Pairing properties, pseudogap phase and dynamics of vortices in a unitary Fermi gas

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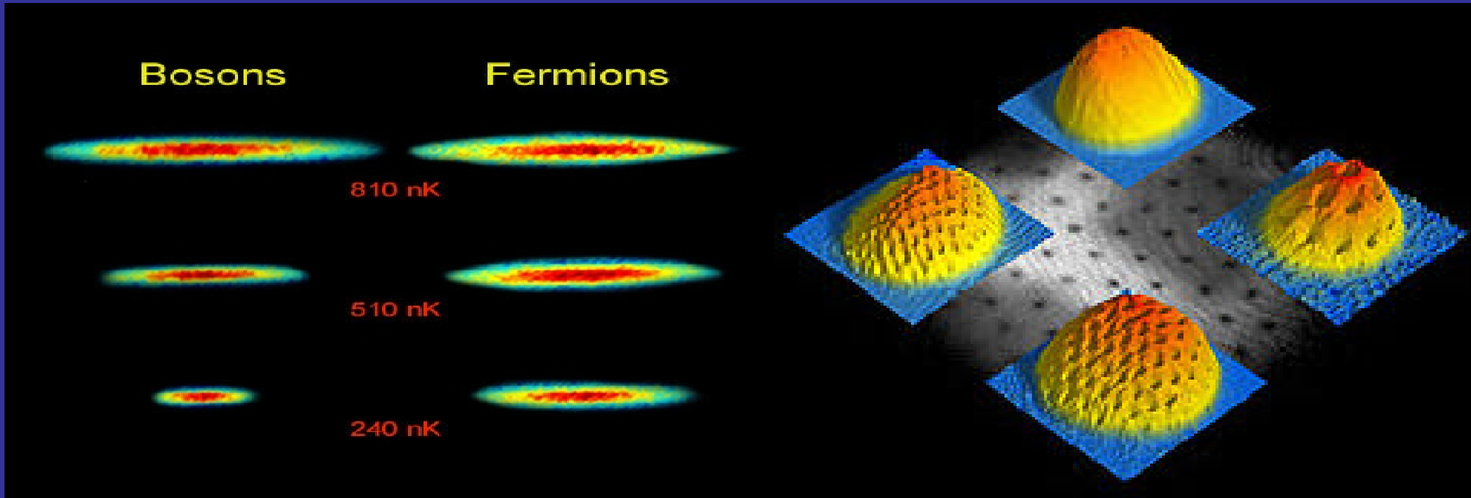


Outline

Why to study a unitary Fermi gas?
Universality of the unitary regime. BCS-BEC crossover.

Equation of state for the uniform Fermi gas in the unitary regime. Critical temperature. Pairing gap. Experiment vs. theory.

Unitary Fermi gas as a high-Tc superconductor:
onset of the pseudogap phase.

Nonequilibrium phenomena: generation and dynamics of superfluid vortices. Exotic topologies of superfluid vortices: vortex rings.

What is a unitary gas?

A gas of interacting fermions is in the unitary regime if the average separation between particles is large compared to their size (range of interaction), but small compared to their scattering length.

$n\, r_0^3 \ll 1$ $n\, |a|^3 \gg 1$

n - particle density
a - scattering length
r_0 - effective range

$$\text{i.e. } r_0 \to 0, a \to \pm\infty$$

NONPERTURBATIVE REGIME

System is dilute but strongly interacting!

UNIVERSALITY: $E = \xi_0 E_{FG}$

AT FINITE TEMPERATURE: $E(T) = \xi\left(\frac{T}{\varepsilon_F}\right) E_{FG}, \quad \xi(0) = \xi_0$

Thermodynamics of the unitary Fermi gas

$$\text{ENERGY:}\quad E(x)=\frac{3}{5}\xi(x)\varepsilon_F N;\quad x=\frac{T}{\varepsilon_F}$$

$$C_V=T\frac{\partial S}{\partial T}=\frac{\partial E}{\partial T}=\frac{3}{5}N\xi'(x)\Rightarrow S(x)=\frac{3}{5}N\int_0^x\frac{\xi'(y)}{y}dy$$

$$\text{ENTROPY/PARTICLE:}\quad \sigma(x)=\frac{S(x)}{N}=\frac{3}{5}\int_0^x\frac{\xi'(y)}{y}dy$$

$$\text{FREE ENERGY:}\ F=E-TS=\frac{3}{5}\varphi(x)\varepsilon_F N$$

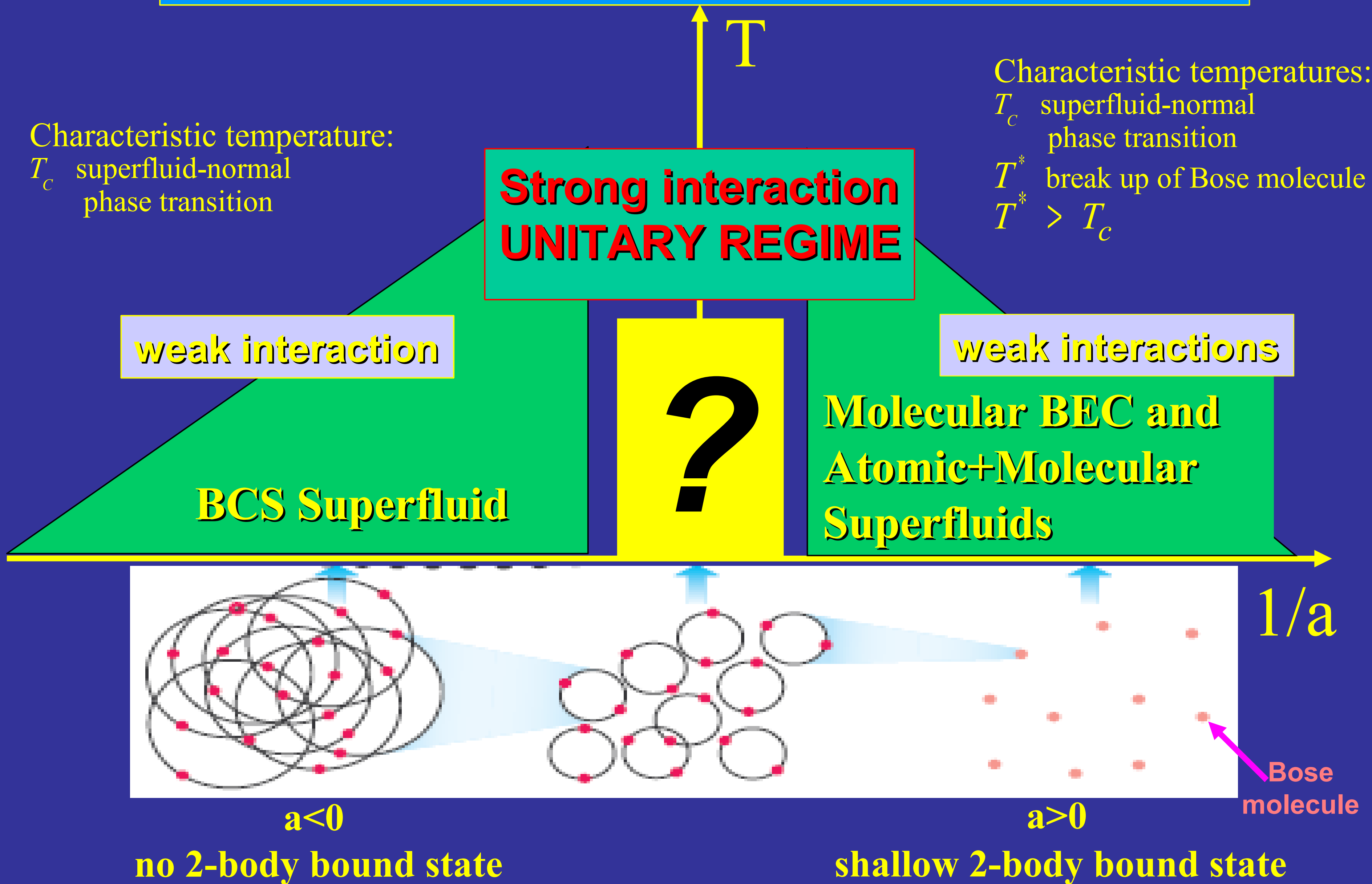
$$\varphi(x)=\xi(x)-x\sigma(x)$$

$$\text{PRESSURE:}\quad P=-\frac{\partial E}{\partial V}=\frac{2}{5}\xi(x)\varepsilon_F\frac{N}{V}$$

$$PV=\frac{2}{3}E$$

Note the similarity to the ideal Fermi gas

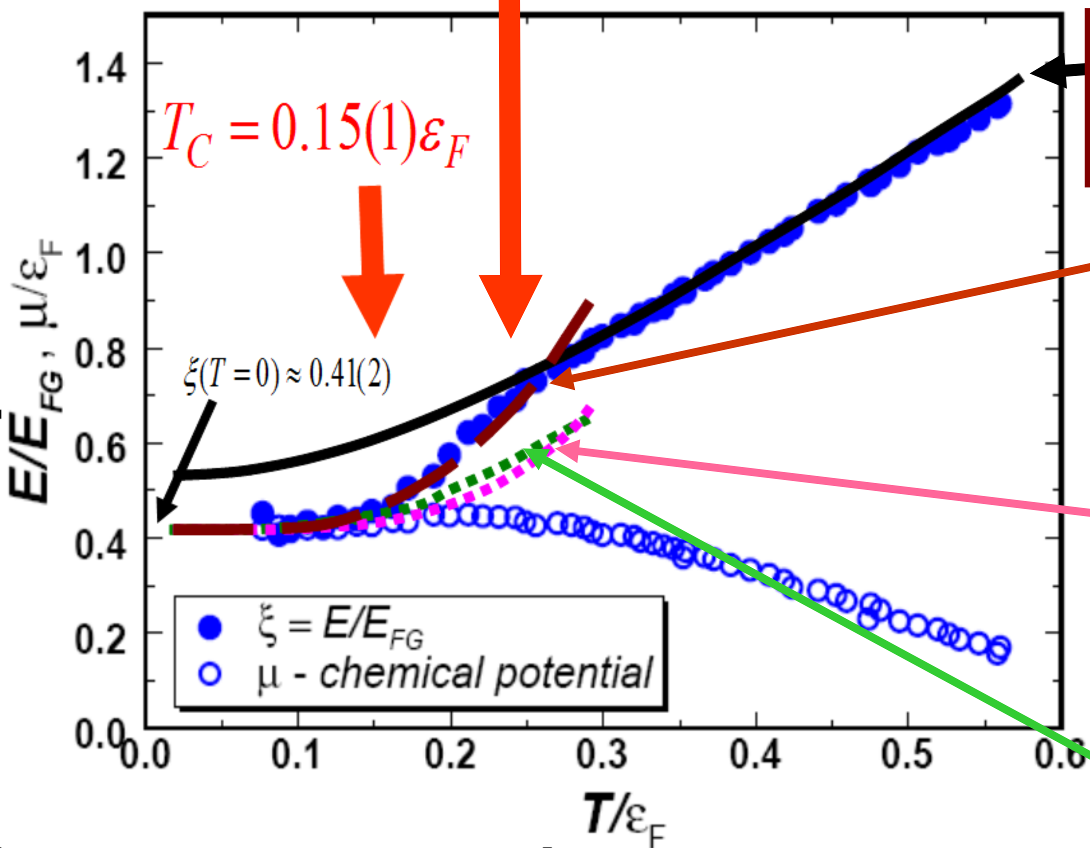
Expected phases of a two species dilute Fermi system
BCS-BEC crossover



Equation of state from QMC (Path Integral Monte Carlo)

a = ±∞

Deviation from Normal Fermi Gas



Normal Fermi Gas
(with vertical offset, solid line)

Bogoliubov-Anderson phonons and quasiparticle contribution
(dashed line)

Bogoliubov-Anderson phonons contribution only (dotted line)

Quasi-particle contribution only
(dotted line)

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

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

$$E_{\text{phonons}}(T) = \frac{3}{5}\varepsilon_F N \frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}}\left(\frac{T}{\varepsilon_F}\right)^4, \qquad \xi_s \approx 0.41$$

A. Bulgac, J.E. Drut, P. Magierski,PRL96,090404(2006)

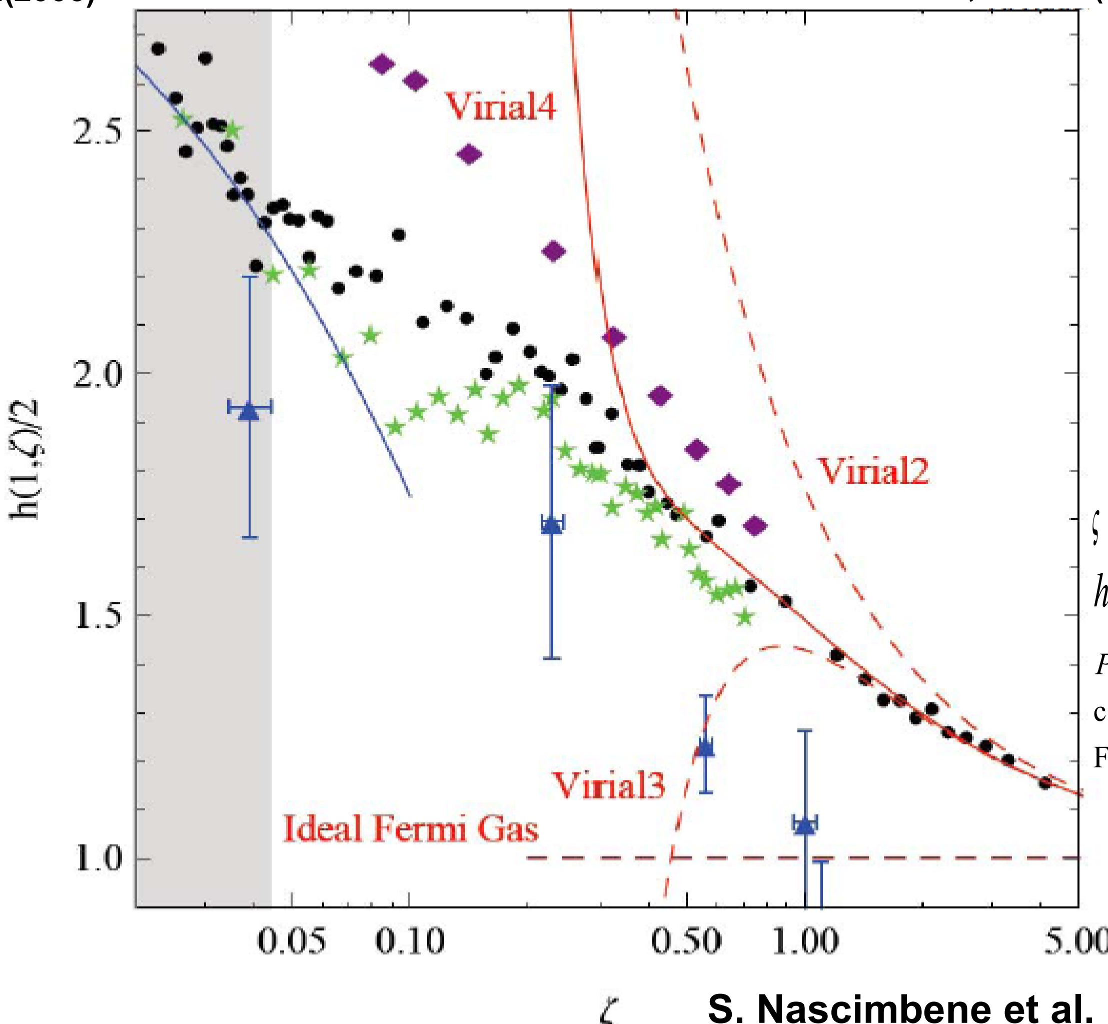
Comparison with Many-Body Theories (1)

Diagram. MC
Burovski et al.
PRL96, 160402(2006)

QMC
Bulgac, Drut, Magierski,
PRL99, 120401(2006)

Diagram. + analytic
Haussmann et al.
PRA75, 023610(2007)

Experiment



$\zeta = e^{-\mu\beta}$

$h(1,\zeta)/2 = P(\mu, T)/(2P_1(\mu, T))$

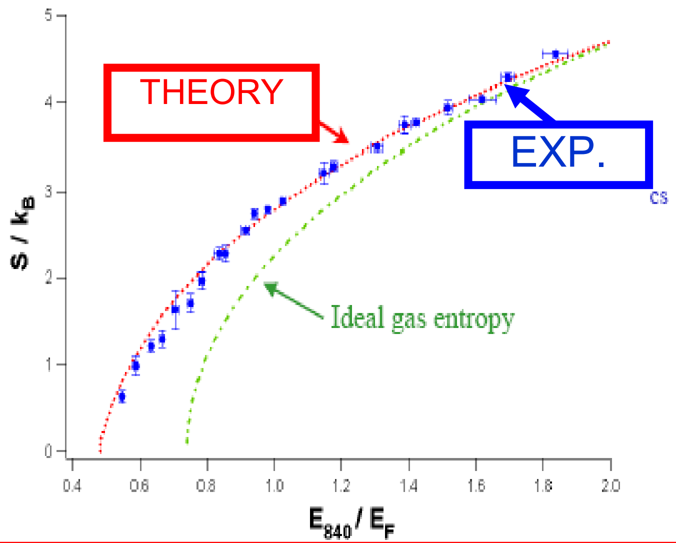
$P_1(\mu, T)$ - pressure of a single component of the noninteracting Fermi gas

S. Nascimbene et al. Nature 463, 1057 (2010)

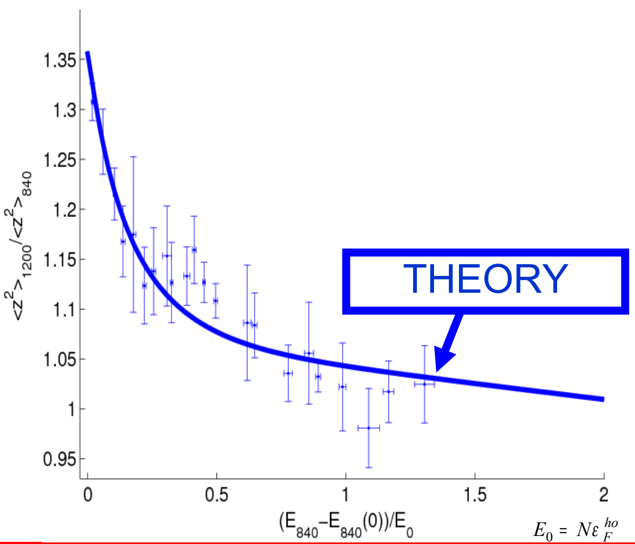
From a talk given by C. Salomon, June 2nd, 2010, Saclay

Unitary Fermi gas (^{6}Li atoms) in a harmonic trap

Experiment:
Luo, Clancy, Joseph, Kinast, Thomas, Phys. Rev. Lett. 98, 080402, (2007)

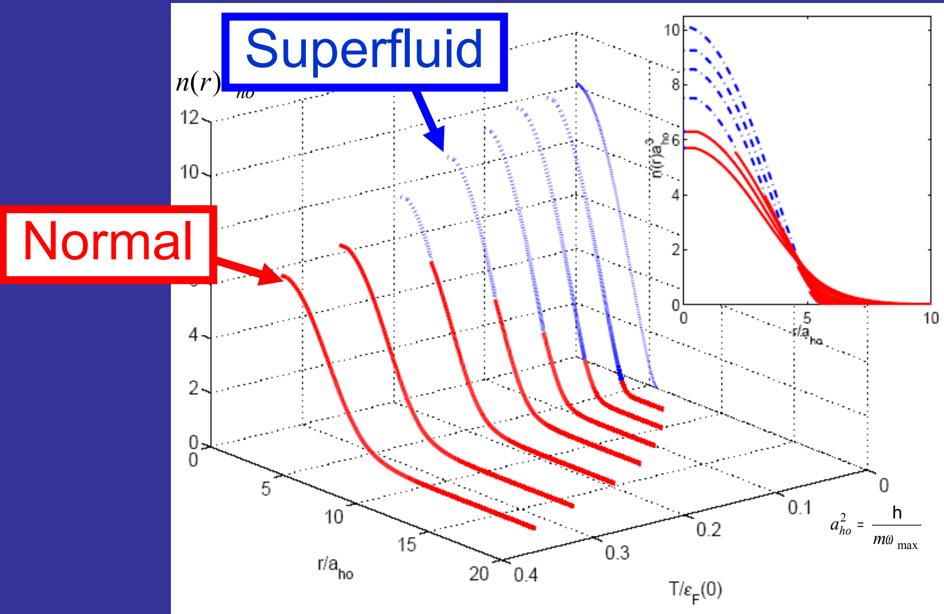


Entropy as a function of energy (relative to the ground state) for the unitary Fermi gas in the harmonic trap.



Ratio of the mean square cloud size at B=1200G to its value at unitarity (B=840G) as a function of the energy. Experimental data are denoted by point with error bars.

$B = 1200G$ corresponds to: $1/k_F a \approx -0.75$



Full *ab initio* theory (no free parameters): LDA + QMC input
Bulgac, Drut, Magierski, Phys. Rev. Lett. 99, 120401 (2007)

$\varepsilon_F(0)$ - Fermi energy at the center of the trap

The radial (along shortest axis) density profiles of the atomic cloud at various temperatures.

Superfluidity in ultra cold atomic gas

Eagles (1960), Leggett (1980), Nozieres and Schmitt-Rink (1985), Randeria *et al.* (1993),…

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

$$\Delta(T=0) = \alpha \frac{\hbar^2 k_F^2}{2m} e^{\left(\pi/2k_F a\right)};\quad \frac{\Delta(T=0)}{T_C} \approx 1.7 \quad \text{if} \quad k_F|a| << 1;\quad \frac{\varepsilon_F}{\Delta} >> 1$$

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

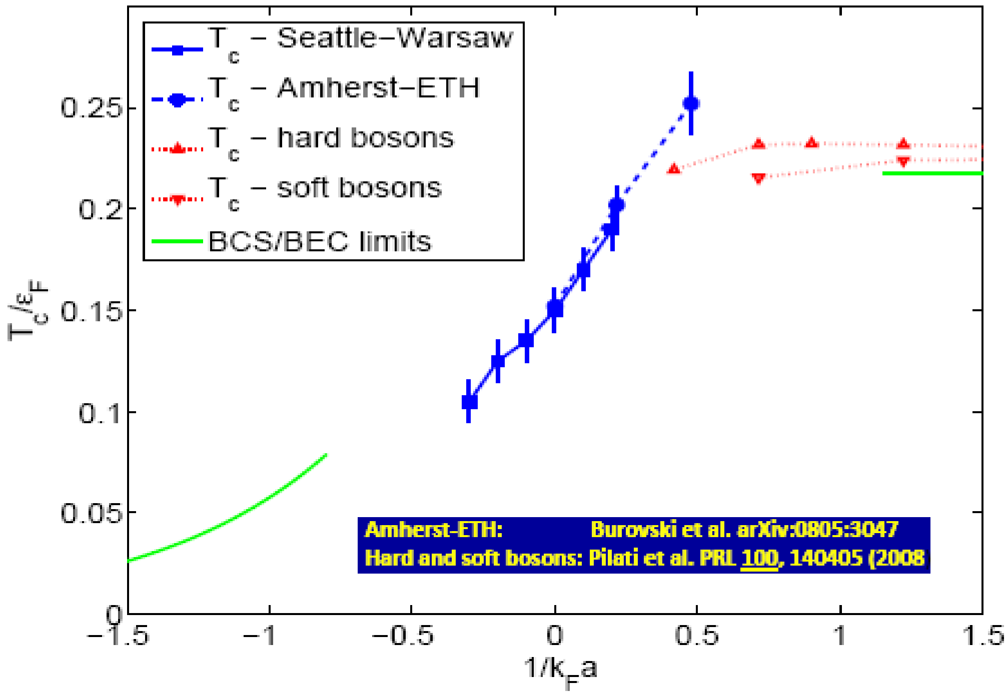
$$\Delta(T=0) = 0.50(1)\varepsilon_F;\quad \frac{\Delta(T=0)}{T_C} \approx 3.3 \quad \text{(it is not a BCS superfluid!)}$$

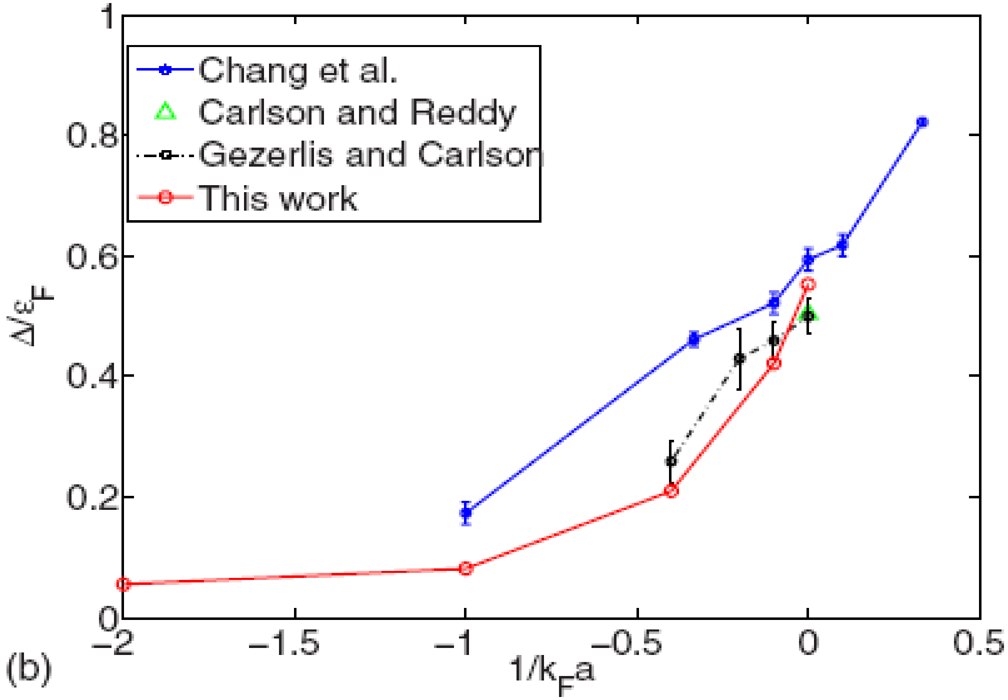
$$E_{normal} = 0.54 E_{FG};\quad E_{superfluid} = 0.40 E_{FG}$$

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

$$\varepsilon_b = -\frac{\hbar^2}{ma^2} \text{ - boson bounding energy;}\quad a_{bb} = 0.6\, a > 0 \text{ - effective boson-boson interaction}$$

$$T_C \approx 3.31 \frac{\hbar^2 n_b^{2/3}}{m}\left(1 + c(a n_b^{1/3})\right) \text{ - Bose-Einstein condensation temp.};\quad T^* \sim \frac{1}{a^2} \text{ - break up of Bose molecule}$$





Results in the vicinity of the unitary limit:

-Critical temperature

-Pairing gap at T=0

Note that

- at unitarity: $\Delta / \varepsilon_F \approx 0.5$

BCS theory predicts:

$$\Delta(T=0)/T_C \approx 1.7$$

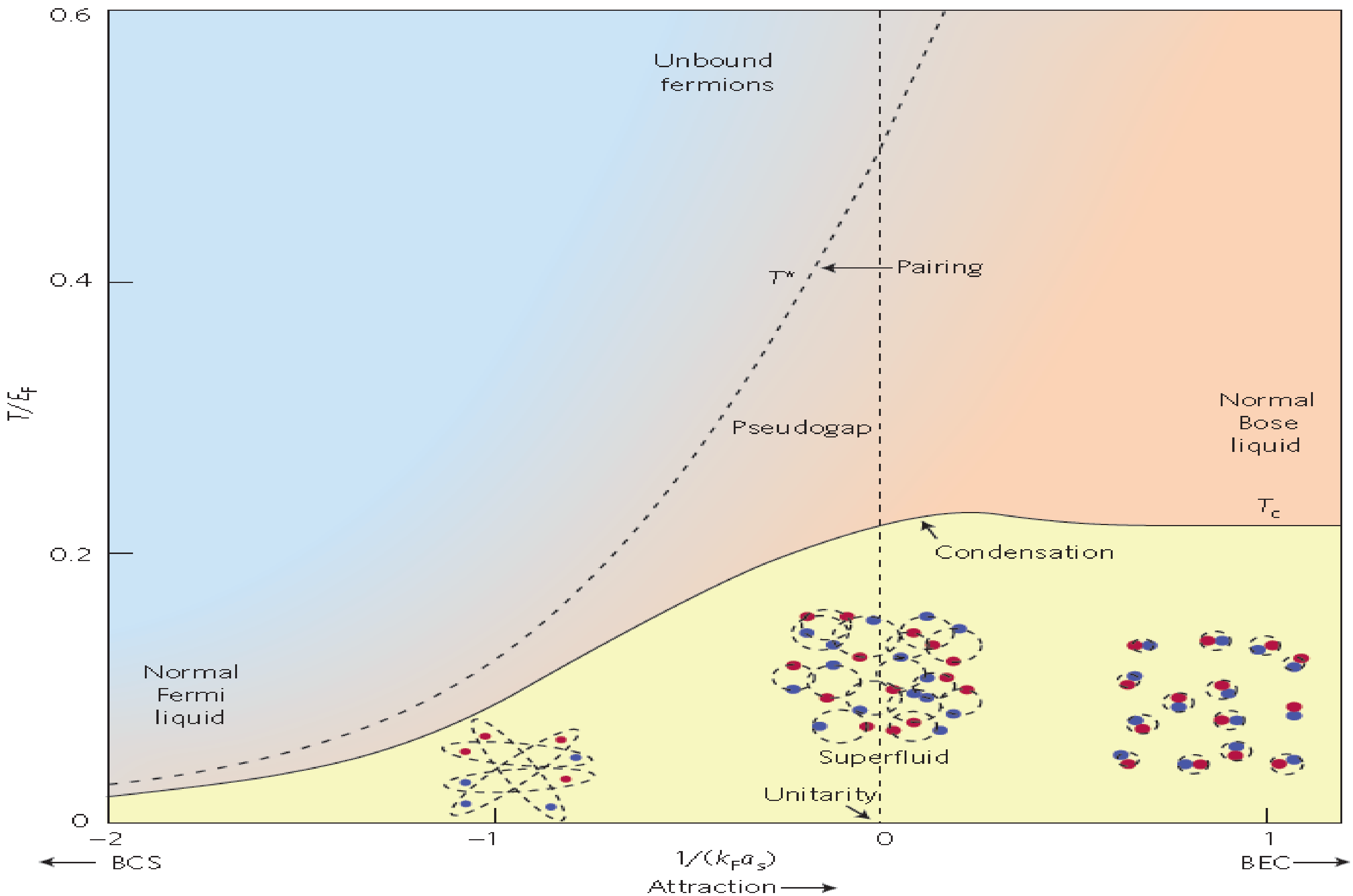
At unitarity:

$$\Delta(T=0)/T_C \approx 3.3$$

This is NOT a BCS superfluid!

Bulgac, Drut, Magierski, PRA78, 023625(2008)

Nature of the superfluid-normal phase transition in the vicinity of the unitary regime



Spectral weight function: $A(\vec{p},\omega)$

$$G^{ret/adv}(\vec{p},\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega'\frac{A(\vec{p},\omega')}{\omega-\omega'\pm i0^{+}}$$

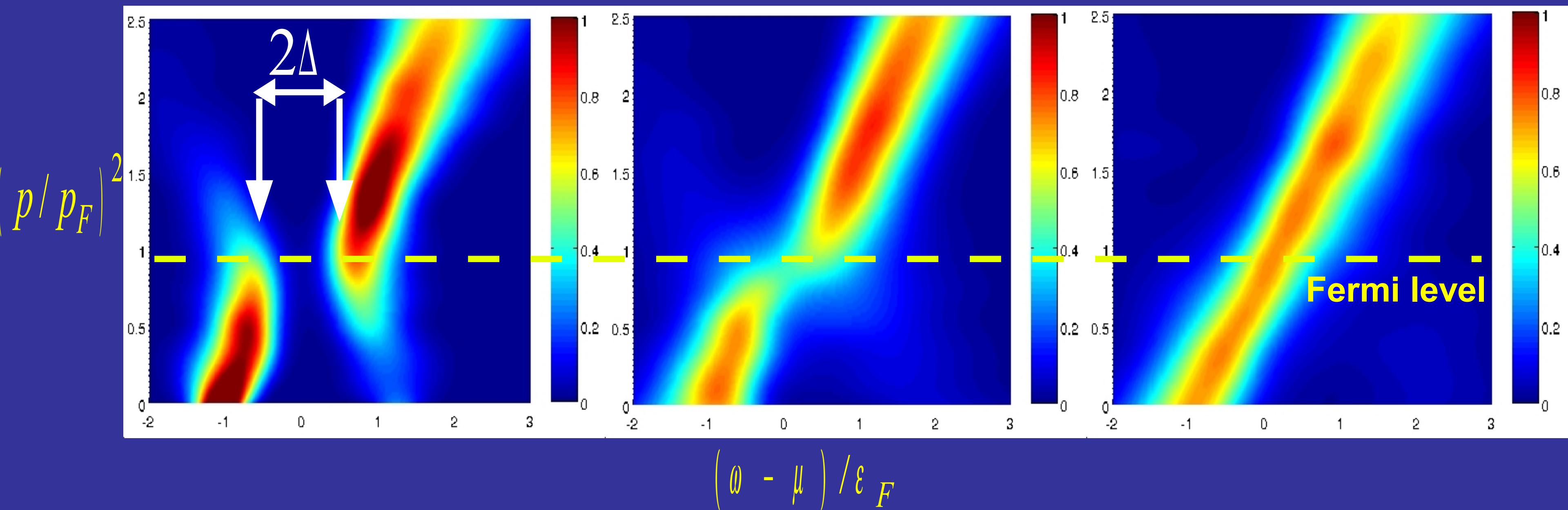
$$G(\vec{p},\tau)=-\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\omega A(\vec{p},\omega)\frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}$$

From Monte Carlo calcs.

$$G(\vec{p},\tau)=\frac{1}{Z}Tr\{e^{-(\beta-\tau)(\hat{H}-\mu\hat{N})}\hat{\psi}_{\uparrow}(\vec{p})e^{-\tau(\hat{H}-\mu\hat{N})}\hat{\psi}_{\uparrow}^{+}(\vec{p})\}$$

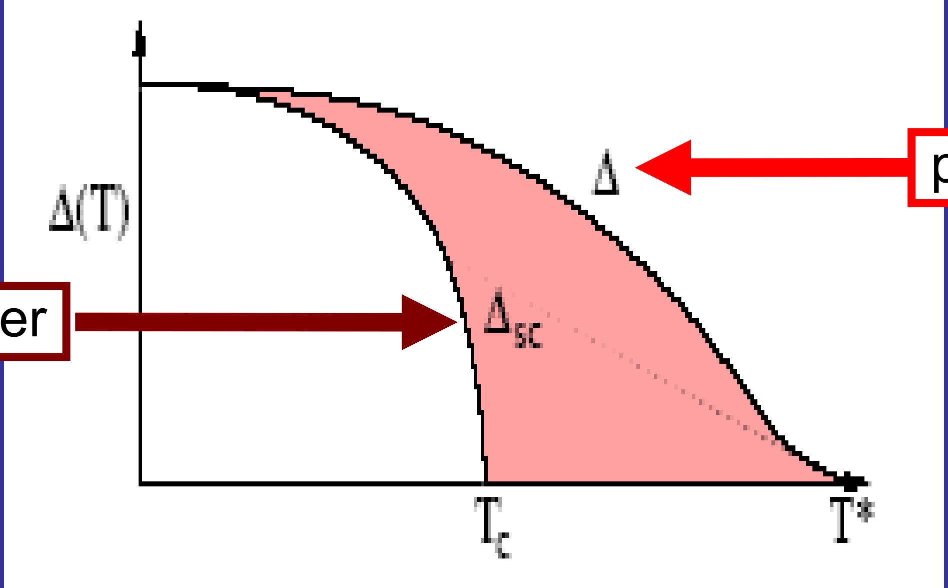
Spectral weight function from MC calc. for $1/k_F a=0.2$

Superfluid region (T=0.13) Pseudogap phase (T=0.22) Normal Fermi gas (T=0.26)



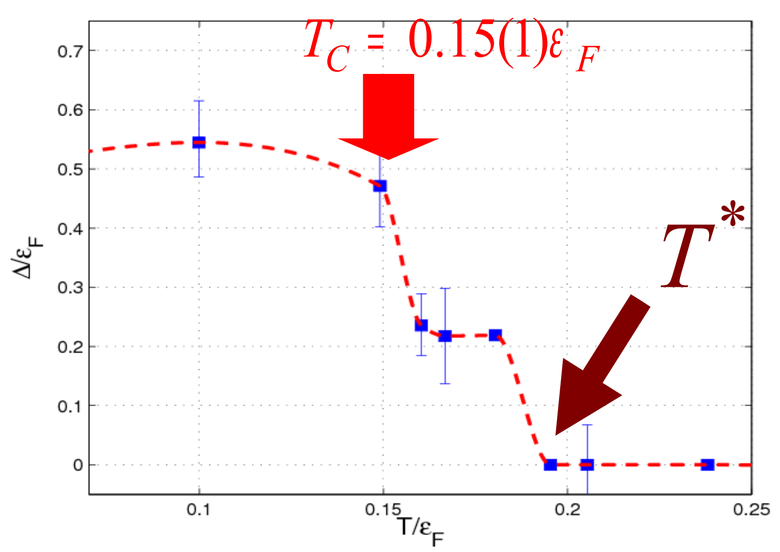
Pairing gap and pseudogap

Outside the BCS regime close to the unitary limit, but still before BEC, superconductivity/superfluidity emerge out of a very exotic, non-Fermi liquid normal state



pseudogap

order parameter

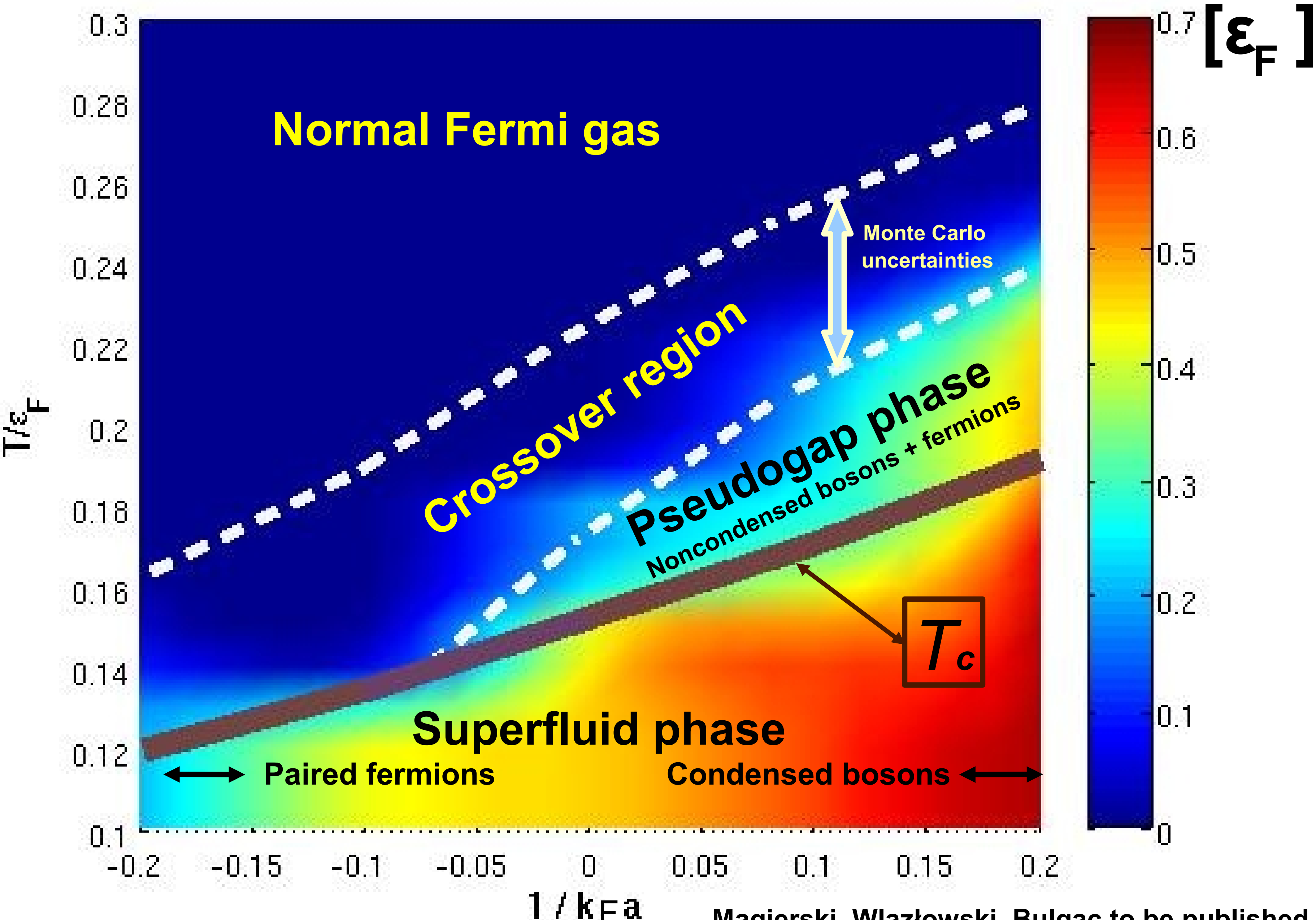


Monte Carlo calculations at the unitary regime

The onset of superconductivity occurs in the presence of fermionic pairs!

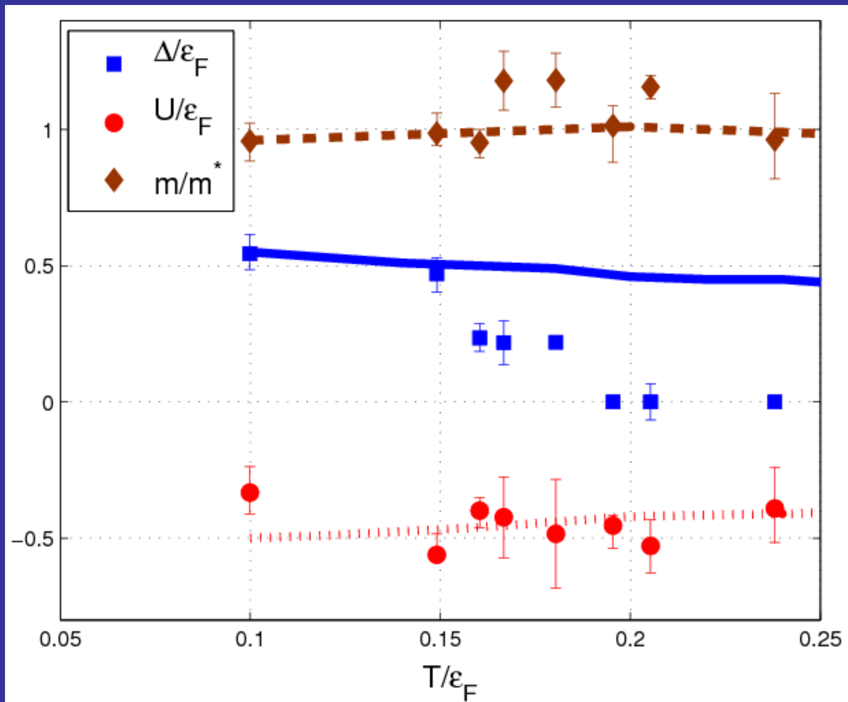
P.Magierski, G. Wlazłowski, A. Bulgac, J.E. Drut, PRL103, 210403 (2009)

Gap in the single particle fermionic spectrum from MC calcs.



Magierski, Wlazłowski, Bulgac to be published

Single-particle properties

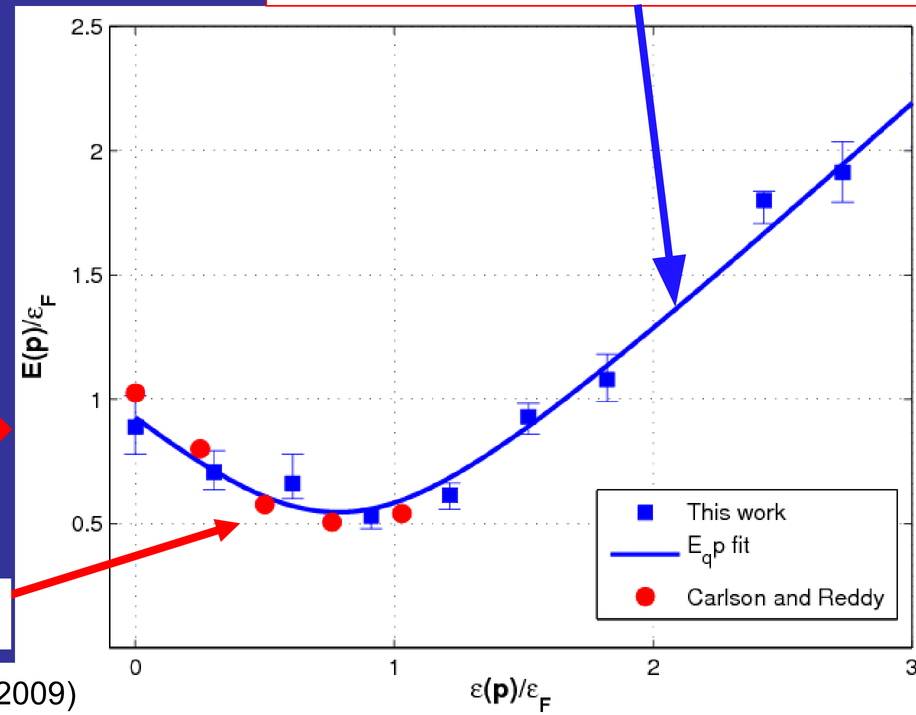


Effective mass: $m^* = (1.0 \pm 0.2)m$

Mean-field potential: $U = (-0.5 \pm 0.2)\varepsilon_F$

Weak temperature dependence!

$$E(\boldsymbol{p}) = \sqrt{\left(\frac{\alpha p^2}{2} + U - \mu\right)^2 + \Delta^2},$$



Quasiparticle spectrum extracted from spectral weight function at $T = 0.1\varepsilon_F$

Fixed node MC calcs. at T=0

P.Magierski, G. Wlazłowski, A. Bulgac, J.E. Drut, PRL103, 210403 (2009)

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

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

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

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

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

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 diverges.

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

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

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

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

One has to introduce position and momentum dependent running coupling constant.

SLDA energy density functional at unitarity

$$\varepsilon(\vec{r}) = \left[\alpha \frac{\tau_c(\vec{r})}{2} - \Delta(\vec{r})\nu_c(\vec{r})\right] + \beta \frac{3(3\pi^2)^{2/3} n^{5/3}(\vec{r})}{5}$$

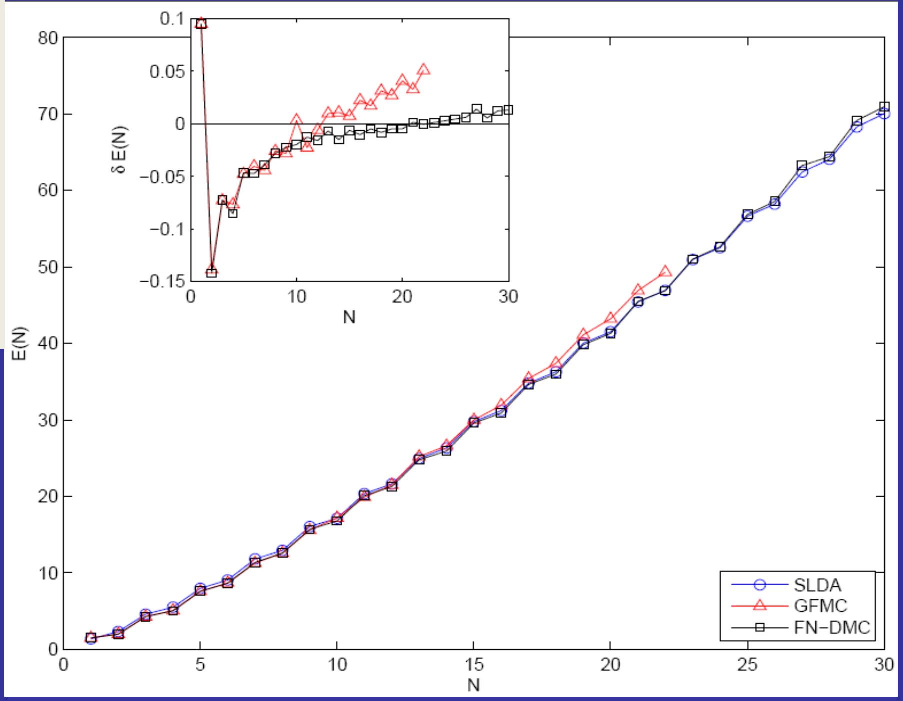
$$n(\vec{r}) = 2\sum_{0<E_k<E_c} \left|\mathrm{v}_k(\vec{r})\right|^2, \quad \tau_c(\vec{r}) = 2\sum_{0<E_k<E_c} \left|\vec{\nabla}\mathrm{v}_k(\vec{r})\right|^2,$$

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

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

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

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)

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

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

$$\begin{cases} [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathrm{u}_i(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)] \mathrm{v}_i(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{u}_i(\vec{r},t)}{\partial t} \\ [\Delta^*(\vec{r},t) + \Delta^*_{ext}(\vec{r},t)] \mathrm{u}_i(\vec{r},t) - [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathrm{v}_i(\vec{r},t) = i\hbar \dfrac{\partial \mathrm{v}_i(\vec{r},t)}{\partial t} \end{cases}$$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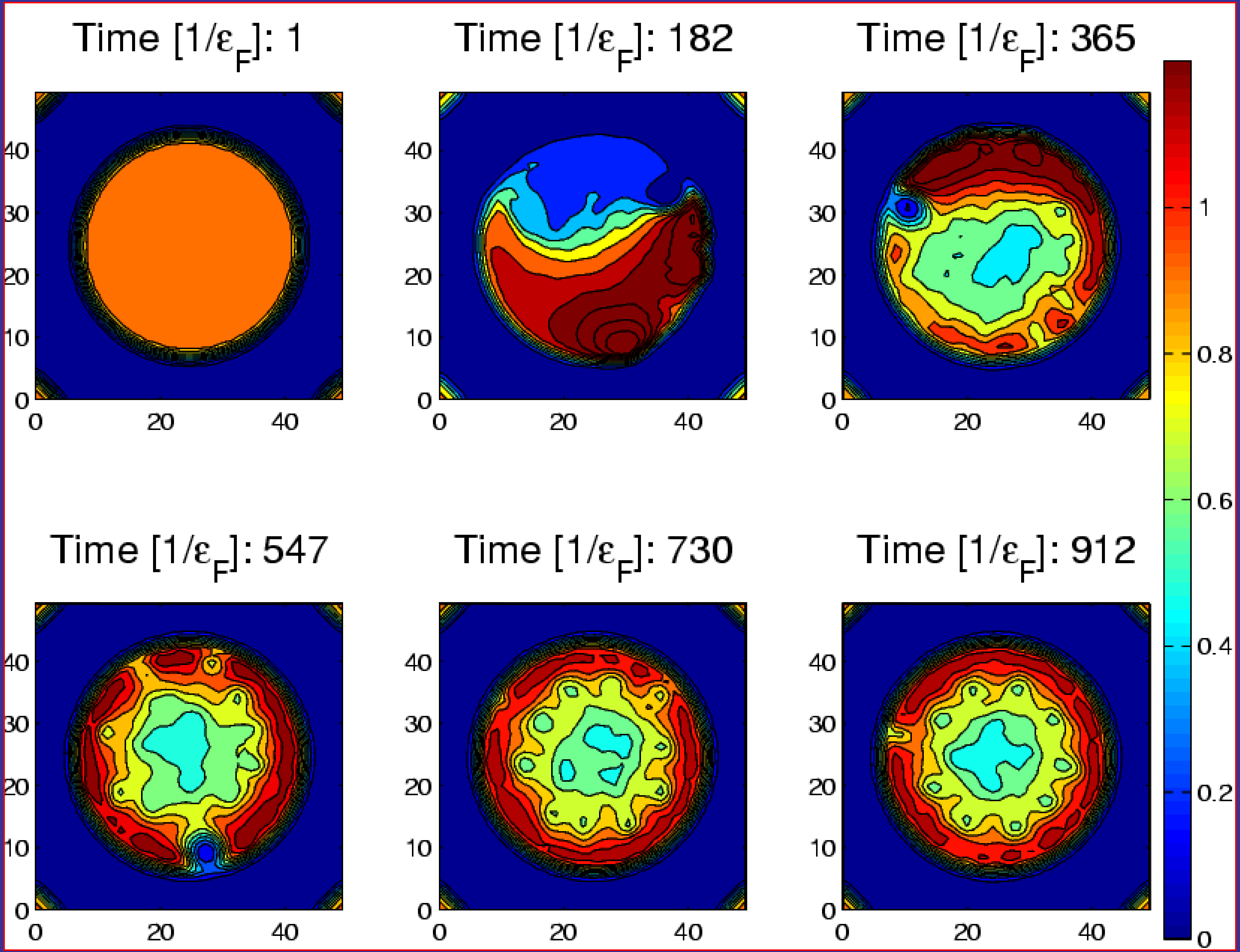
- **The system is placed on a 3D spatial lattice**
- **Derivatives are computed with FFTW**
- **Fully self-consistent treatment with Galilean invariance**
- **No symmetry restrictions**
- **Number of quasiparticle wave functions is of the order of the number of spatial lattice points**
- **Initial state is the ground state of the SLDA (formally like HFB/BdG)**
- **The code was implementation on JaguarPf (NCCS) and Franklin (NERSC)**

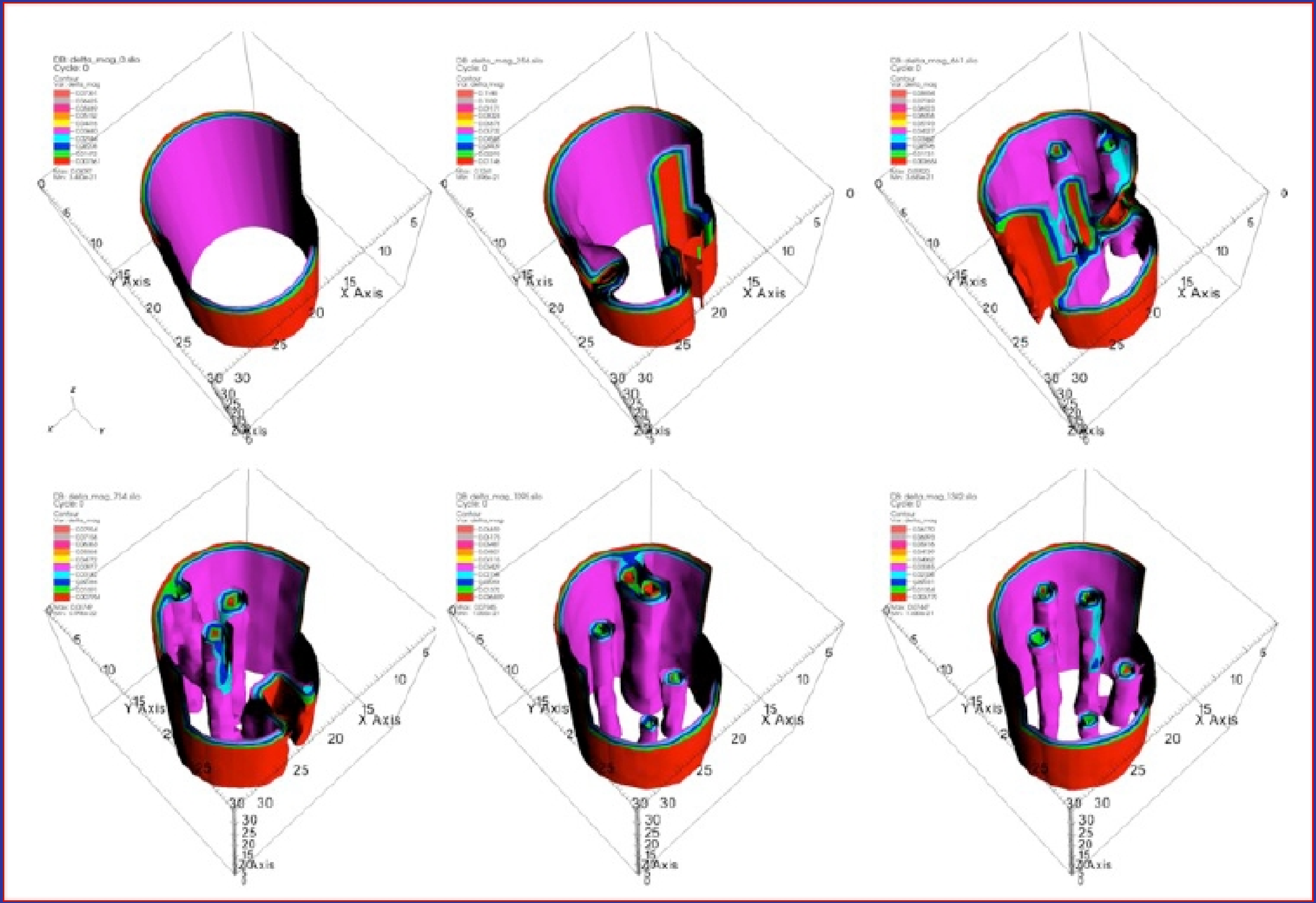
I will present two examples, illustrating the complex time-dependent dynamics in 2D/3D of a unitary Fermi superfluid excited with various external probes.

In each case we solved on JaguarPf or Franklin the TDSLDA equations for a 32^3 and 32^2 *96 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!



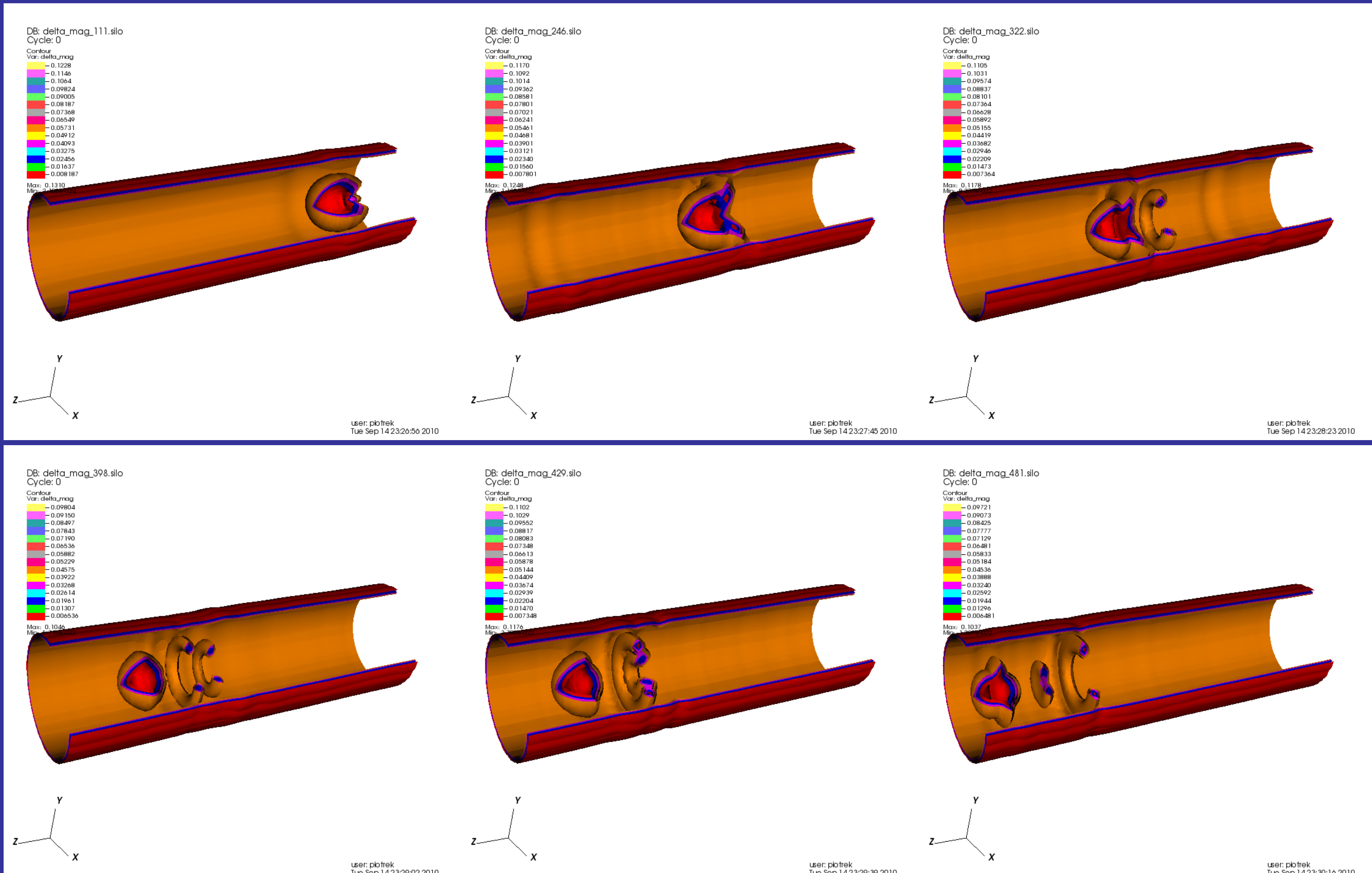
Density cut through a stirred unitary Fermi gas at various times.



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

Exotic vortex topologies: dynamics of vortex rings

Heavy spherical object moving through the superfluid unitary Fermi gas



__We created a set of accurate and efficient tools for studies of large,__
__superfluid Fermi systems.__

They 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**

__APPLICATIONS:__ - Dynamics of unitary Fermi gas
- Dynamics of atomic nuclei: neutron capture, induced fission, fussion, low energy nuclear reaction, etc.

Summary

- ✓ The properties of the Unitary Fermi Gas (UFG) are defined by the number density and the temperature only → *universal properties.*

- ✓ UFG is stable and superfluid at zero temperature.

- ✓ Thermodynamic properties are known from *ab initio* calculations and most of them were confirmed by experiment.

- ✓ The pairing gap and quasiparticle spectrum was determined in ✓*ab initio* calculations at zero and finite temperatures.

- ✓ UFG demonstrates the pseudogap behavior (challenge for the finite temperature DFT).

- ✓ In the time-dependent regime one finds an incredible rich range of new qualitative phenomena.