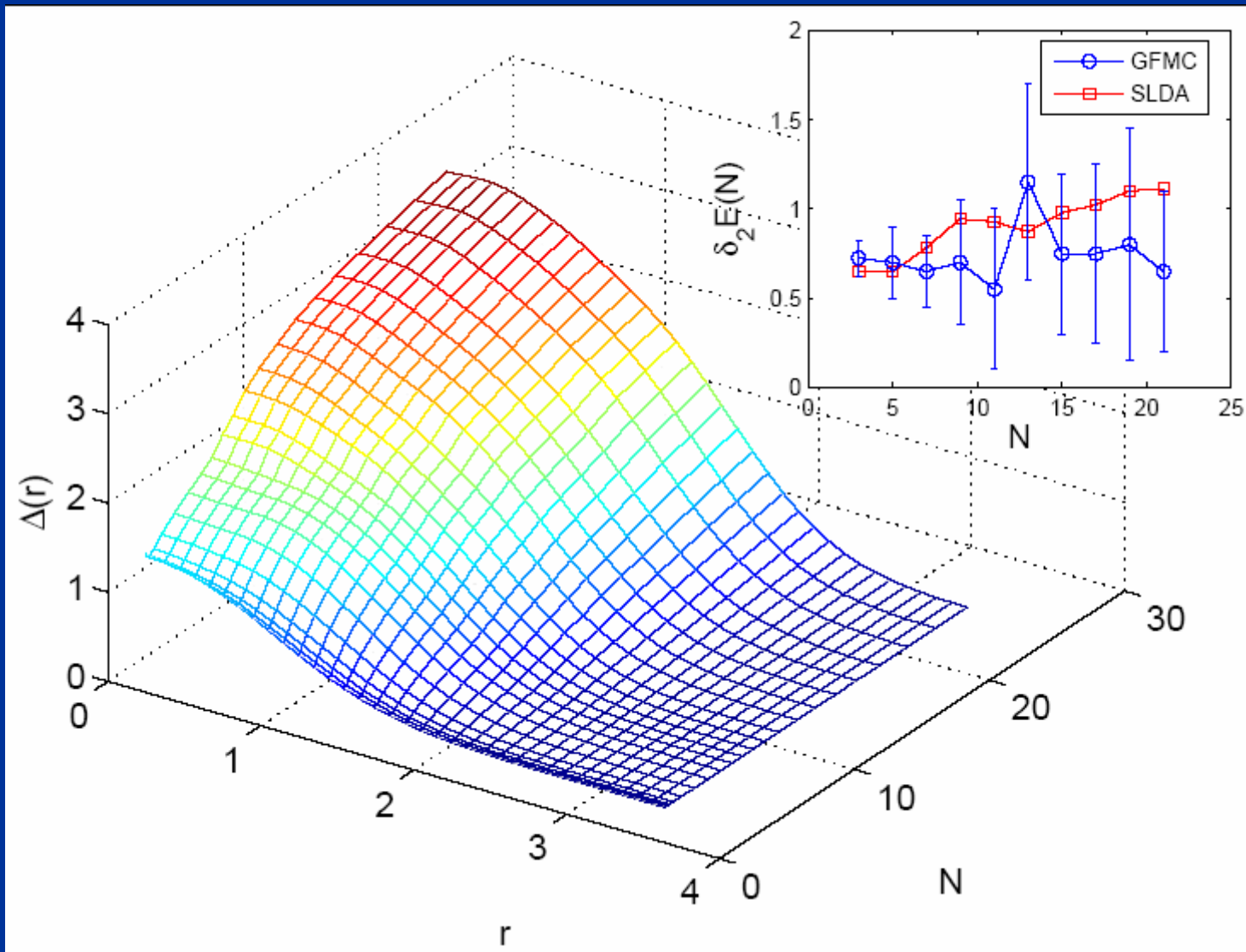
SLDA - Extension of Kohn-Sham approach to superfluid Fermi systems

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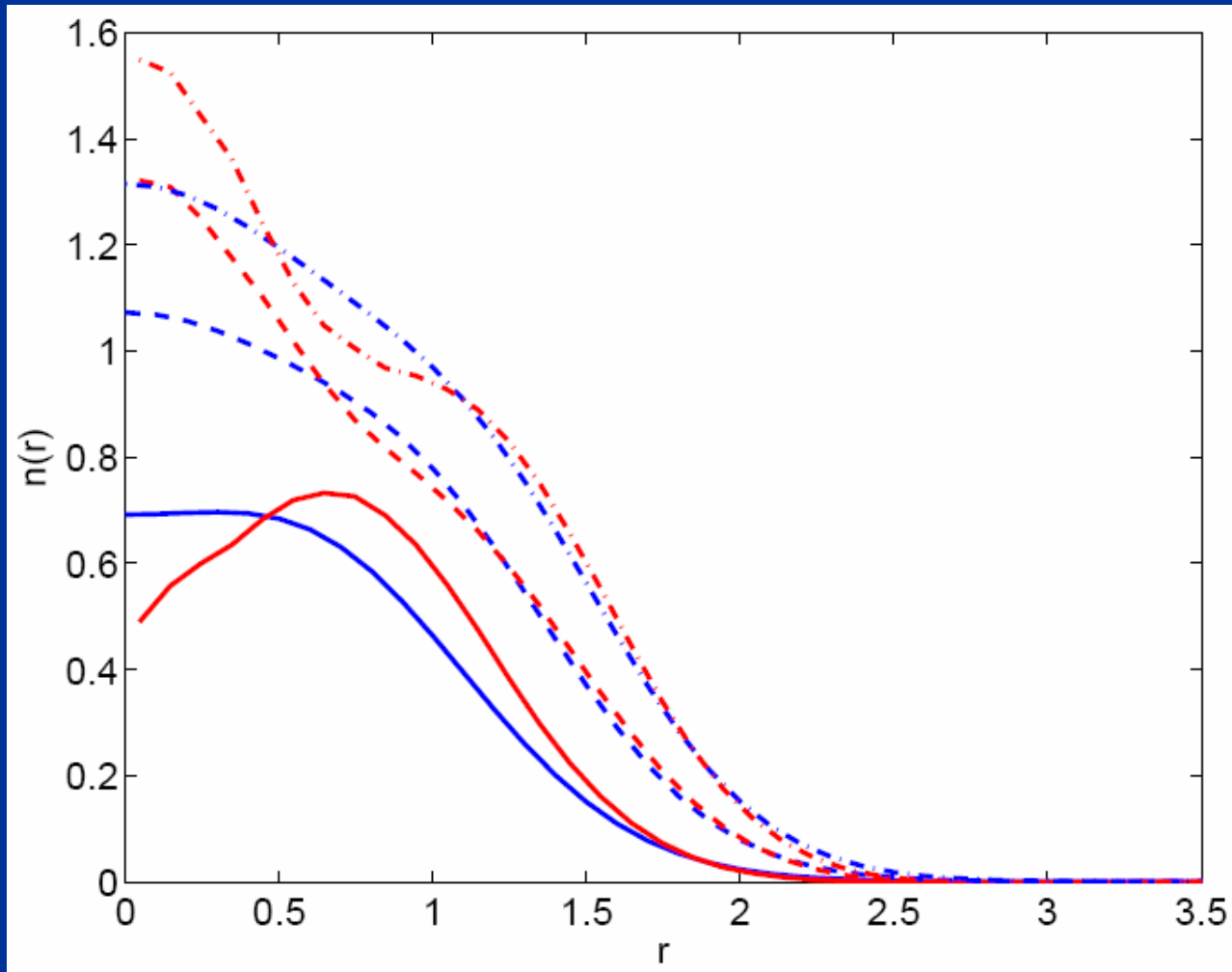
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$$\begin{pmatrix} T + U(\vec{r}) - \mu & \Delta(\vec{r}) \\ \Delta^*(\vec{r}) & -(T + U(\vec{r}) - \mu) \end{pmatrix} \begin{pmatrix} \mathbf{u}_k(\vec{r}) \\ \mathbf{v}_k(\vec{r}) \end{pmatrix} = E_k \begin{pmatrix} \mathbf{u}_k(\vec{r}) \\ \mathbf{v}_k(\vec{r})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



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



**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

Extension to excited states

Extension to time dependent problems

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

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