# Generation and Dynamics of Vortices in a Superfluid Unitary Gas

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**DE-FC02-07ER41457 (SciDAC-UNEDF)**

**Outline:**

- **What is a unitary gas?**
- **DFT extension to superfluid systems and its further extension to time-dependent phenomena**
- **A rare excitation mode in unitary Fermi gases: The Higgs mode**
- **The birth and life of vortices in a unitary Fermi gas in real time**

## Why would one want to study a unitary gas?

**One reason:**

**(for the nerds, I mean the hard-core theorists,**
**not for the phenomenologists)**

**Bertsch's 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.***

**What are the scattering length and the effective range?**

$$k \ \text{cotan}\ \delta_0 = -\frac{1}{a} + \frac{1}{2} r_0 k^2 + \cdots$$

$$\sigma = \frac{4\pi}{k^2} \sin^2 \delta_0 + \cdots = 4\pi a^2 + \cdots$$

**If the energy is small only the s-wave is relevant.**

**Let us consider a very old and simple example:**
**the hydrogen atom.**

**The ground state energy could only be a function of:**

- ✓ **Electron charge**
- ✓ **Electron mass**
- ✓ **Planck's constant**

**and then trivial dimensional arguments lead to**

$$E_{gs} = \frac{e^4 m}{\hbar^2} \times \frac{1}{2}$$

**Only the factor ½ requires some hard work.**

# Let us turn now to dilute fermion matter

**The ground state energy is given by a function:**

$$E_{gs} = f(N, V, \hbar, m, a, r_0)$$

**Taking the scattering length to infinity and the range of the interaction to zero, we are left with:**

$$E_{gs} = F(N, V, \hbar, m) = \frac{3}{5}\varepsilon_F N \times \xi$$

$$\frac{N}{V} = \frac{k_F^3}{3\pi^2}, \qquad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

**Pure number (dimensionless)**

*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.*

**Why? Besides pure theoretical curiosity, this problem is relevant to neutron stars!**

**In 1999 it was not yet clear, either theoretically or experimentally, whether such fermion matter is stable or not! A number of people argued that under such conditions Fermionic matter is unstable.**

- ***systems of bosons are unstable (Efimov effect)***
- ***systems of three or more fermion species are unstable (Efimov effect)***

**• Baker (LANL, winner of the MBX challenge) concluded that the system is stable. See also Heiselberg (entry to the same competition)**

**• Carlson *et al* (2003) Fixed-Node Green Function Monte Carlo and Astrakharchik *et al* (2004) FN-DMC provided the best theoretical estimates for the ground state energy of such systems.**

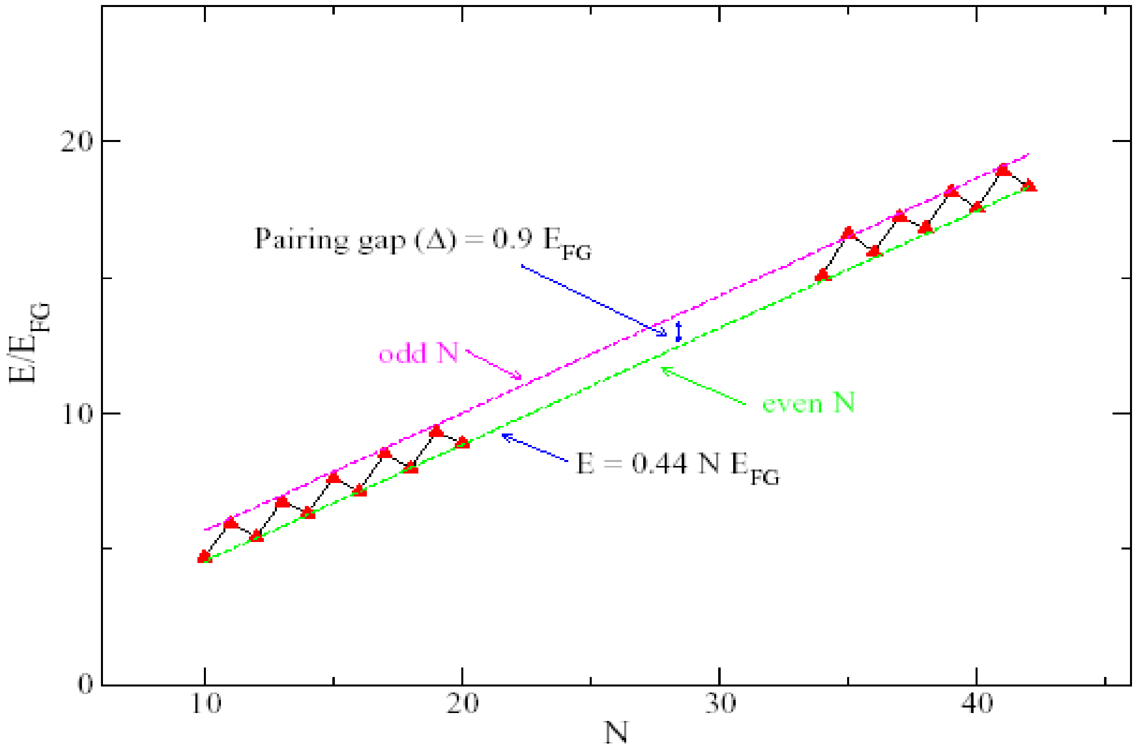
**Carlson *et al* (2003) have also shown that the system has a huge pairing gap !**

$$E_{gs} = \frac{3}{5}\varepsilon_F N \times \xi \qquad \Delta = \varepsilon_F \times \varsigma$$

$$\xi = 0.40(1), \qquad \zeta = 0.50(1)$$

**• Thomas' Duke group (2002) demonstrated experimentally that such systems are (meta)stable.**

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




Result for $ak_F = -\infty$

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

**Green Function Monte Carlo with Fixed Nodes**
**Chang, Carlson, Pandharipande and Schmidt, PRL 91, 050401 (2003)**

**The initial Bertsch's Many Body challenge has evolved over time and became the problem of *Fermions in the Unitary Regime***

**And this is part of the BCS-BEC crossover problem**

**The system is very dilute, but strongly interacting!**

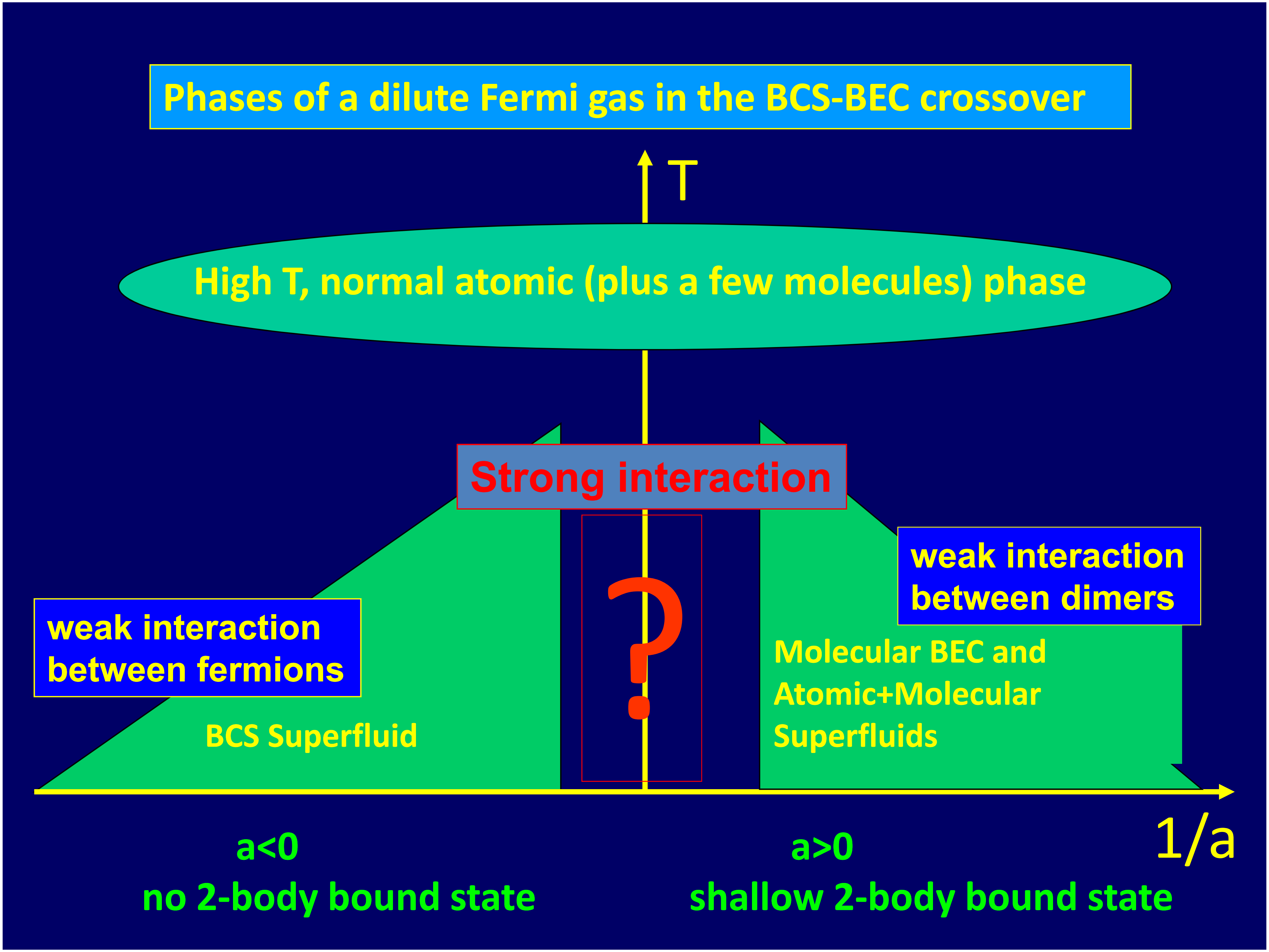
$$\boxed{n\, r_0^3 \ll 1} \qquad \boxed{n\, |a|^3 \gg 1}$$

**n - number density**

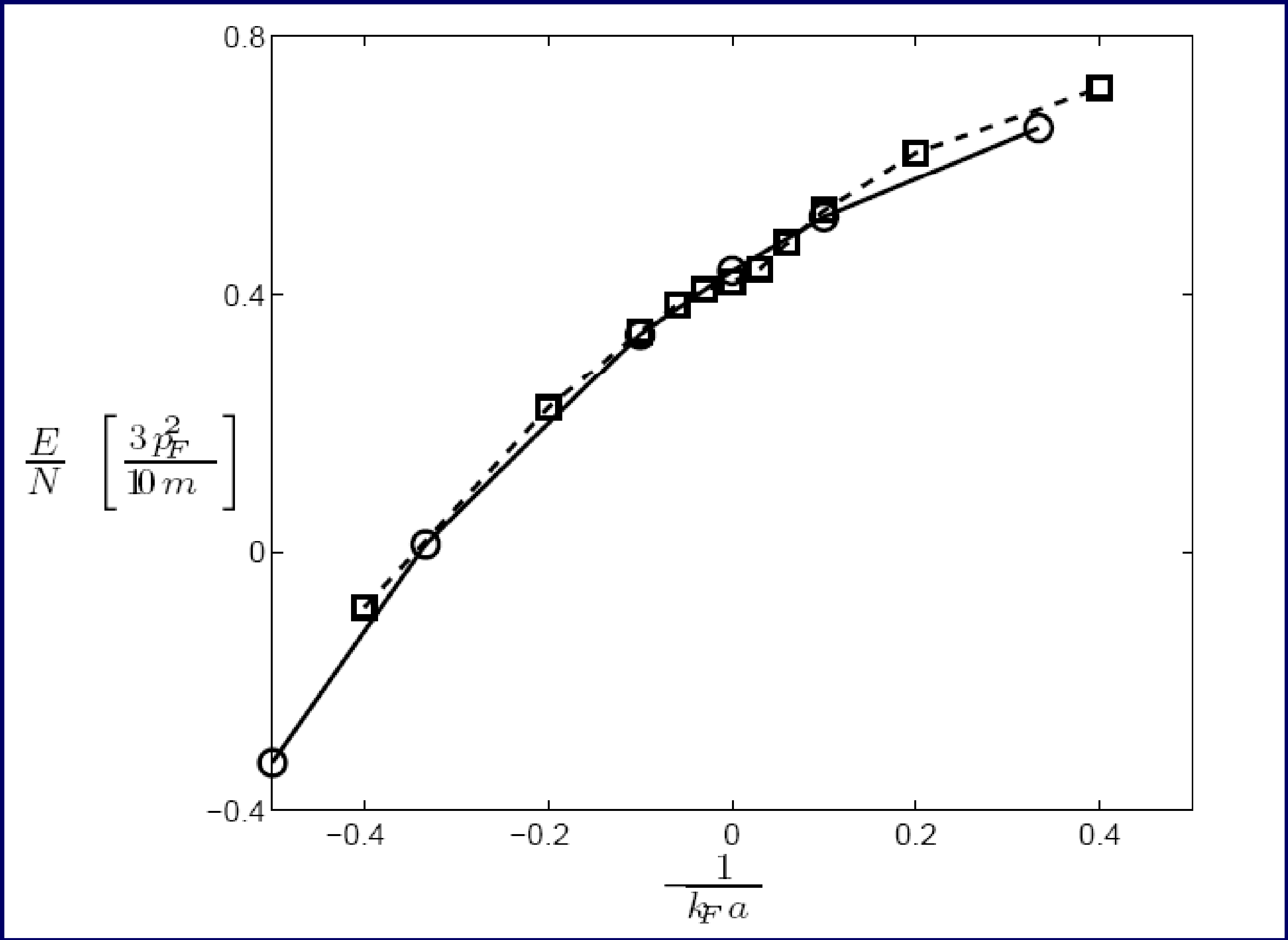
$$\boxed{r_0 \ll n^{-1/3} \approx \lambda_F/2 \ll |a|}$$

**$r_0$ - range of interaction**

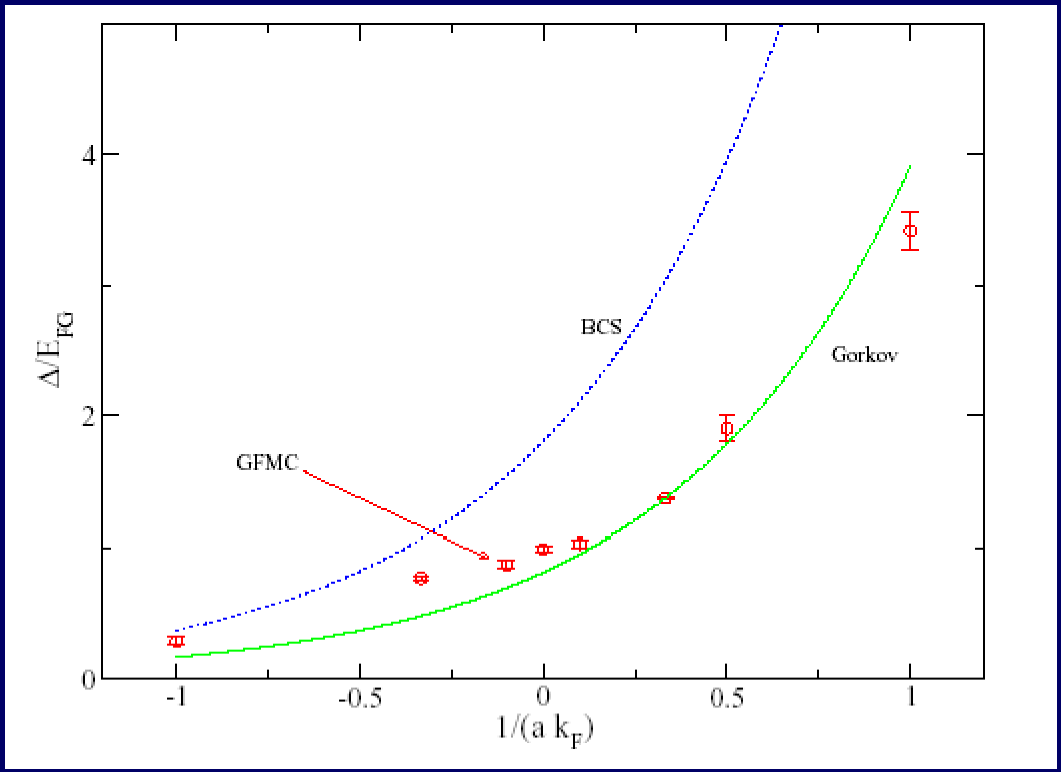
**a - scattering length**


Phases of a dilute Fermi gas in the BCS-BEC crossover
T
High T, normal atomic (plus a few molecules) phase
Strong interaction
?
weak interaction between dimers
weak interaction between fermions
Molecular BEC and Atomic+Molecular Superfluids
BCS Superfluid
1/a
a<0
no 2-body bound state
a>0
shallow 2-body bound state

BEC side BCS side




**Solid line with open circles – Chang *et al.* PRA, 70, 043602 (2004)**
**Dashed line with squares - Astrakharchik *et al.* PRL 93, 200404 (2004)**




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

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

**Fixed node GFMC results: S.-Y. Chang *et al.* PRA 70, 043602 (2004)**

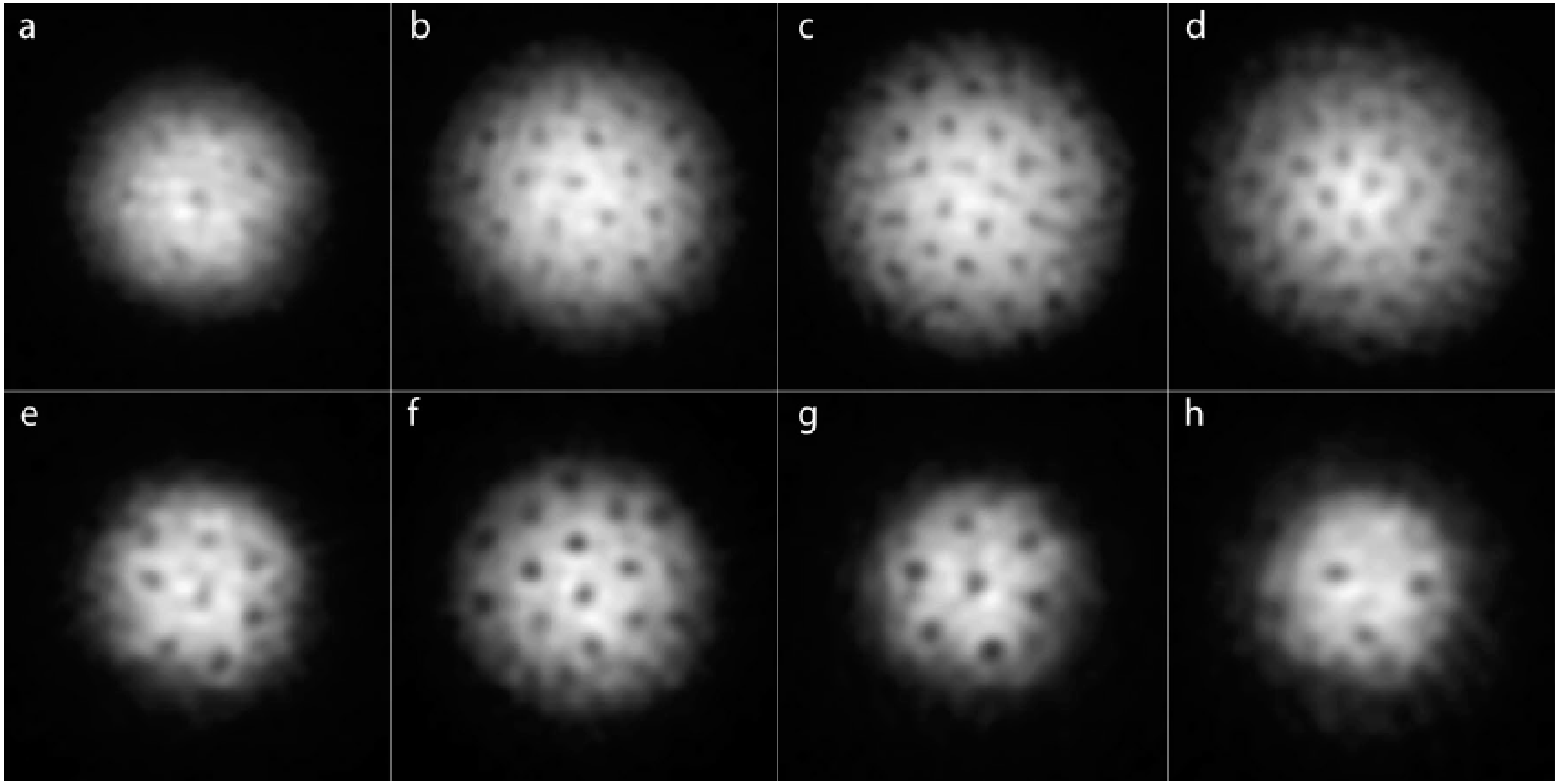
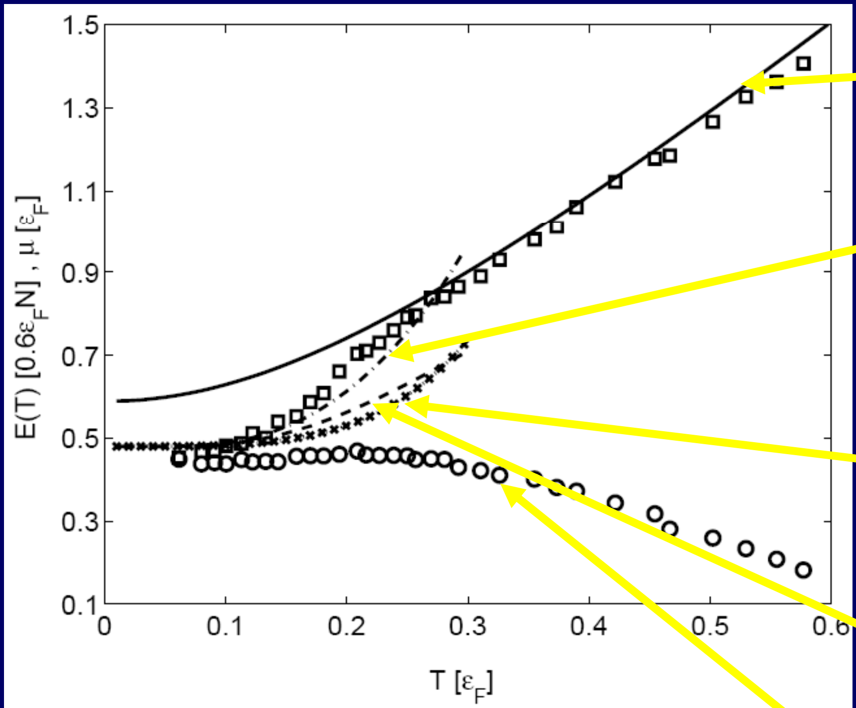



Fig. 2: Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) to 500 ms (b-h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were (a) 740 G, (b) 766 G, (c) 792 G, (d) 812 G, (e) 833 G, (f) 843 G, (g) 853 G and (h) 863 G. The field of view of each image is $880\ \mu\mathrm{m} \times 880\ \mu\mathrm{m}$.

**Zweirlein *et al.* Nature 435, 1047 (2005)**

# Finite temperature properties from QMC

**a = ±∞**




**Normal Fermi Gas (with vertical offset, solid line)**

**Bogoliubov-Anderson phonons and quasiparticle contribution (dot-dashed line )**

**Bogoliubov-Anderson phonons contribution only**

**Quasi-particles contribution only (dashed line)**

**μ - chemical potential (circles)**

$$E_{\text{phonons}}(T) = \frac{3}{5}\varepsilon_F N \; \frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}}\left(\frac{T}{\varepsilon_F}\right)^4, \qquad \xi_s \approx 0.44$$

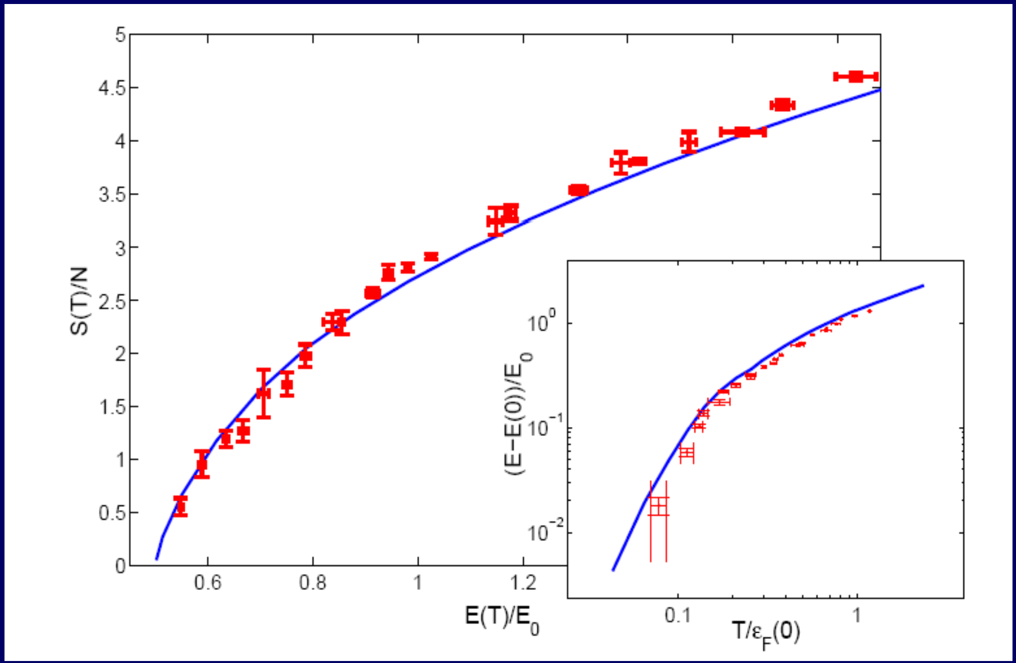
$$E_{\text{quasi-particles}}(T) = \frac{3}{5}\varepsilon_F N \; \frac{5}{2}\sqrt{\frac{2\pi\Delta^3 T}{\varepsilon_F^4}} \exp\left(-\frac{\Delta}{T}\right)$$

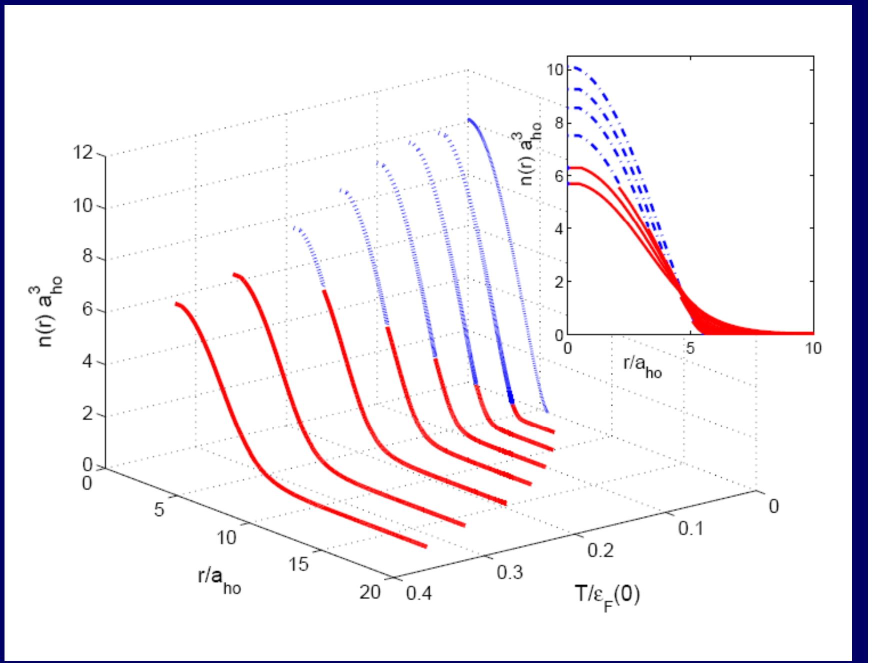
$$\Delta = \left(\frac{2}{e}\right)^{7/3} \varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$


**Bulgac, Drut, and Magierski**
**Phys. Rev. Lett. 96, 090404 (2006)**

**Experiment (about 100,000 atoms in a trap):**

***Measurement of the Entropy and Critical Temperature of a Strongly Interacting Fermi Gas,***
**Luo, Clancy, Joseph, Kinast, and Thomas, Phys. Rev. Lett. <u>98</u>, 080402 (2007)**

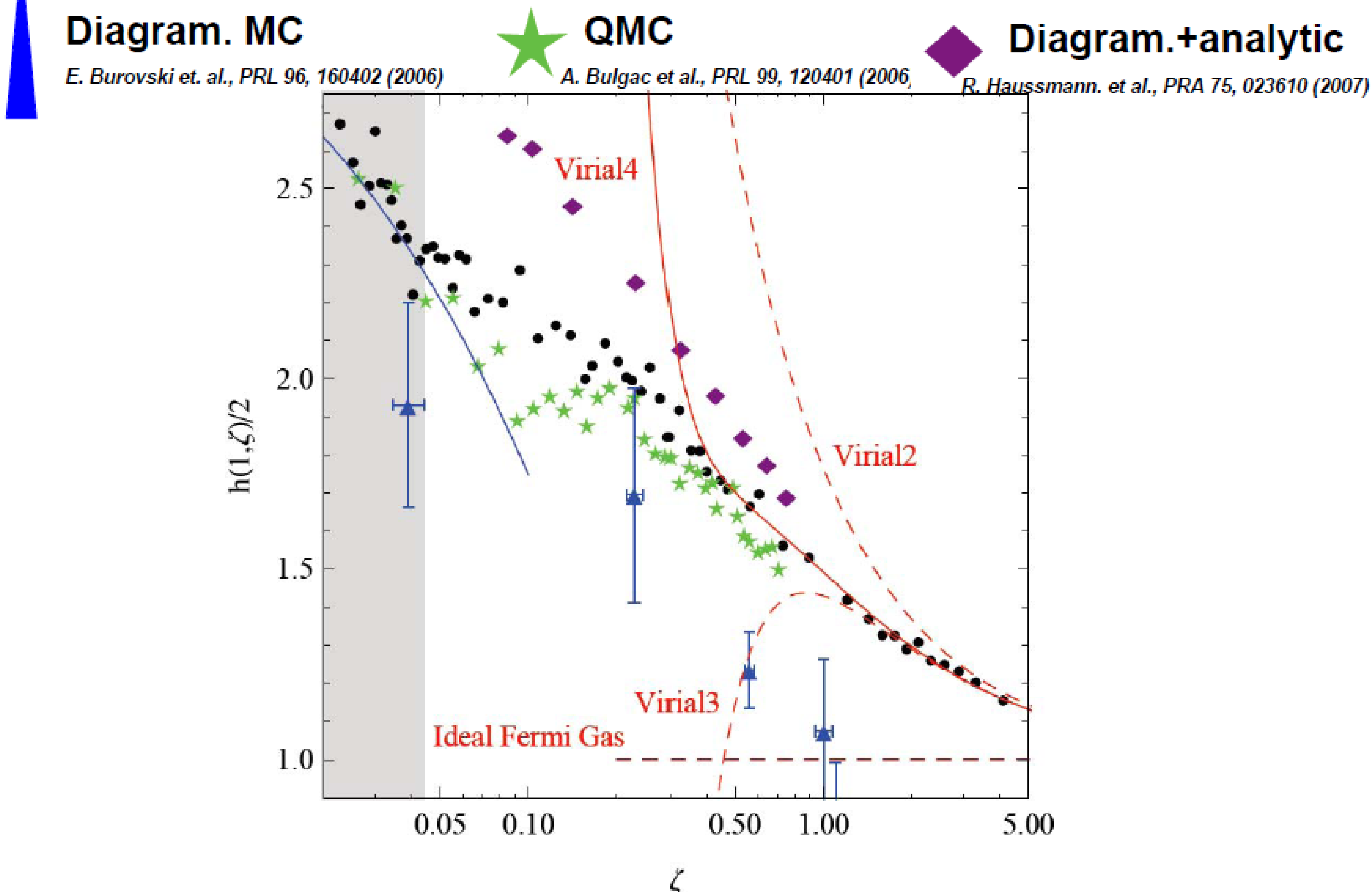



**Full *ab initio* theory (no free parameters)**

**Bulgac, Drut, and Magierski, Phys. Rev. Lett. <u>99</u>, 120401 (2007)**

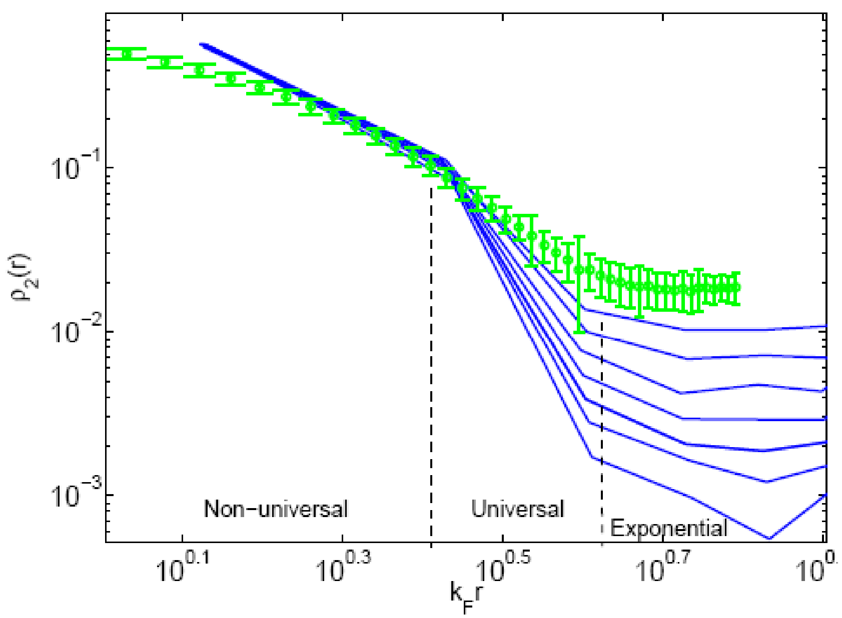
# Comparison with Many-Body Theories (1)

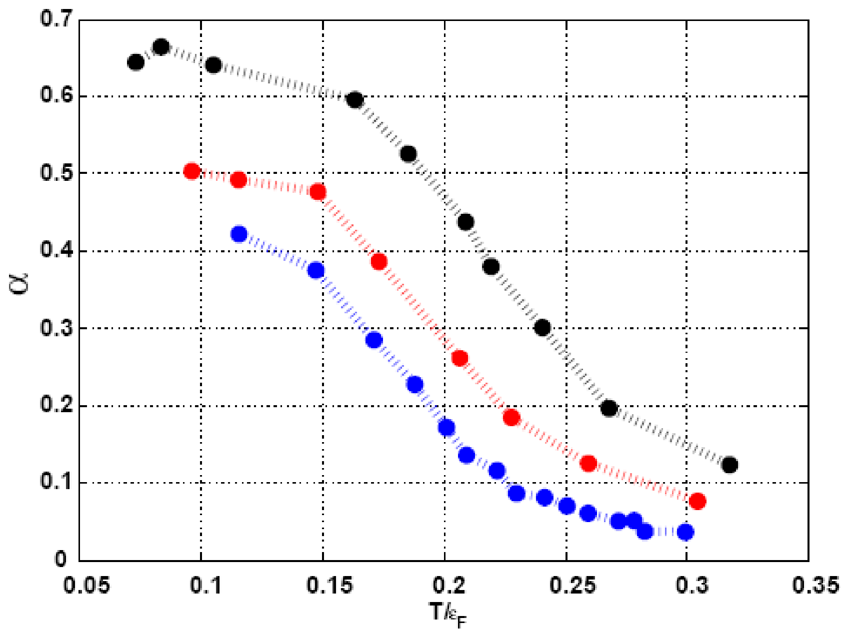



**From a talk given by C. Salomon, June 2nd, 2010, Saclay**

# Long range order, superfluidity and condensate fraction

## O. Penrose (1951), O. Penrose and L. Onsager (1956), C.N. Yang (1962)



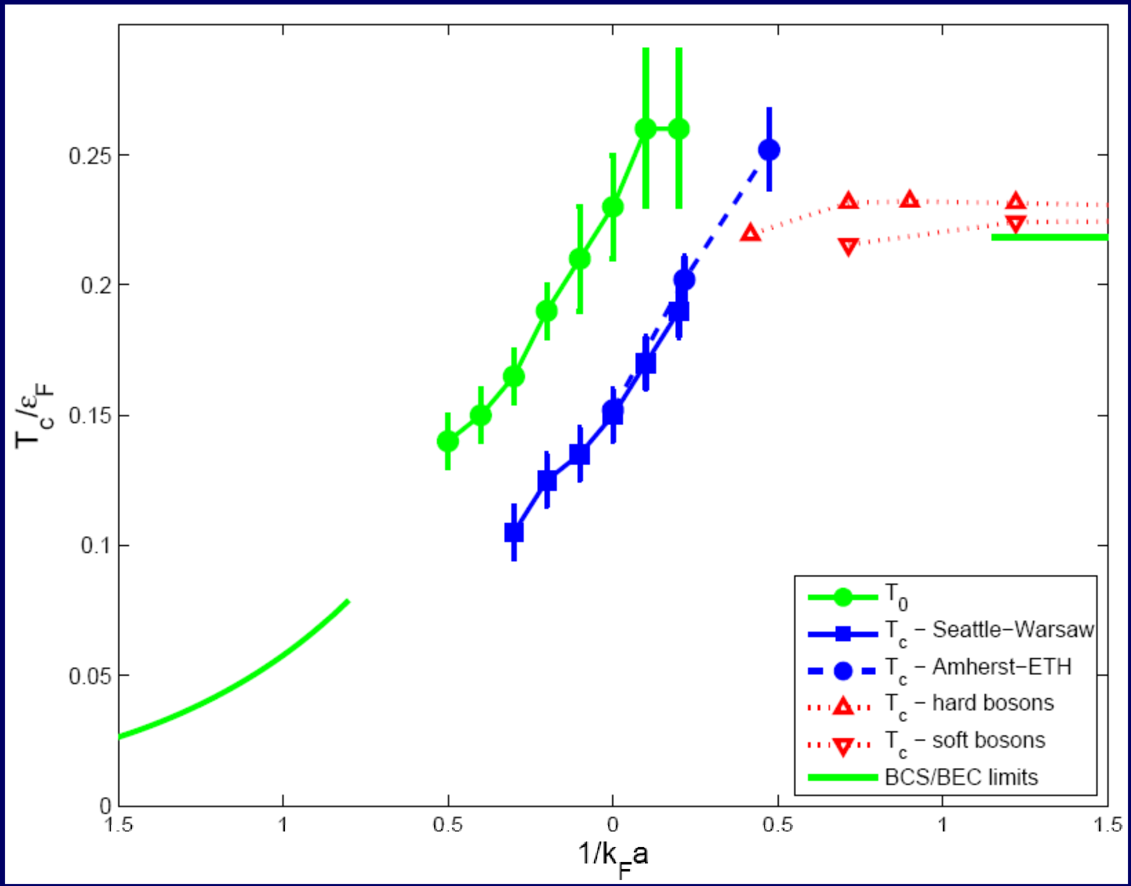




$$g_2(\vec{r}) = \left(\frac{2}{N}\right)^2 \int d^3\vec{r}_1 \int d^3\vec{r}_2 \left\langle \psi^\dagger_\uparrow(\vec{r}_1+\vec{r})\psi^\dagger_\downarrow(\vec{r}_2+\vec{r})\psi_\downarrow(\vec{r}_2)\psi_\uparrow(\vec{r}_2)\right\rangle$$

$$\alpha = \lim_{r\to\infty} \frac{N}{2} g_2(\vec{r}) - n(\vec{r})^2, \qquad n(\vec{r}) = \frac{2}{N}\int d^3\vec{r}_1 \left\langle \psi^\dagger_\uparrow(\vec{r}_1+\vec{r})\psi_\uparrow(\vec{r}_1)\right\rangle$$

**Bulgac, Drut, and Magierski, Phys. Rev. A <u>78</u>, 023625 (2008)**

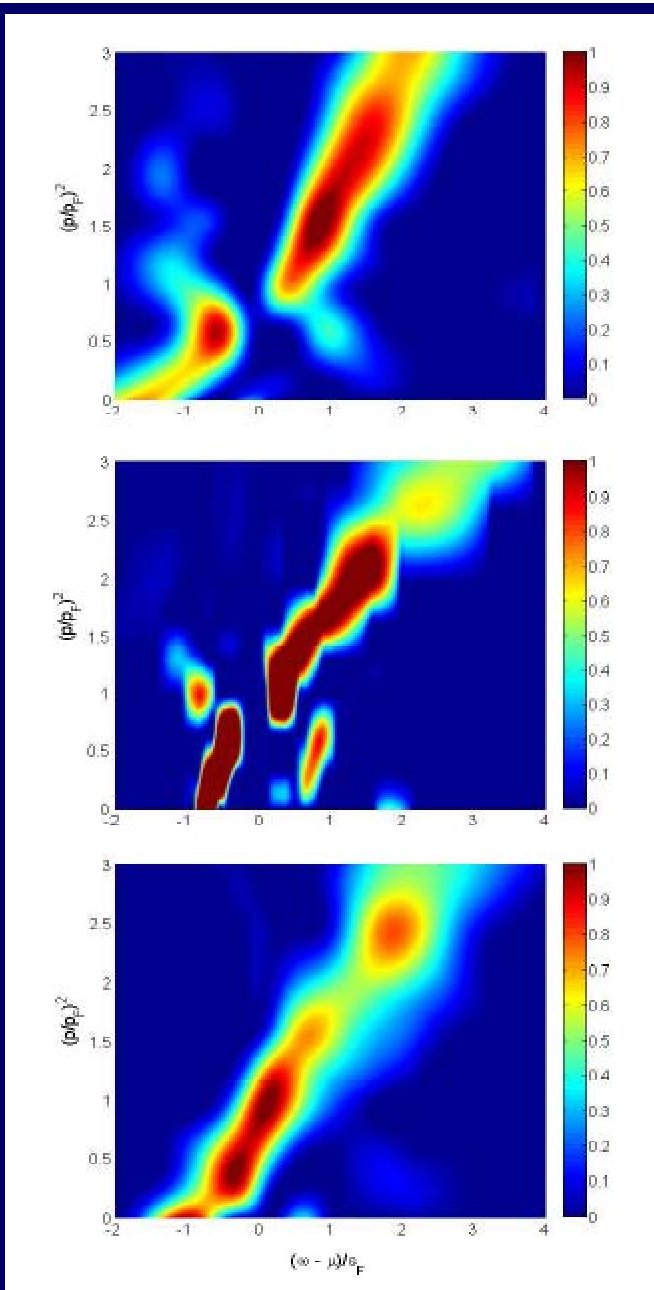
# Critical temperature for superfluid to normal transition




Bulgac, Drut, and Magierski, Phys. Rev. A 78, 023625 (2008)

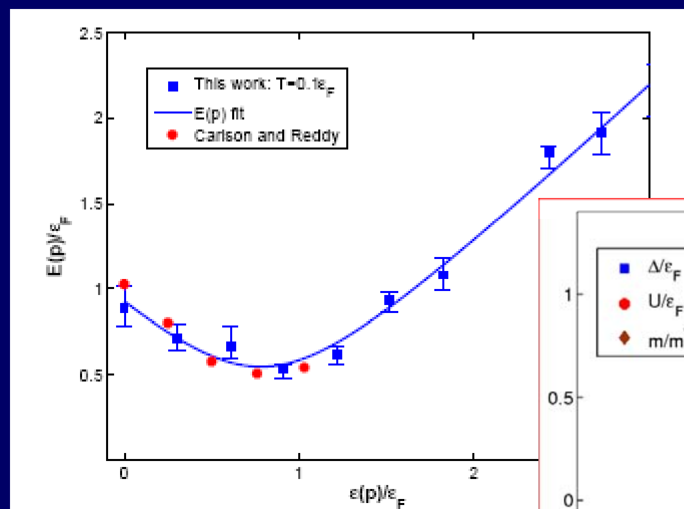
**Amherst-ETH:** Burovski et al. Phys. Rev. Lett. 101, 090402 (2008)

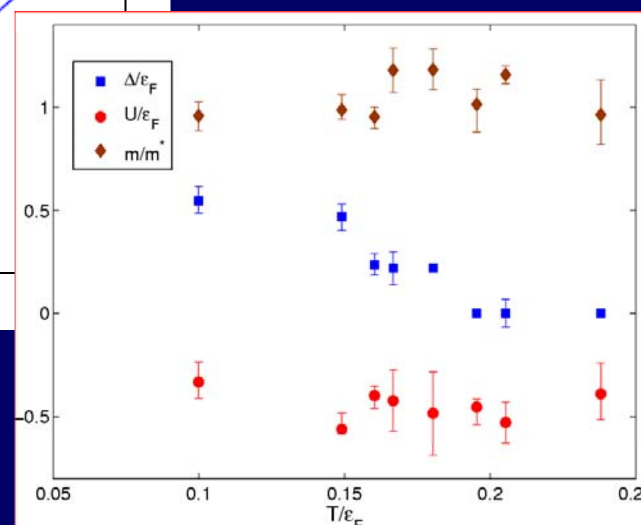
**Hard and soft bosons:** Pilati et al. PRL 100, 140405 (2008)




$$G(p,\tau)=\frac{1}{Z}\mathrm{Tr}\left\{\exp\left[-(\beta-\tau)(H-\mu N)\right]\psi^{\dagger}(p)\times \exp\left[-\tau(H-\mu N)\right]\psi(p)\right\}$$

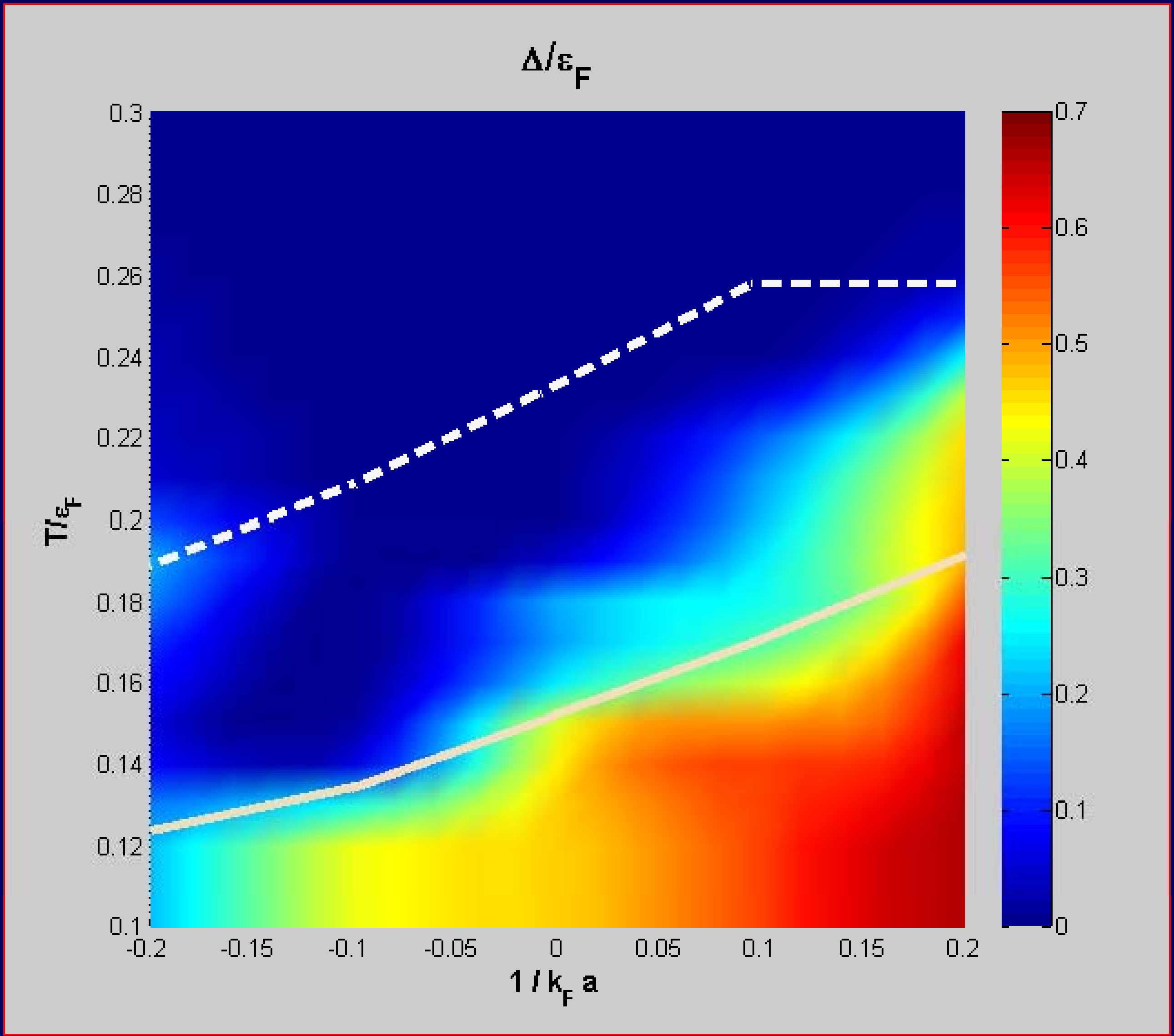
$$=-\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, A(p,\omega)\frac{\exp(-\omega\tau)}{1+\exp(-\omega\beta)}$$



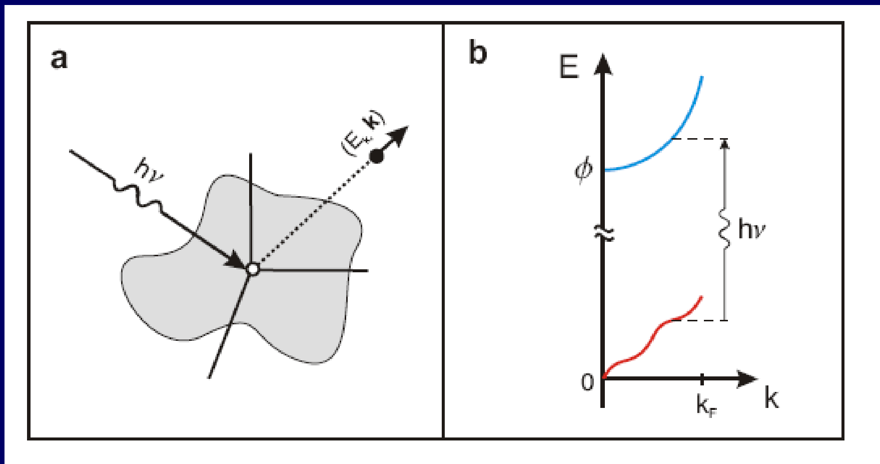

**Magierski, Wlazlowski, Bulgac, and Drut**
**Phys. Rev. Lett. 103, 210403 (2009)**

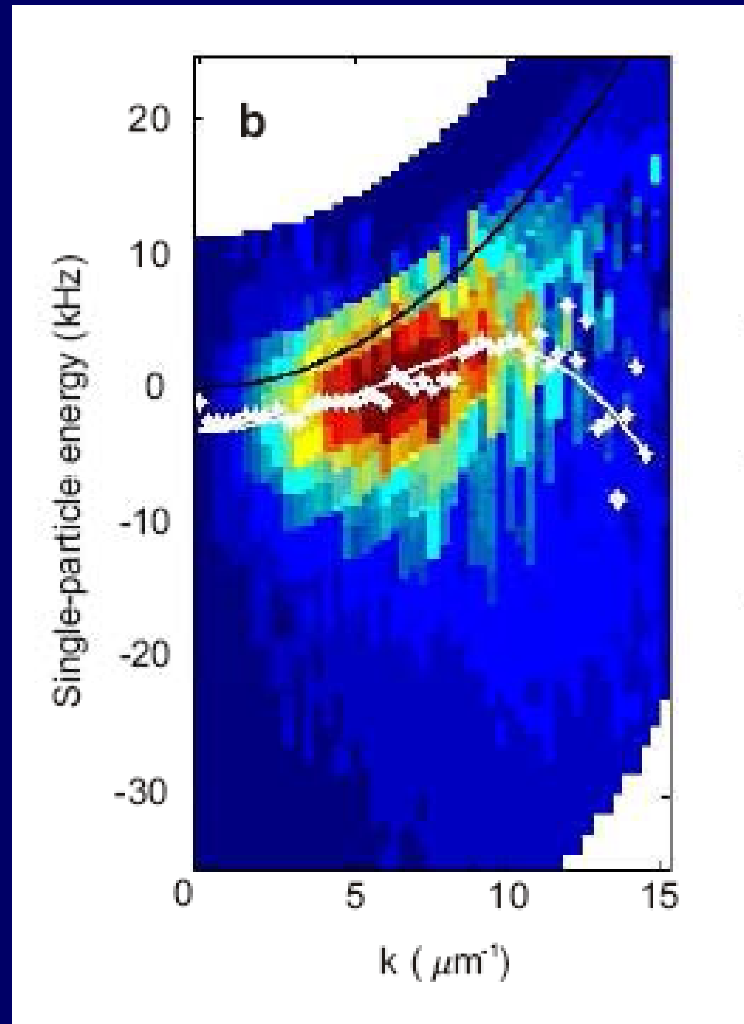
**The pseudo-gap vanishes at ≈ $T_0$**




**The pseudogap around the unitary point**

**Onset around** $1/k_F a \approx -0.1$



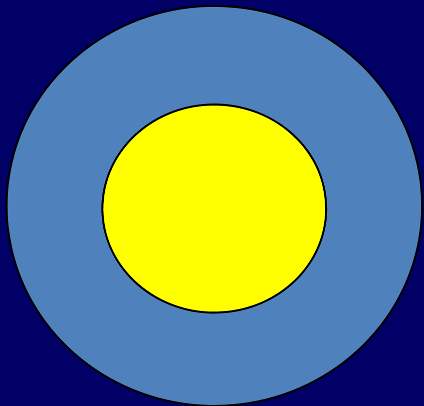

$$E(N) + h\nu = E(N-1) + E_k + \frac{\hbar^2 k^2}{2m} + \phi$$

***Using photoemission spectroscopy to probe a strongly interacting Fermi gas***

**Stewart, Gaebler, and Jin, Nature, <u>454</u>, 744 (2008)**

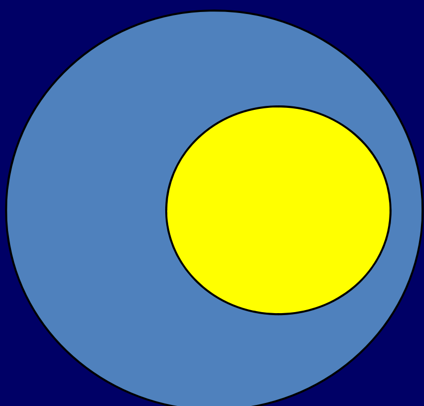
**What happens when there are not enough partners for everyone to pair with?**

**What theory tells us?**

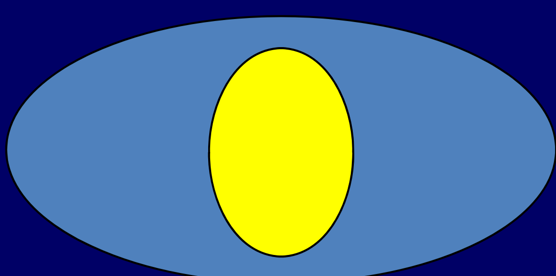


**Green – Fermi sphere of spin-up fermions**
**Yellow – Fermi sphere of spin-down fermions**

$$\text{If} \quad \left|\mu_\uparrow - \mu_\downarrow\right| < \frac{\Delta}{\sqrt{2}} \ \text{ the same solution as for } \mu_\uparrow = \mu_\downarrow$$



**LOFF/FFLO solution (1964)**
**Pairing gap becomes a spatially varying function**
**Translational invariance broken**

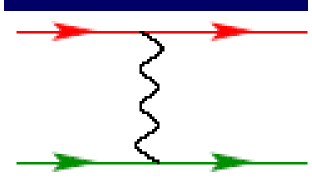


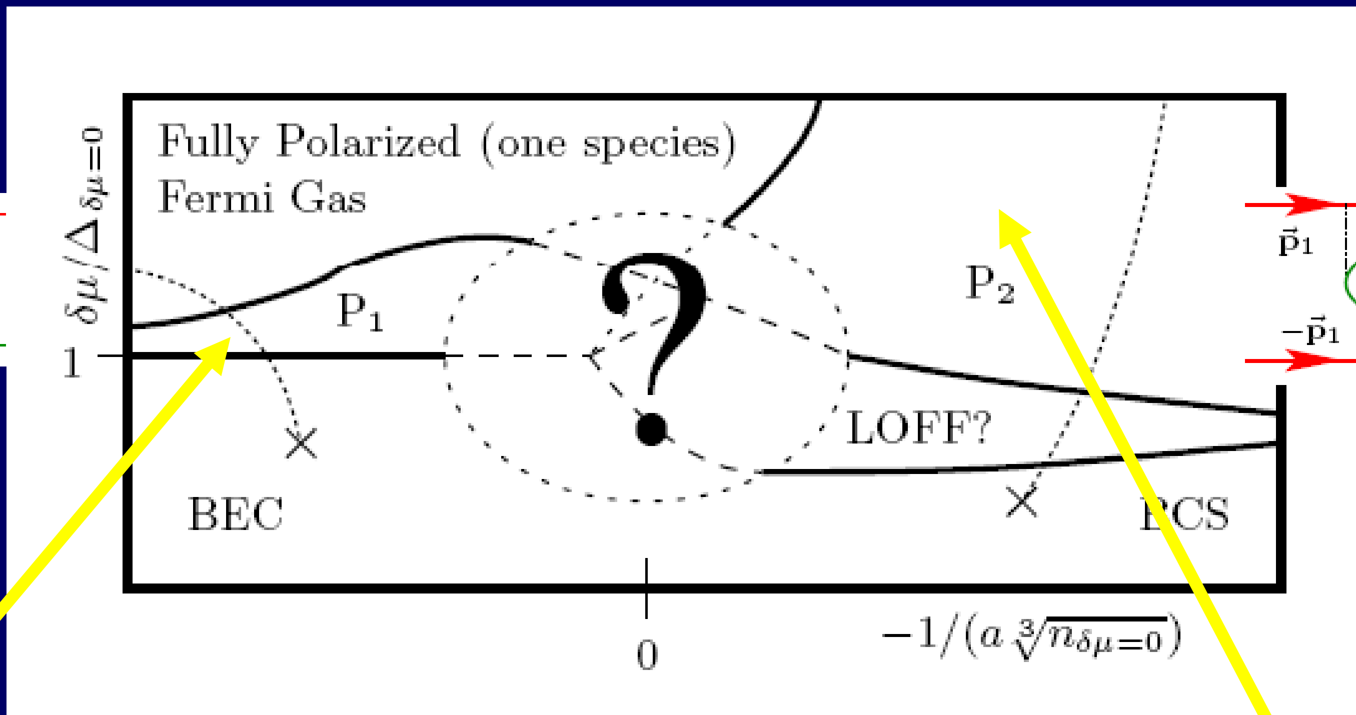
**Muether and Sedrakian (2002)**
**Translational invariant solution**
**Rotational invariance broken**

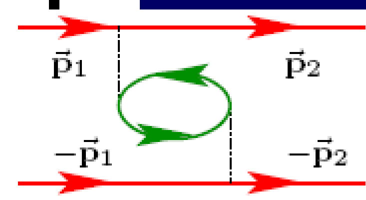
## What we think is happening in spin imbalanced systems?

**Induced P-wave superfluidity**

**Two new superfluid phases where before they were not expected**





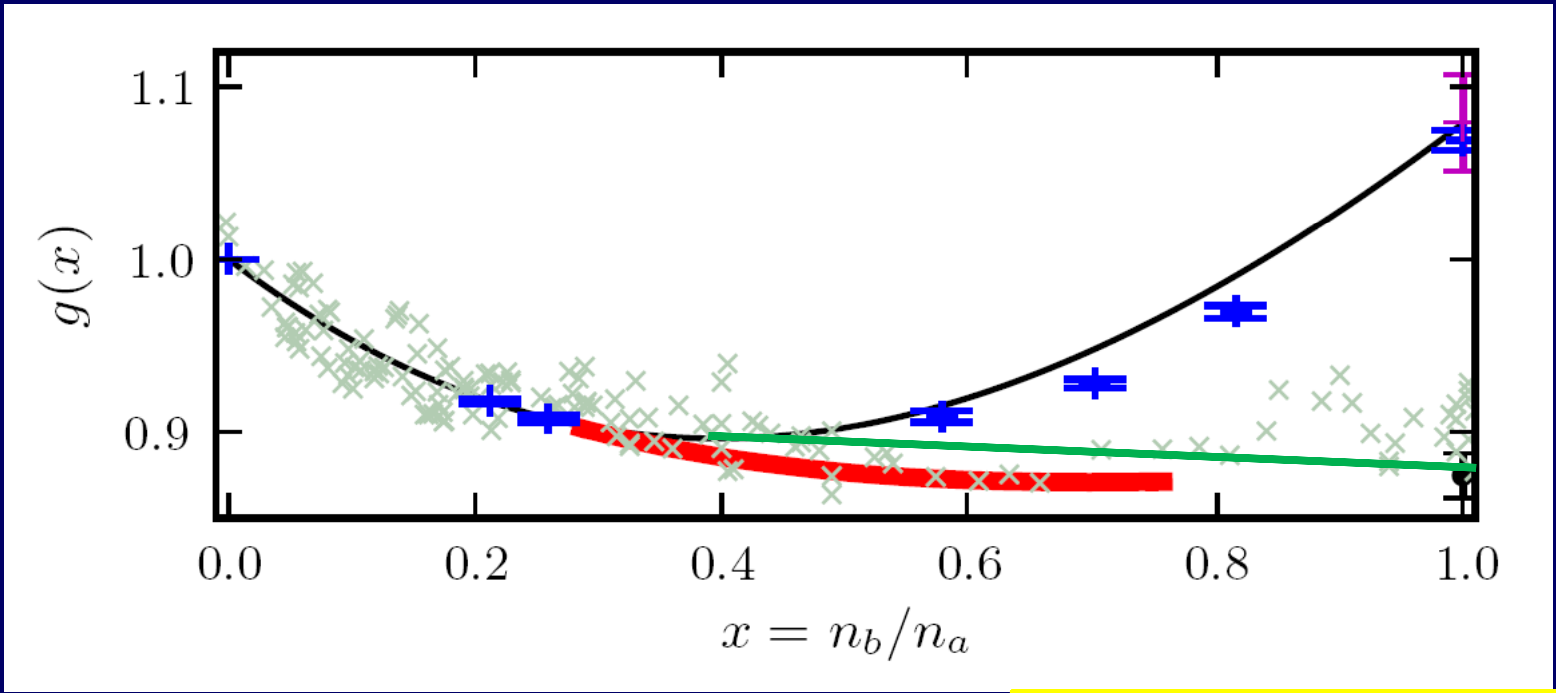




**One Bose superfluid coexisting with one P-wave Fermi superfluid**

**Two coexisting P-wave Fermi superfluids**

**Bulgac, Forbes, Schwenk, Phys. Rev. Lett. 97, 020402 (2006)**

# A refined EOS for spin unbalanced systems




Bulgac and Forbes,
Phys. Rev. Lett. 101, 215301 (2008)

**Red line: Larkin-Ovchinnikov phase**

**Black line:** normal part of the energy density
**Blue points:** DMC calculations for normal state, Lobo et al, PRL 97, 200403 (2006)
**Gray crosses:** experimental EOS due to Shin, Phys. Rev. A 77, 041603(R) (2008)

$$E(n_a, n_b) = \frac{3}{5}\frac{(6\pi^2)^{2/3}\hbar^2}{2m}\left[n_a g\left(\frac{n_b}{n_a}\right)\right]^{5/3}$$

# We need also to treat inhomogeneous systems!

- Monte Carlo (feasible for small particle numbers only)

- Density Functional Theory (large particle numbers)

  1) one needs to find an Energy Density Functional (EDF)
  and 2) to extend DFT to superfluid phenomena

**Density Functional Theory (DFT)**
**Hohenberg and Kohn, 1964**

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

**particle density only!**

**Local Density Approximation (LDA) Kohn and Sham, 1965**

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

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

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

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

**Kohn-Sham equations**

## Kohn-Sham theorem

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

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

$$n(\vec{r})=\left\langle\Psi_0\left|\sum_{i}^{N}\delta(\vec{r}-\vec{r}_i)\right|\Psi_0\right\rangle$$

**Injective map (one-to-one)**

$$\boxed{\Psi_0(1,2,\ldots N)\quad\Leftrightarrow\quad V_{ext}(\vec{r})\quad\Leftrightarrow\quad n(\vec{r})}$$

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

$$n(\vec{r})=\sum_{i}^{N}\left|\varphi_i(\vec{r})\right|^2,\qquad\tau(\vec{r})=\sum_{i}^{N}\left|\vec{\nabla}\varphi_i(\vec{r})\right|^2$$

**Universal functional of particle density alone**

**Independent of external potential**

**Normal Fermi systems only!**

However, not everyone is normal!

## Superconductivity and superfluidity in Fermi systems

| | |
|---|---|
| ✓ Dilute atomic Fermi gases | $T_c \approx 10^{-9}$ 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

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

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

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

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

**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 $\Delta$ diverges.**

# The SLDA (renormalized) equations

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

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

$$\begin{cases} [h(\vec{r})-\mu]\mathrm{u}_\mathrm{i}(\vec{r}) + \Delta(\vec{r})\mathrm{v}_\mathrm{i}(\vec{r}) = E_i\mathrm{u}_\mathrm{i}(\vec{r}) \\ \Delta^*(\vec{r})\mathrm{u}_\mathrm{i}(\vec{r}) - [h(\vec{r})-\mu]\mathrm{v}_\mathrm{i}(\vec{r}) = E_i\mathrm{v}_\mathrm{i}(\vec{r}) \end{cases} \qquad \begin{cases} h(\vec{r}) = -\vec{\nabla}\dfrac{\hbar^2}{2m(\vec{r})}\vec{\nabla} + U(\vec{r}) \\ \Delta(\vec{r}) = -g_{\text{eff}}(\vec{r})\nu_c(\vec{r}) \end{cases}$$

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

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

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

**Position and momentum dependent running coupling constant**
**Observables are (obviously) independent of cut-off energy (when chosen properly).**

# The SLDA (DFT) energy density functional at unitarity for equal numbers of spin-up and spin-down fermions

$$\varepsilon(\vec{r}) = \overbrace{\left[\alpha \frac{\tau_c(\vec{r})}{2} - \Delta(\vec{r})\nu_c(\vec{r})\right]}^{\text{Only this combination is cutoff independent}} + \beta \frac{3(3\pi^2)^{2/3} n^{5/3}(\vec{r})}{5}$$

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

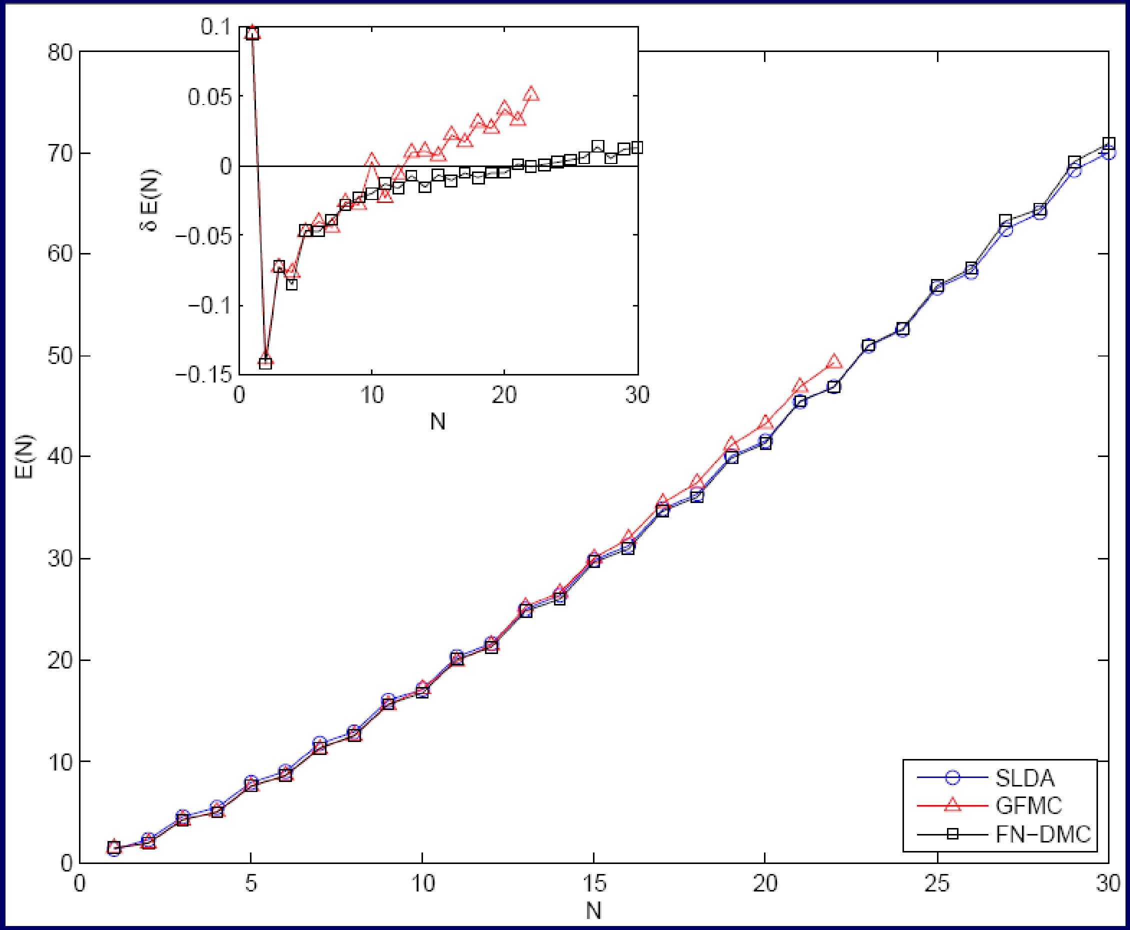
$$\nu_c(\vec{r}) = \sum_{0<E<E_c} \mathrm{u}_\mathrm{k}(\vec{r})\mathrm{v}_\mathrm{k}^*(\vec{r})$$

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

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

**$\alpha$ can take any positive value,**
**but the best results are obtained when $\alpha$ is fixed by the qp-spectrum**

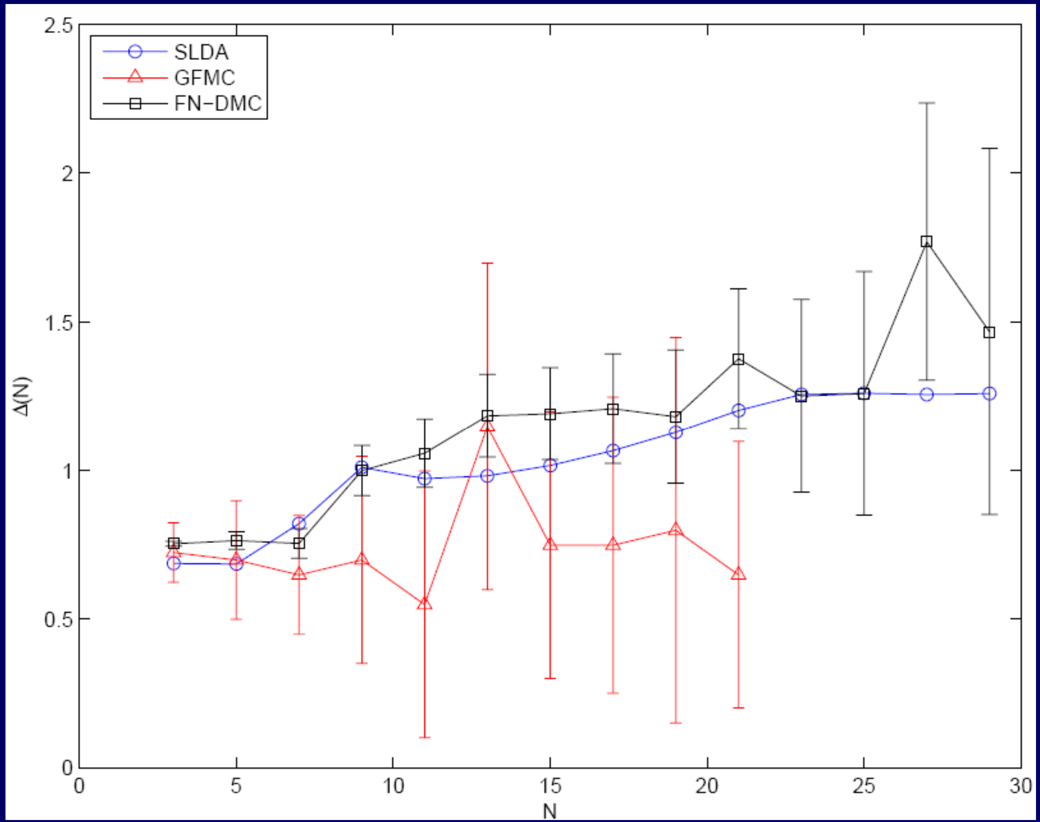
# Fermions at unitarity in a harmonic trap
# Total energies E(N)




**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)**

# Fermions at unitarity in a harmonic trap
# Pairing gaps




$$\Delta(N) = \frac{E(N+1) - 2E(N) + E(N-1)}{2}, \quad \text{for odd } N$$

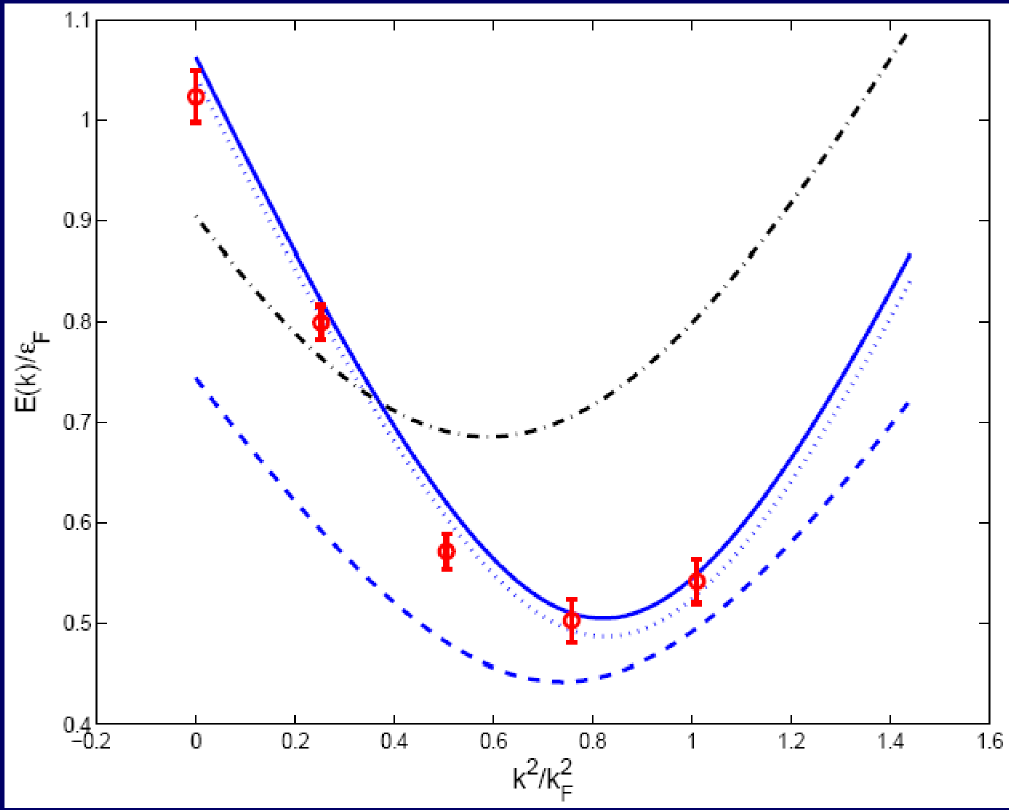
**GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007)**

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

**PRA 76, 053613 (2007)**

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

# Quasiparticle spectrum in homogeneous matter

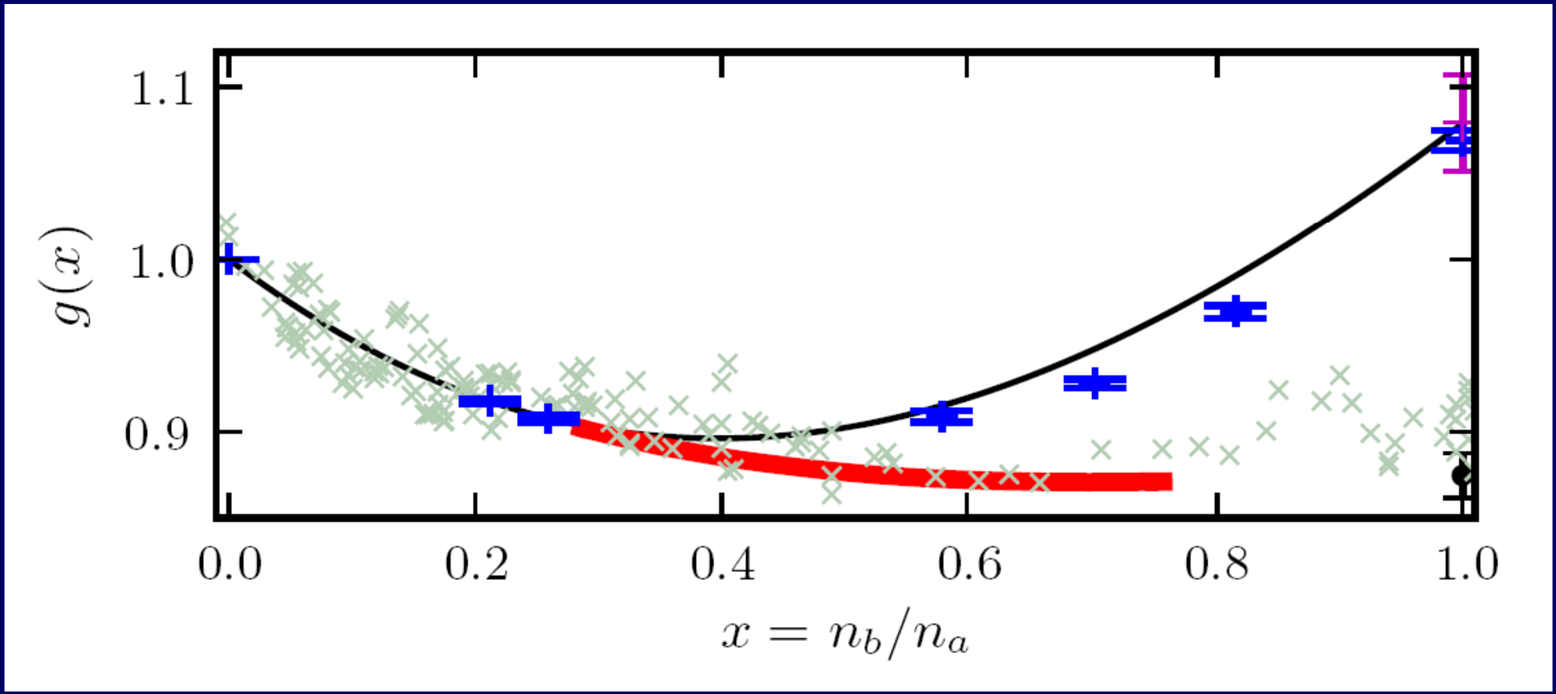



**NB! In DFT one does not try to reproduce the single-particle spectrum ( only the Fermi level)**

**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**

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

## EOS for spin polarized systems



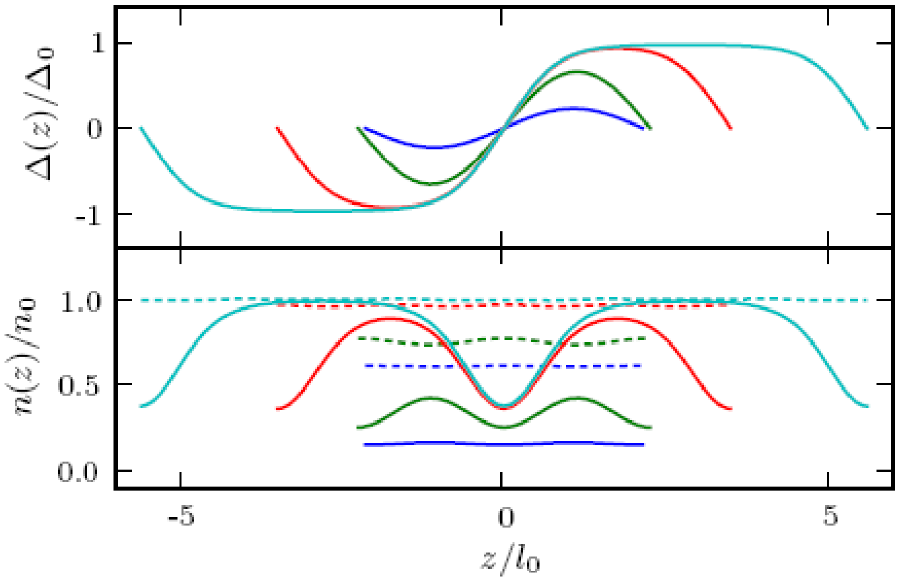

**Red line: Larkin-Ovchinnikov phase (unitary Fermi supersolid)**

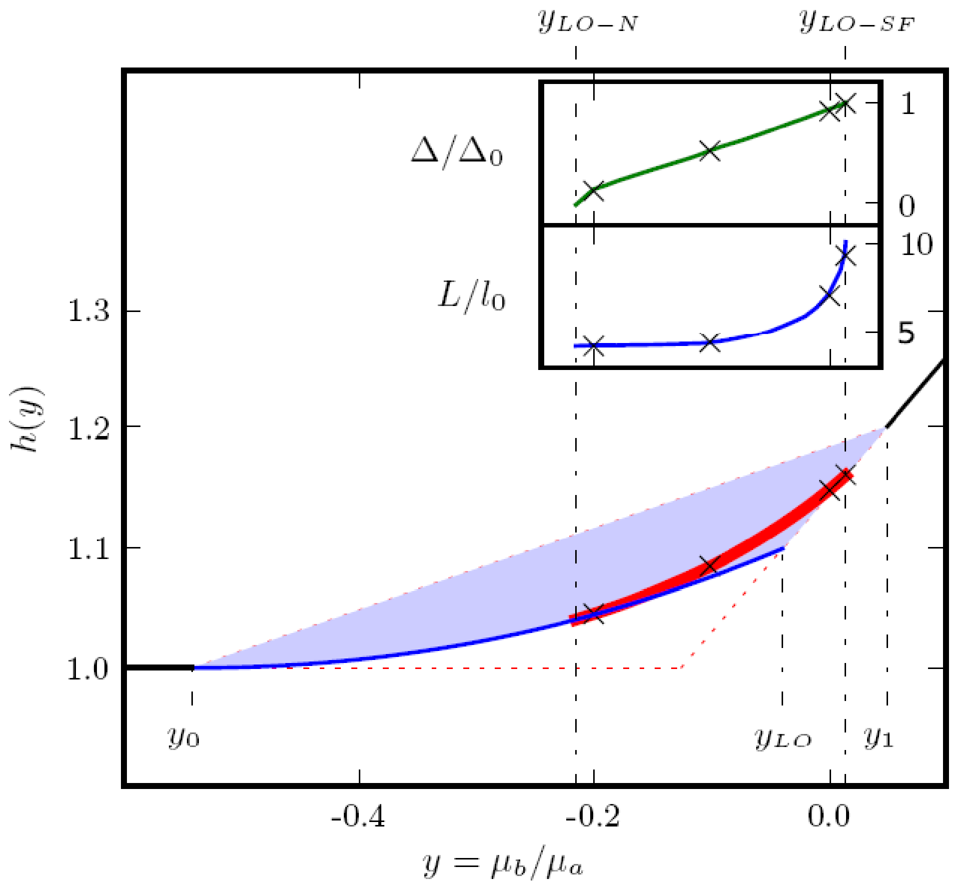
**Black line:** normal part of the energy density
**Blue points:** DMC calculations for normal state, Lobo et al, PRL 97, 200403 (2006)
**Gray crosses:** experimental EOS due to Shin, Phys. Rev. A 77, 041603(R) (2008)

$$E(n_a, n_b) = \frac{3}{5}\frac{(6\pi^2)^{2/3}\hbar^2}{2m}\left[n_a g\left(\frac{n_b}{n_a}\right)\right]^{5/3}$$

**Bulgac and Forbes,**
**Phys. Rev. Lett. 101, 215301 (2008)**

# A Unitary Fermi Supersolid: the Larkin-Ovchinnikov phase




Bulgac and Forbes
PRL 101, 215301 (2008)

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

# Formalism for Time Dependent Phenomena

**The time-dependent density functional theory is viewed in general as a reformulation of the exact quantum mechanical time evolution of a many-body system when only one-body properties are considered.**

**A.K. Rajagopal and J. Callaway, Phys. Rev. B 7, 1912 (1973)**
**V. Peuckert, J. Phys. C 11, 4945 (1978)**
**E. Runge and E.K.U. Gross, Phys. Rev. Lett. 52, 997 (1984)**

**http://www.tddft.org**

$$E(t) = \int d^3r \left[ \varepsilon(n(\vec{r},t), \tau(\vec{r},t), \nu(\vec{r},t), \underline{\vec{j}(\vec{r},t)}) + V_{ext}(\vec{r},t)\, n(\vec{r},t) + \ldots \right]$$

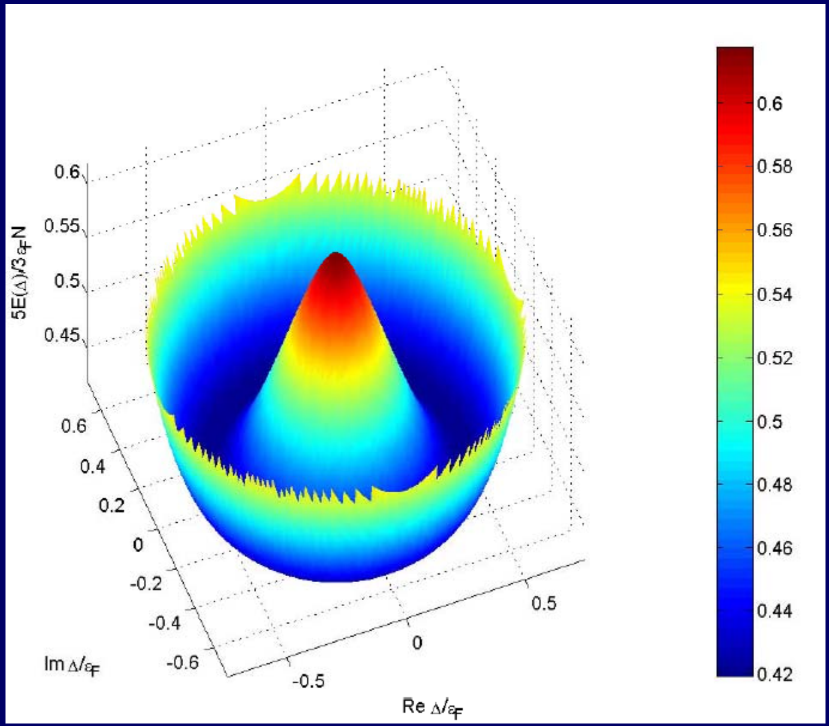
$$\begin{cases} [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu]\mathrm{u_i}(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)]\mathrm{v_i}(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{u_i}(\vec{r},t)}{\partial t} \\ [\Delta^*(\vec{r},t) + \Delta^*_{ext}(\vec{r},t)]\mathrm{u_i}(\vec{r},t) - [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu]\mathrm{v_i}(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{v_i}(\vec{r},t)}{\partial t} \end{cases}$$

**For time-dependent phenomena one has to add currents.**

A rare excitation mode:

the Higgs pairing mode.

# Energy of a Fermi system as a function of the pairing gap




$$\dot{n} + \vec{\nabla}\cdot\left[\vec{v}n\right] = 0$$

$$m\dot{\vec{v}} + \vec{\nabla}\left\{\frac{m\vec{v}^{\,2}}{2} + \mu\left[n\right]\right\} = 0$$

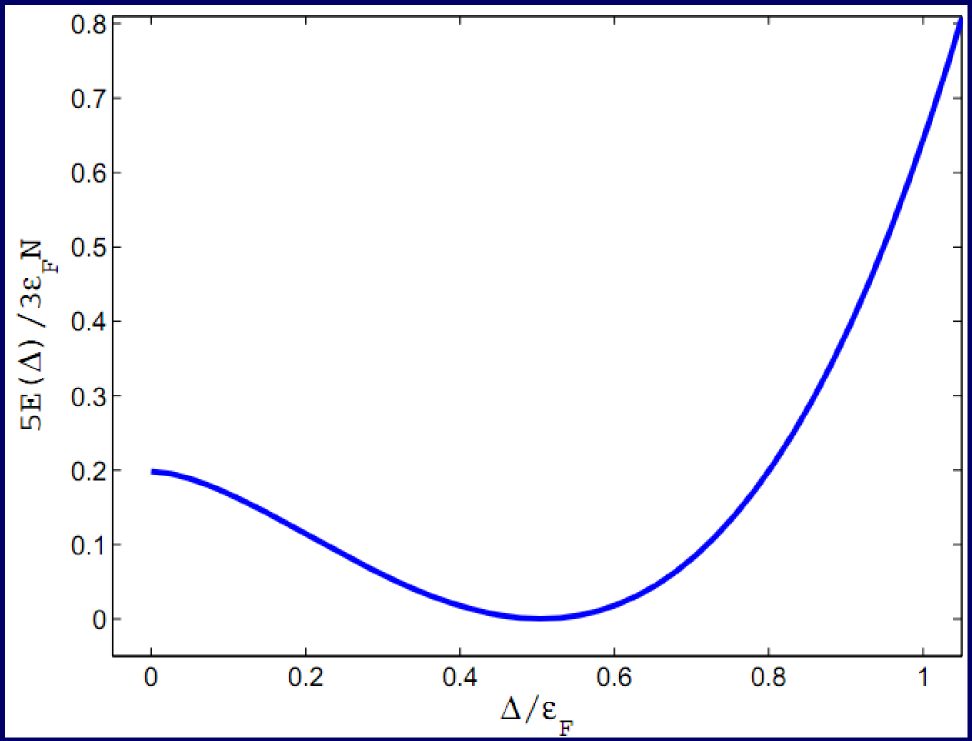
$$i\hbar\dot{\Psi}(\vec{r},t) = -\frac{\hbar^2\Delta}{4m}\Psi(\vec{r},t) + U\left(\left|\Psi(\vec{r},t)\right|^2\right)\Psi(\vec{r},t)$$

**Quantum hydrodynamics**

**“Landau-Ginzburg” equation**

## Higgs mode

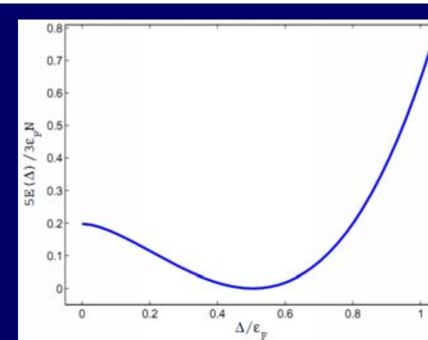
**Small amplitude oscillations of the modulus of the order parameter (pairing gap)**

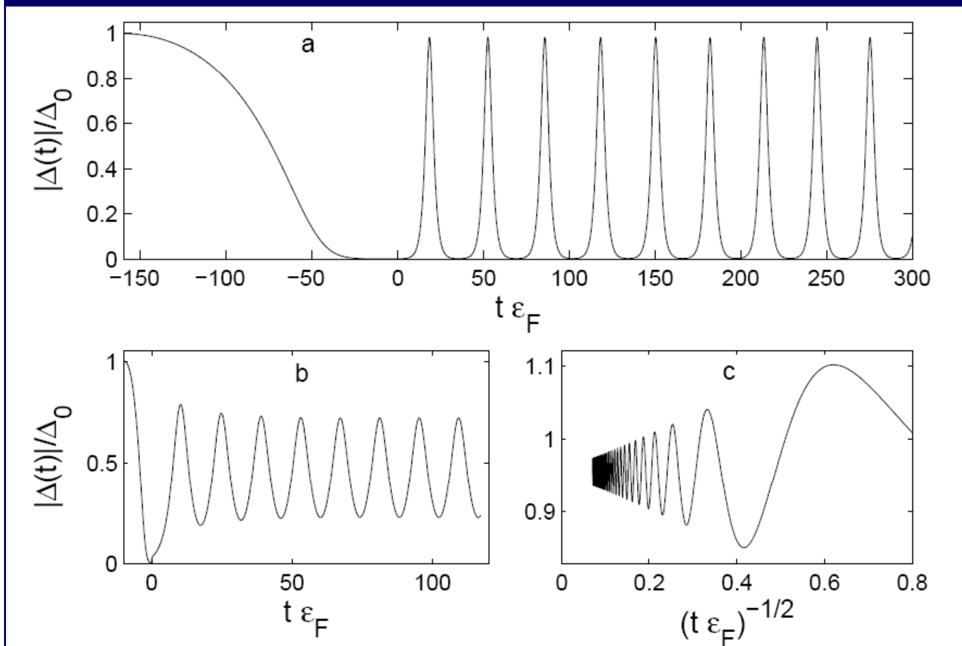


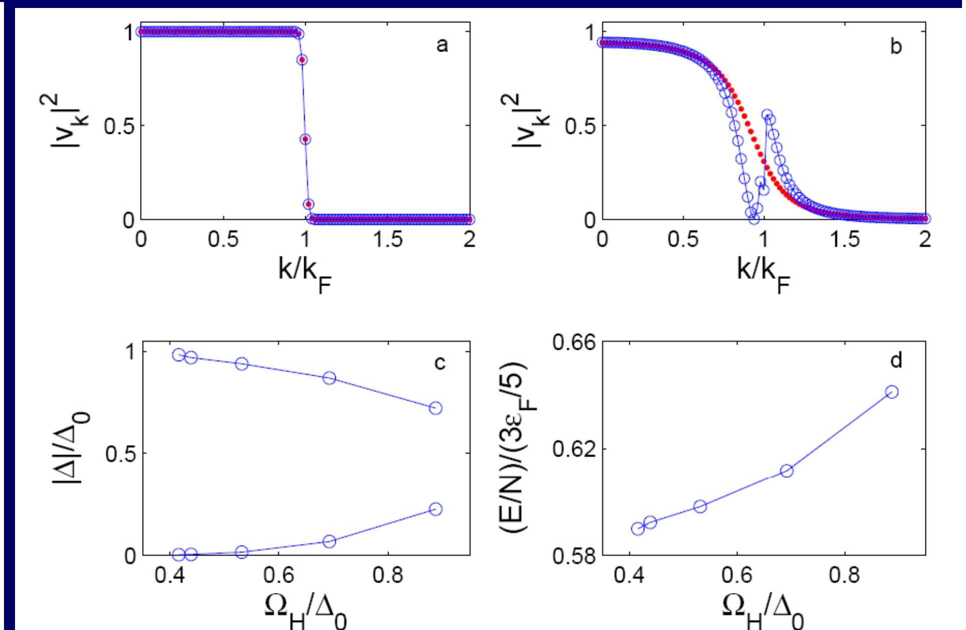

$$\hbar\Omega_H = 2\Delta_0$$

**This mode has a bit more complex character**
***cf.*** **Volkov and Kogan (1972)**

# Response of a unitary Fermi system to changing the scattering length with time





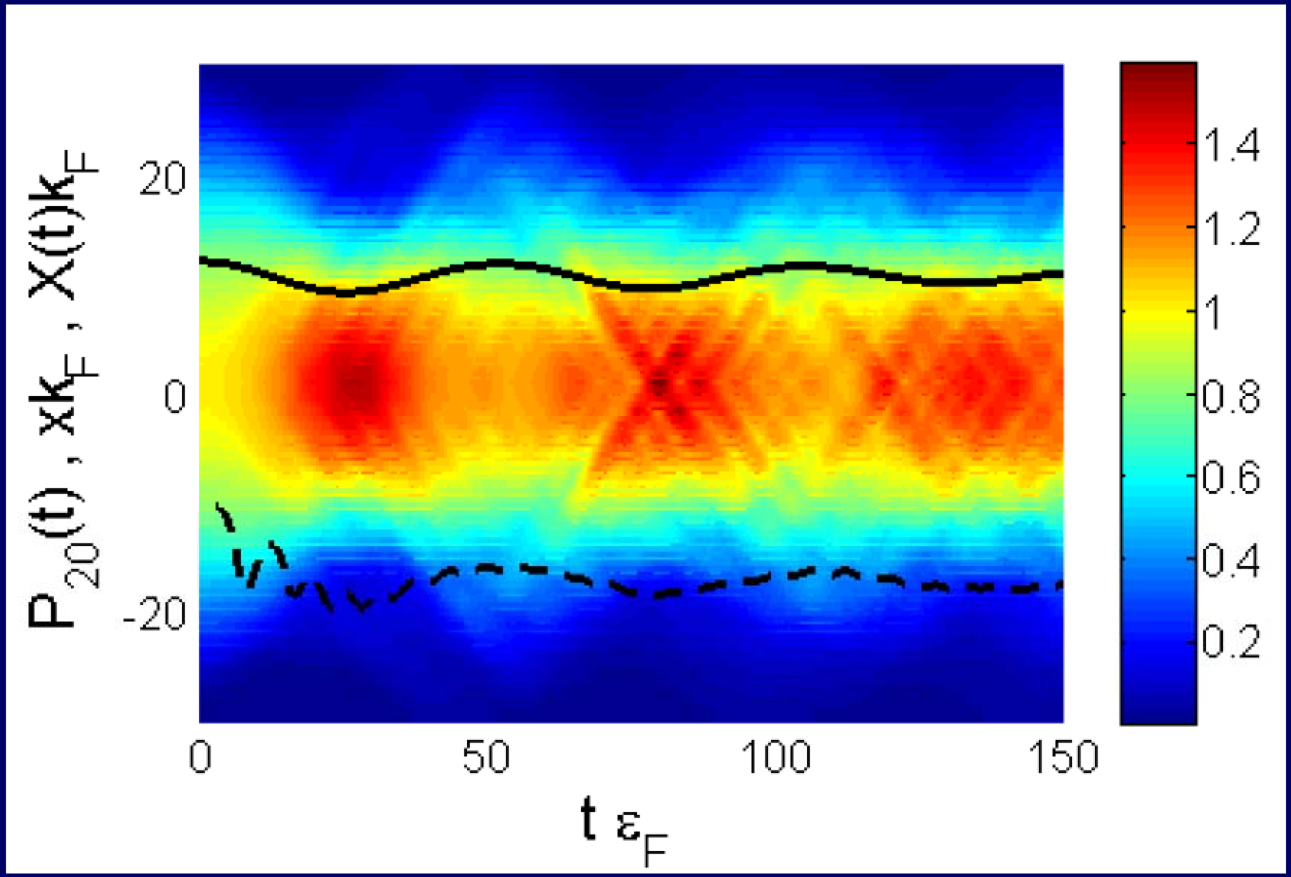

- All these modes have a very low frequency below the pairing gap and a very large amplitude and very large excitation energy

- None of these modes can be described either within Quantum Hydrodynamics or Landau-Ginzburg like approaches


Bulgac and Yoon, Phys. Rev. Lett. 102, 085302 (2009)

## 3D unitary Fermi gas confined to a 1D ho potential well (pancake)

**New qualitative excitation mode of a superfluid Fermi system (non-spherical Fermi momentum distribution)**




**Black solid line – Time dependence of the cloud radius**
**Black dashed line – Time dependence of the quadrupole moment of momentum distribution**

Bulgac and Yoon, Phys. Rev. Lett. 102, 085302 (2009)

**Full 3D implementation of TD-SLDA is a petaflop problem and has been completed by now.**

**Bulgac and Roche, J. Phys. Conf. Series 125, 012064 (2008)**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10,000 | Predictive and Accurate Monte Carlo-based Simulations for Mott Insulators, Cuprate Superconductors, and Nanoscale Systems
4,096 | Intermittency and Star Formation in Turbulent Molecular Clouds
2,292 | Climate-Science Computational End Station Development and Grand Challenge Team
2,160 | CHiMES: Coupled High-Resolution Modeling of the Earth System

## TDSLDA
## (equations look like TDHFB/TDBdG)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix} = \begin{pmatrix} \hat{h}_{\uparrow\uparrow}(\vec{r},t)-\mu & 0 & 0 & \Delta(\vec{r},t) \\ 0 & \hat{h}_{\downarrow\downarrow}(\vec{r},t)-\mu & -\Delta(\vec{r},t) & 0 \\ 0 & -\Delta^*(\vec{r},t) & -\hat{h}^*_{\uparrow\uparrow}(\vec{r},t)+\mu & 0 \\ \Delta^*(\vec{r},t) & 0 & 0 & -\hat{h}^*_{\downarrow\downarrow}(\vec{r},t)+\mu \end{pmatrix}\begin{pmatrix} u_{n\uparrow}(\vec{r},t) \\ u_{n\downarrow}(\vec{r},t) \\ v_{n\uparrow}(\vec{r},t) \\ v_{n\downarrow}(\vec{r},t) \end{pmatrix}$$

- **The system is placed on a 3D spatial lattice**
- **Derivatives are computed with FFTW**
- **Fully self-consistent treatment with Galilean invariance**
- **No symmetry restrictions**
- **Number of quasiparticle wave functions is of the order of the number of spatial lattice points**
- **Initial state is the ground state of the SLDA (formally like HFB/BdG)**
- **The code was implementation on JaguarPf (NCCS) and Franklin (NERSC)**

**I will present a few short movies, illustrating the complex time-dependent dynamics in 2D/3D of a unitary Fermi superfluid excited with various external probes.**

**In each case we solved on JaguarPf  or Franklin the TDSLDA equations for a $32^3$ and $48^3$ spatial lattices (approximately for 30k to 40k quasiparticle wavefunctions) for about 10k to 100k time steps using from about 30k to 40k PEs**

***Fully unrestricted calculations!***

**All the movies will be eventually posted at**

**http://www.phys.washington.edu/groups/qmbnt/index.html**

# Critical velocity in a unitary gas

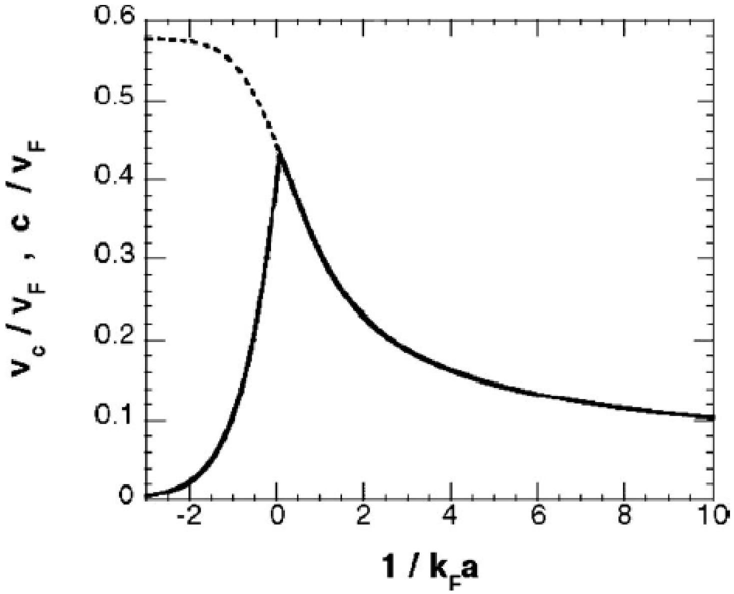



FIG. 20. Landau's critical velocity (in units of the Fermi velocity) calculated along the crossover using BCS mean-field theory. The critical velocity is largest near unitarity. The dashed line is the sound velocity. From Combescot, Kagan, and Stringari, 2006.

**From Giorgini, Pitaevskii and Stringari, Rev. Mod. Phys., 80, 1215 (2008)**

**Study based on BCS/Leggett approximation**

$$c_s = 0.370(5)\mathrm{v}_\mathrm{F}$$

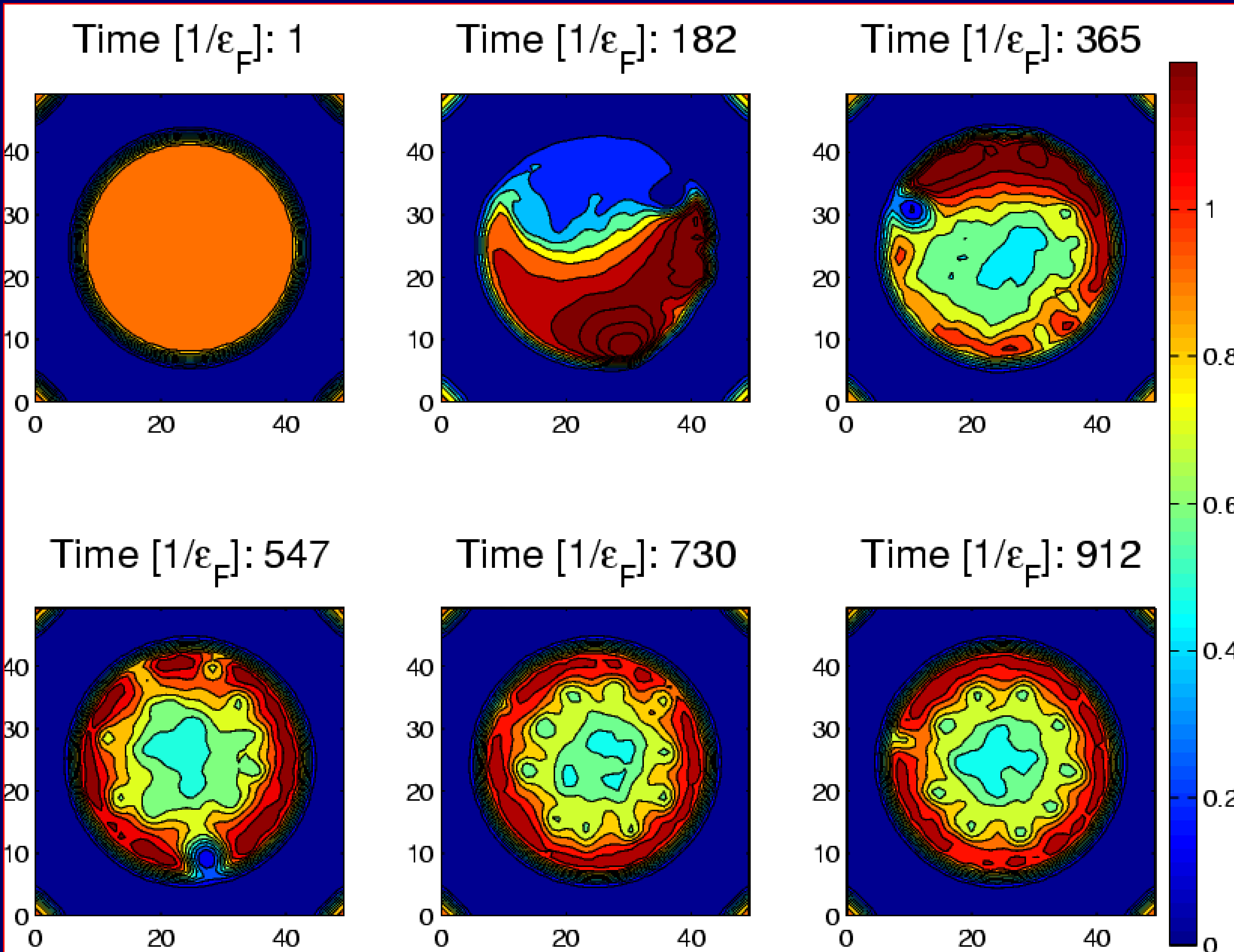
$$\min\left(\frac{\varepsilon_{qp}}{k}\right) = 0.385(3)$$

$$\Rightarrow \quad \mathrm{v}_c = 0.370(5)\mathrm{v}_\mathrm{F}$$

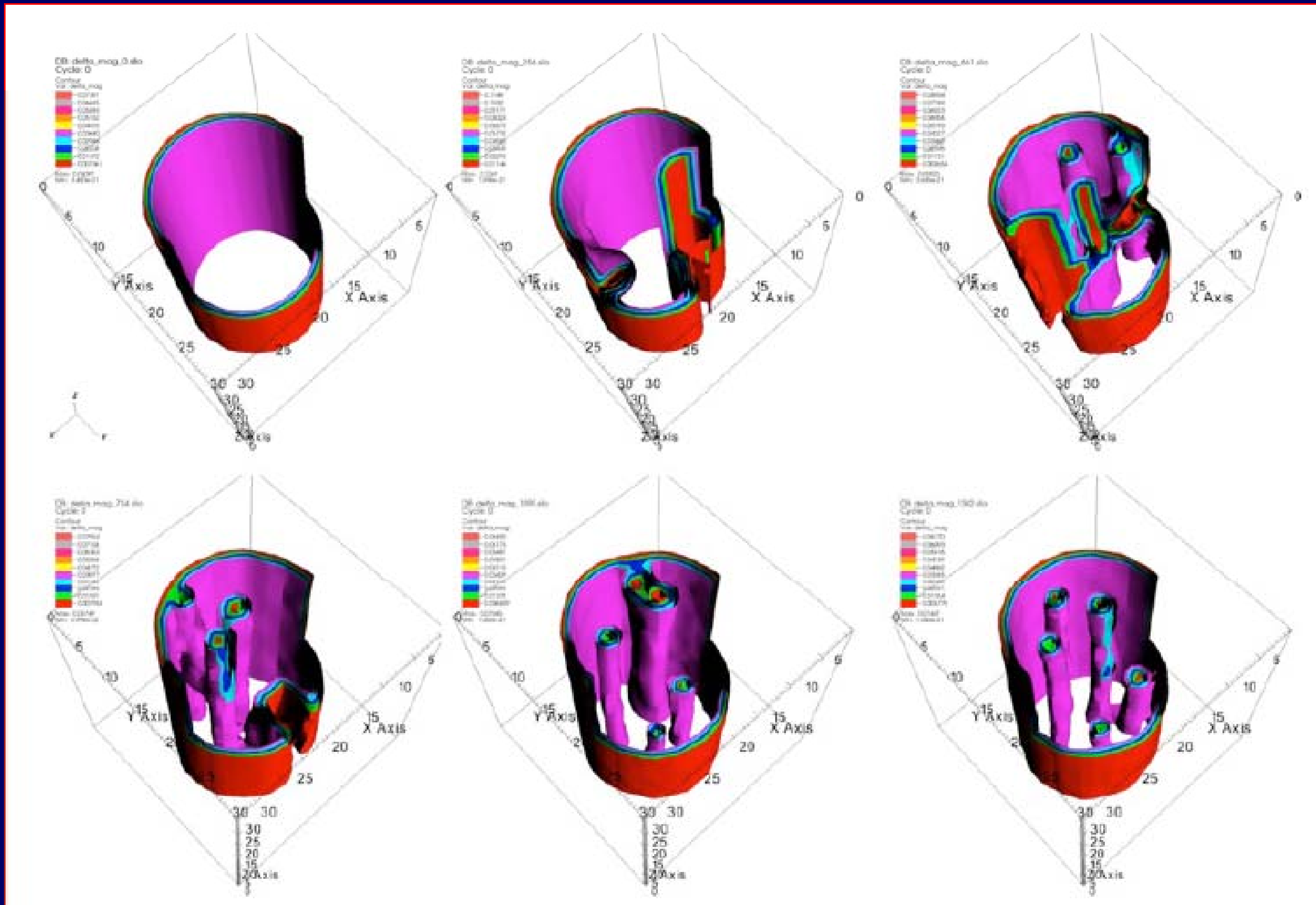
**Values obtained using QMC data**

$$\mathrm{v}_c \approx 0.25(3)\mathrm{v}_F$$

**Miller et al. (MIT, 2007)**




**Density cut through a stirred unitary Fermi gas at various times.**




**Profile of the pairing gap of a stirred unitary Fermi gas at various times.**

• ***<u>We created a set of accurate and efficient tools for the petaflop regime</u>*** **which have been successfully implemented on leadership class computers (Franklin, JaguarPF)**

**• Currently capable of treating large volumes for up to 10,000-20,000 fermions , and for long times, fully self-consistently and with no symmetry restrictions under the action of complex spatio-temporal external probes**

**• The suites of codes can handle systems and phenomena ranging from:**

**ground states properties**
**excited states in the linear response regime,**
**large amplitude collective motion,**
**response to various weak and strong external probes**

**• There is a clear path towards exascale applications and implementation of the Stochastic TD(A)SLDA**

# Properties of the Unitary Fermi Gas (UFG)

✓ The properties of the UFG are defined by the number density and the temperature only → *universal properties*
✓ UFG is stable and superfluid at zero temperature
✓ Full thermodynamic properties are known from *ab initio* calculations and most of them were confirmed by experiment
✓ The quasiparticle spectrum was determined in *ab initio* calculations at zero and finite temperatures
✓ UFG has the highest (relative) critical temperature of all known superfluids
✓ UFG has the highest critical velocity of all known superfluids
✓ The elusive Larkin-Ovchinnikov (FFLO) pairing can be realized under extremely favorable conditions. The system displays the equivalent of charge density waves → supersolid
✓ Extremely favorable conditions to realize induced *P*- or *F*-wave superfluidity
✓ UFG demonstrates the pseudogap behavior
✓ In the time-dependent regime one finds an incredible rich range of new qualitative phenomena (in particular flow with supercritical velocities)