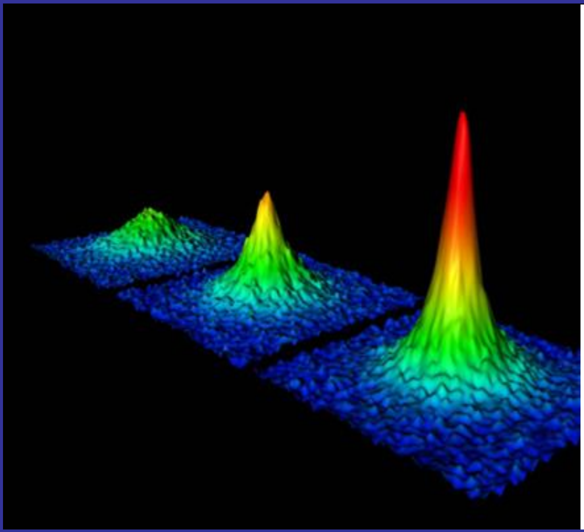
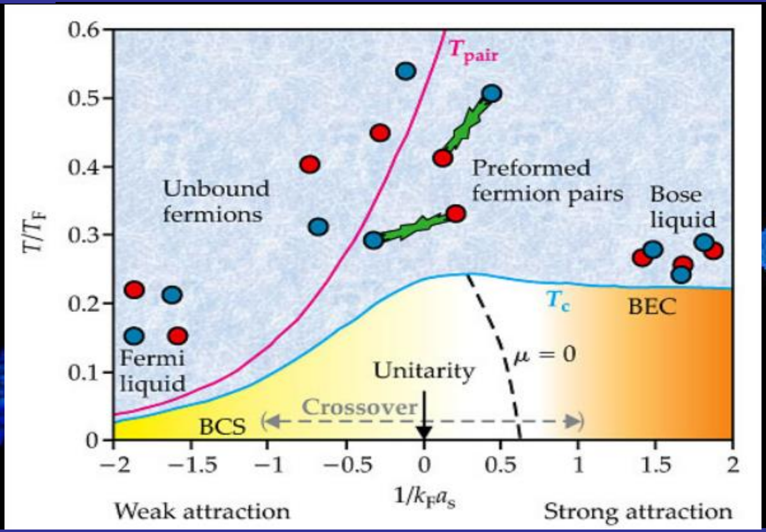
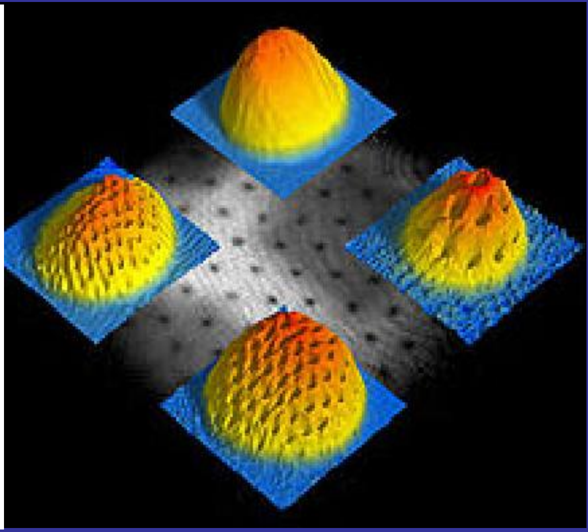
Properties of strongly correlated Fermi gas from Quantum Monte Carlo – constraints on Energy Density Functional







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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: $E(x) = \xi(x) E_{FG}$; $x = T/\varepsilon_F$

$\xi(0) = 0.37(1)$ - Exp. estimate

E_{FG} - Energy of noninteracting Fermi gas

BCS – BEC crossover

Eagles (1969), Leggett (1980): Variational approach

$$|gs\rangle = \prod_k \left(u_k + v_k \hat{a}^\dagger_{k\uparrow} \hat{a}^\dagger_{-k\downarrow} \right) |vacuum\rangle$$ BCS wave function

BCS limit: $\frac{1}{k_F a_s} \to -\infty$

a_s - scattering length

$\mu \to \varepsilon_F$ chemical potential

$\Delta \to \frac{8}{e^2} \varepsilon_F \exp\left(\frac{\pi}{2 k_F a_s} \right)$ pairing gap

Usual BCS solution for small and negative scattering lengths, with exponentially small pairing gap describing the system of spatially overlapping Cooper pairs.

BEC limit: $\frac{1}{k_F a_s} \to +\infty$

$$\mu \to -\frac{\hbar^2}{2 m a_s^2} = -\frac{E_b}{2}$$

$$\Delta \to \frac{4 \varepsilon_F}{\sqrt{3 \pi k_F a_s}}$$

Gas of weakly repelling molecules with binding energy E_b, essentially all at rest (almost pure BEC state)

No singularity within the whole range of scattering length!
Smooth crossover from spatially overlapping Cooper pairs to tightly bound difermionic molecules

Beyond mean field: Nozieres, Schmitt-Rink (1985), Randeria et al.(1993)

Thermodynamics of the unitary Fermi gas

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

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

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

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

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

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

Note the similarity to the ideal Fermi gas

Universal Tan relations

$$\lim_{k\to\infty} n(k) = \frac{C}{k^4}, \qquad {}^1\!/_a >> k >> {}^1\!/_{r_0}, \quad C \text{ - contact}$$

- Contact measures the probability that two fermions of opposite spins are close together.

$$E = \sum_{\sigma=\pm 1} \int \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} \left(n_\sigma(k) - \frac{C}{k^4} \right) + \frac{\hbar^2}{4\pi m a_s} C$$

Total energy of the system

$$\left(\frac{dE}{d(1/a_s)} \right)_S = -\frac{\hbar^2}{4\pi m} C$$

Adiabatic relation

C and 1/a are conjugate thermodynamic variables
1/a – „generalized force"
C - „generalize displacement" – capture physics at short length scales.

Shina Tan, Ann.Phys.323,2971(2008), Ann.Phys.323,2952(2008)

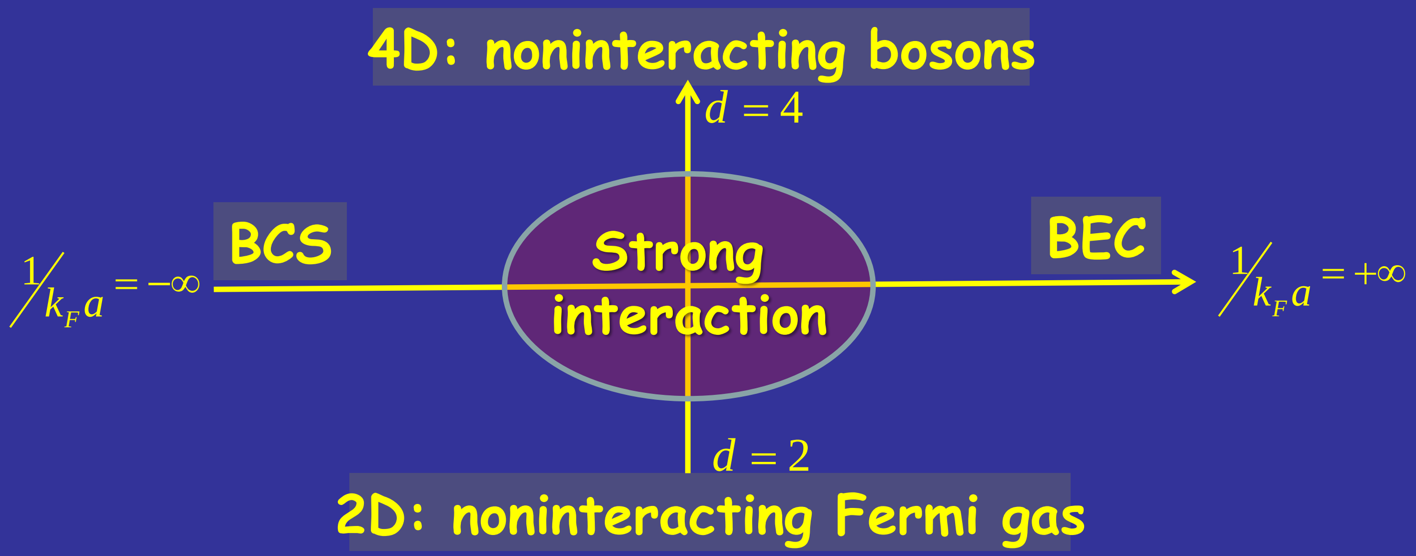
Other theory papers: Tan, Leggett, Braaten, Combescot, Baym, Blume, Werner, Castin, Randeria,Strinati,…

Unitary limit in 2 and 4 dimensions:

$$a \to \infty: \; R(r) \propto \frac{1}{r^{d-2}} + O(r^{4-d}), \quad \textit{Two body wave function for } r \to 0.$$

Intuitive arguments:

- For d=4 $\int R(r)^2 d^d r$ diverges at the origin
- For d=2 the singularity of the wave function disapears = interaction also disapears.



The only nontrivial case of unitary regime is in 3D

Nussinov,Nussinov, Phys.Rev. A74, 053622(2006)

Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = \int d^3r \sum_{s=\uparrow\downarrow} \hat{\psi}_s^\dagger(\vec{r})\left(-\frac{\hbar^2\Delta}{2m}\right)\hat{\psi}_s(\vec{r}) \; - \; g \int d^3r \; \hat{n}_\uparrow(\vec{r})\hat{n}_\downarrow(\vec{r})$$

$$\hat{N} = \int d^3r \; \left(\hat{n}_\uparrow(\vec{r}) + \hat{n}_\downarrow(\vec{r})\right); \;\; \hat{n}_s(\vec{r}) = \hat{\psi}_s^\dagger(\vec{r})\hat{\psi}_s(\vec{r})$$

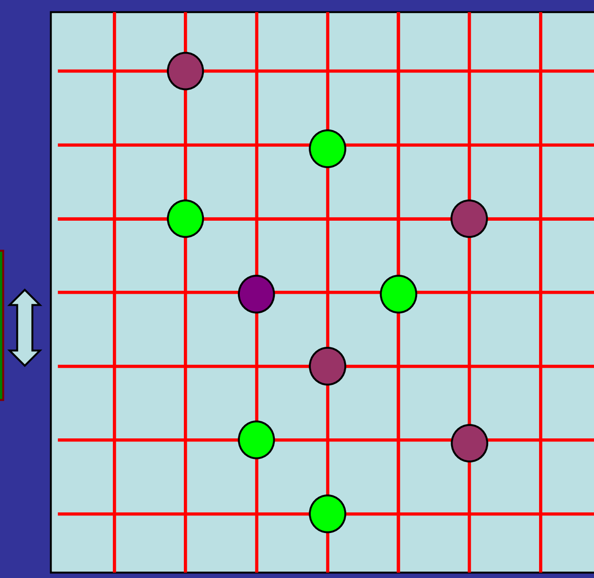
$$\frac{1}{g} = -\frac{m}{4\pi\hbar^2 a} + \frac{mk_{cut}}{2\pi^2\hbar^2}$$

Path Integral Monte Carlo for fermions on 3D lattice

Coordinate space

L –limit for the spatial correlations in the system

$$k_{cut} = \frac{\pi}{\Delta x} \; ; \;\; \Delta x$$



$$Volume = L^3$$

$$lattice\ spacing = \Delta x$$

- Spin up fermion:

- Spin down fermion:

External conditions:

T - temperature

μ - chemical potential

Periodic boundary conditions imposed

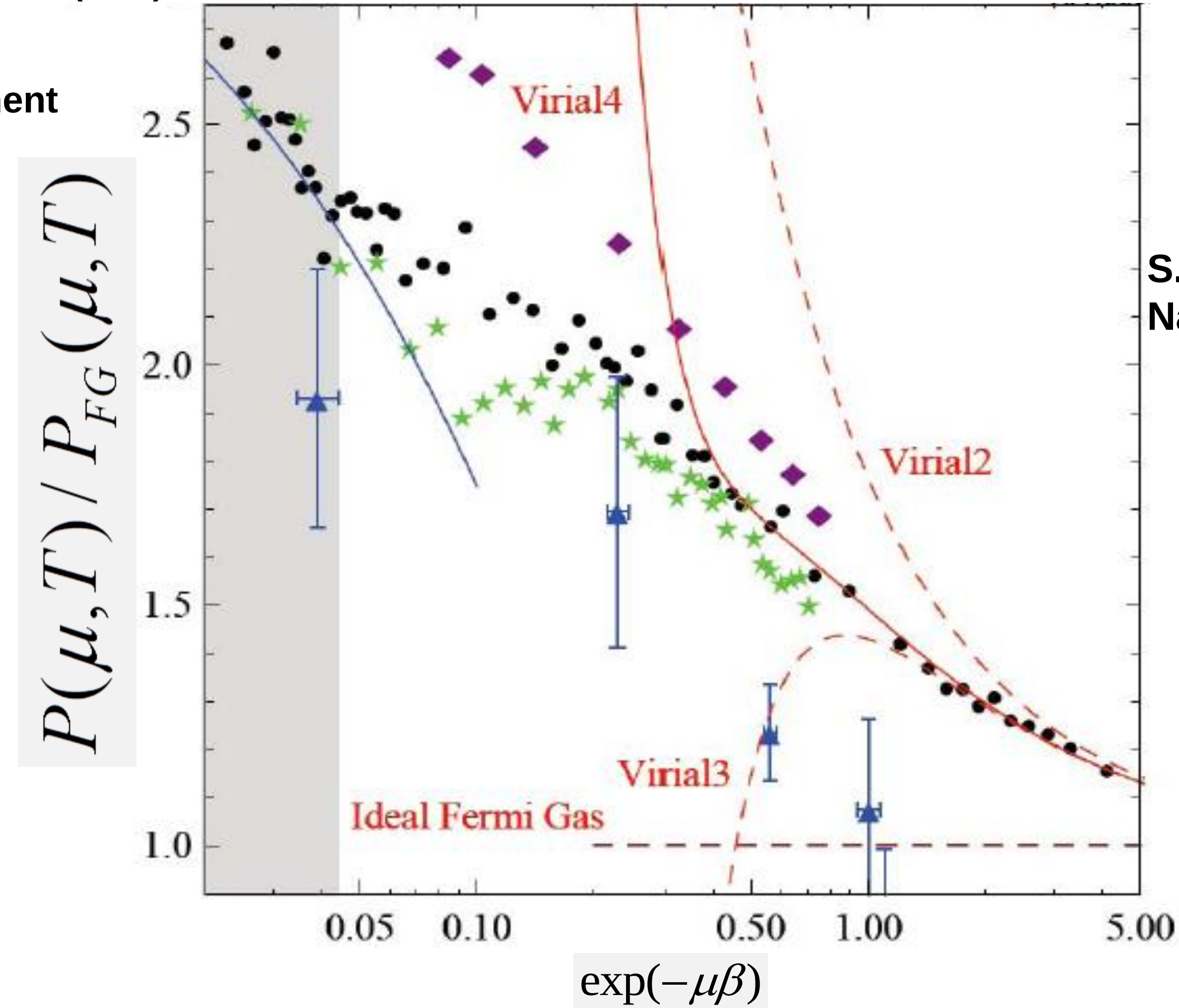
Comparison with Many-Body Theories (1)

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

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

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

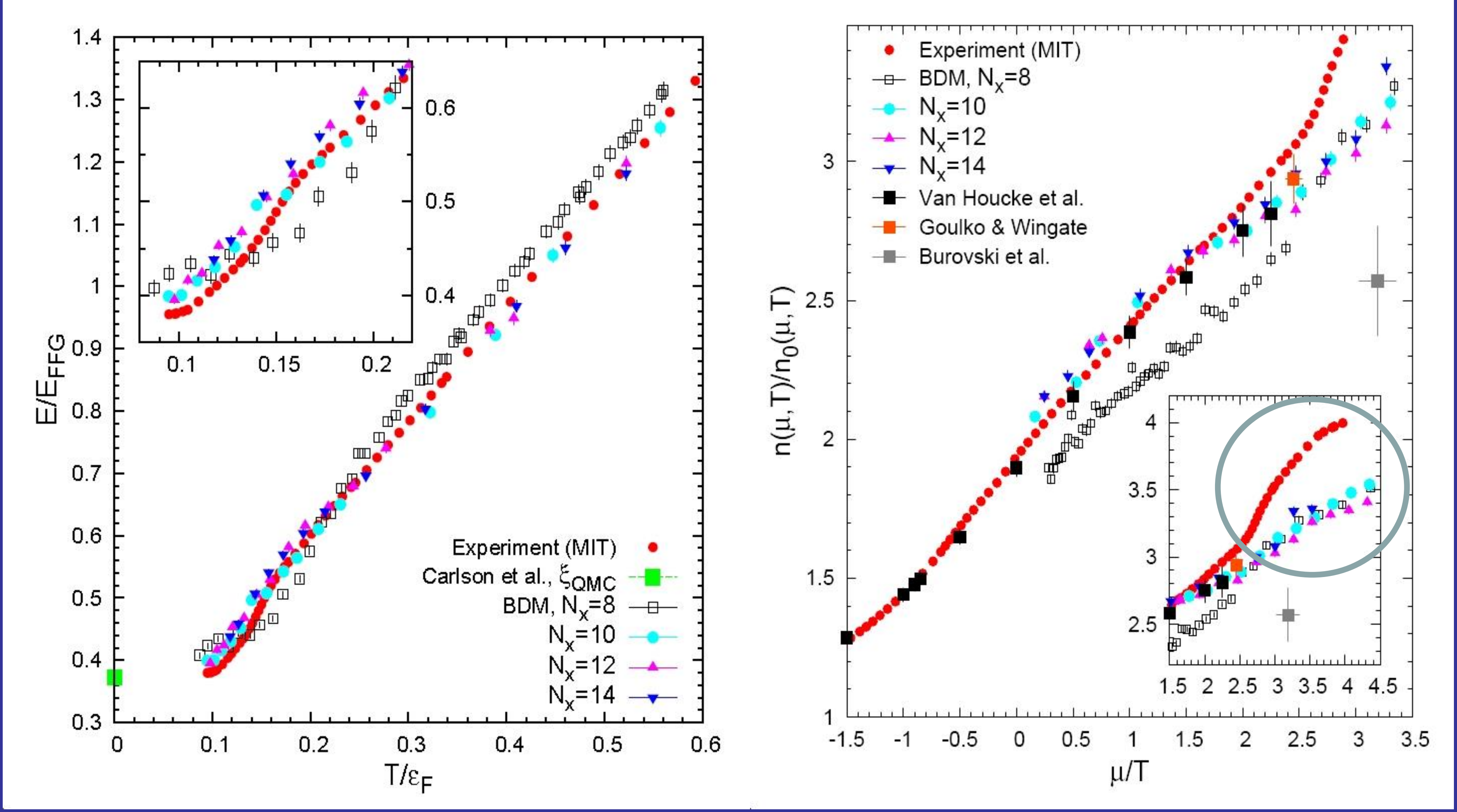
● **Experiment**



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

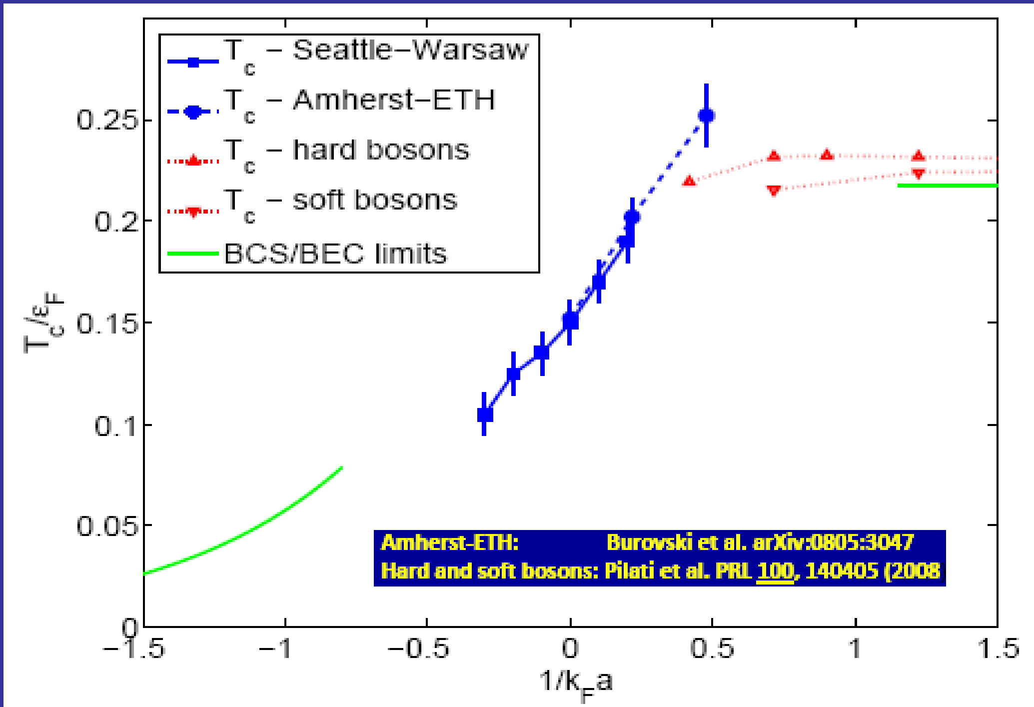
Courtesy of C. Salomon

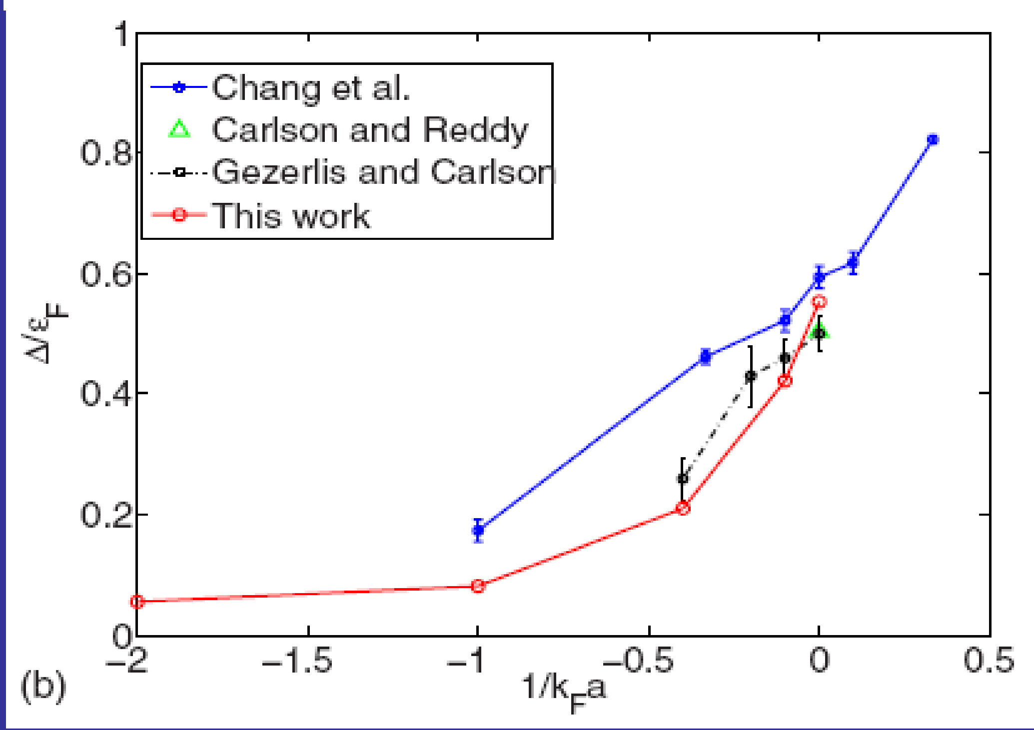
Equation of state of the unitary Fermi gas - current status



Experiment: M.J.H. Ku, A.T. Sommer, L.W. Cheuk, M.W. Zwierlein , Science 335, 563 (2012)

QMC (PIMC + Hybrid Monte Carlo):
J.E.Drut, T.Lähde, G.Wlazłowski, P.Magierski, Phys. Rev. A 85, 051601 (2012)





Results in the vicinity of the unitary limit:

-Critical temperature

-Pairing gap

BCS theory predicts:

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

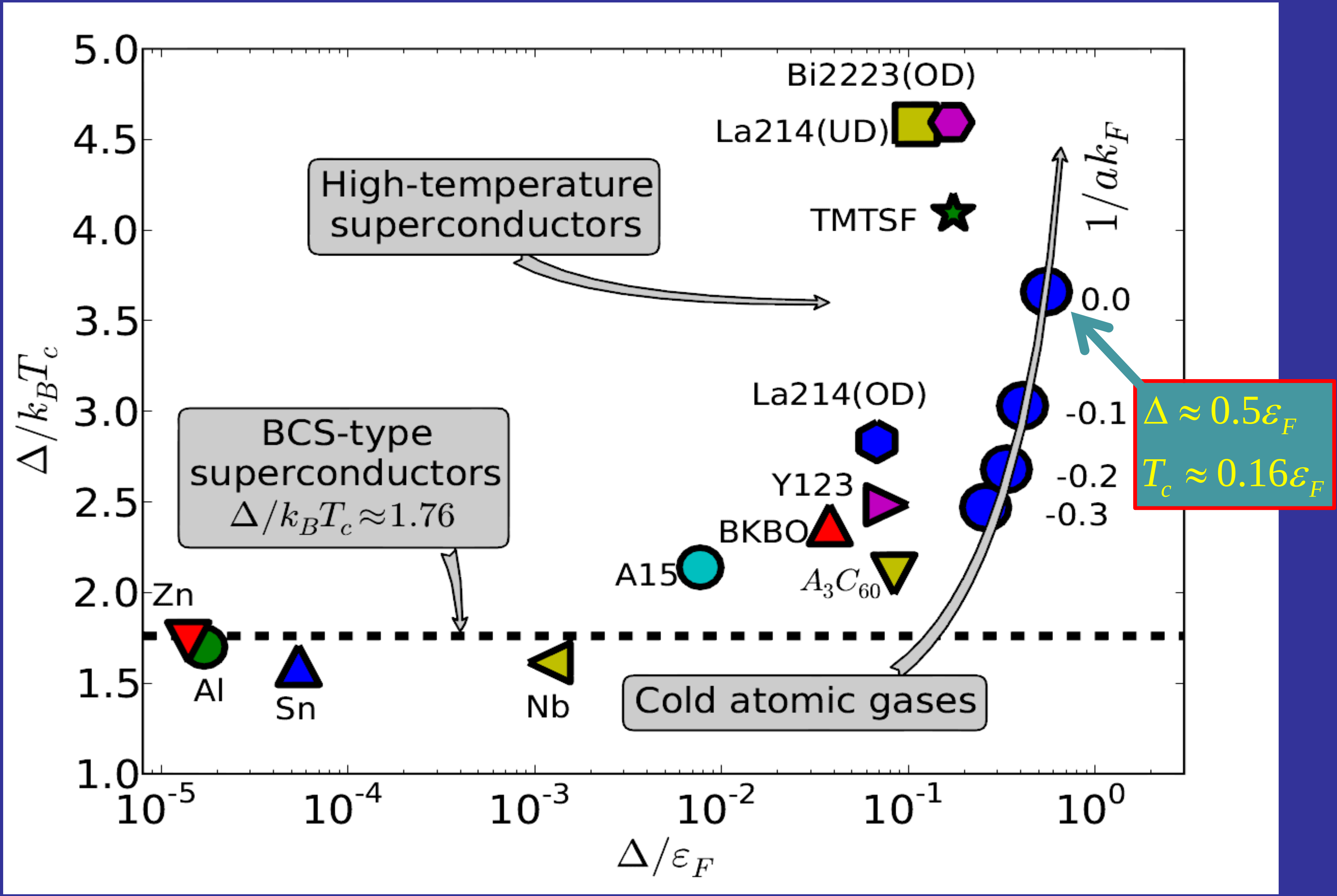
At unitarity:

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

This is NOT a BCS superfluid!

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

Cold atomic gases and high Tc superconductors



From Fischer et al., Rev. Mod. Phys. 79, 353 (2007) & P. Magierski, G. Wlazłowski, A. Bulgac, Phys. Rev. Lett. 107, 145304 (2011)

Pairing gap from spectral function:

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.

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

Constraints

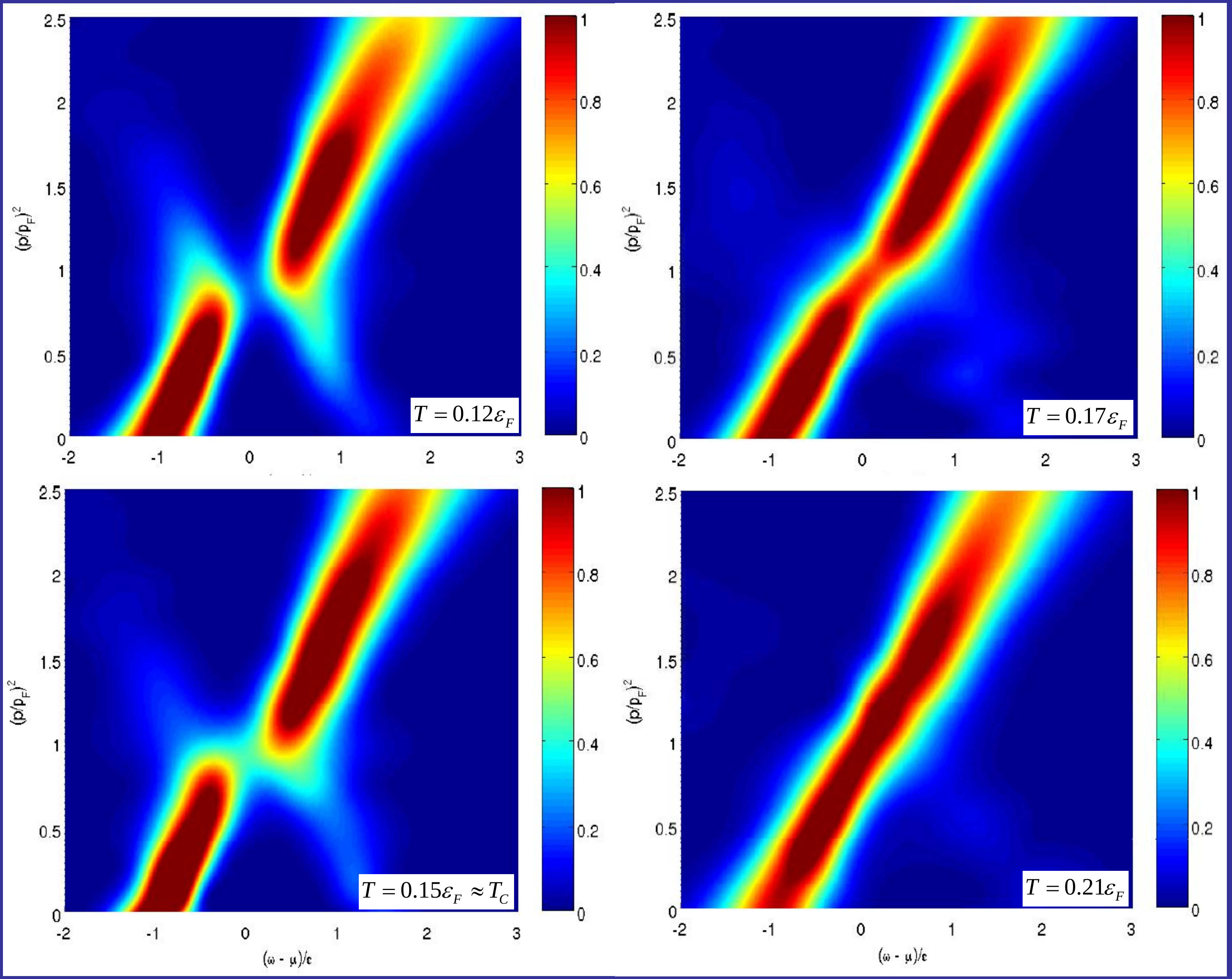
$$\int_{-\infty}^{+\infty} A(\vec{p},\omega)\frac{d\omega}{2\pi}=1$$

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

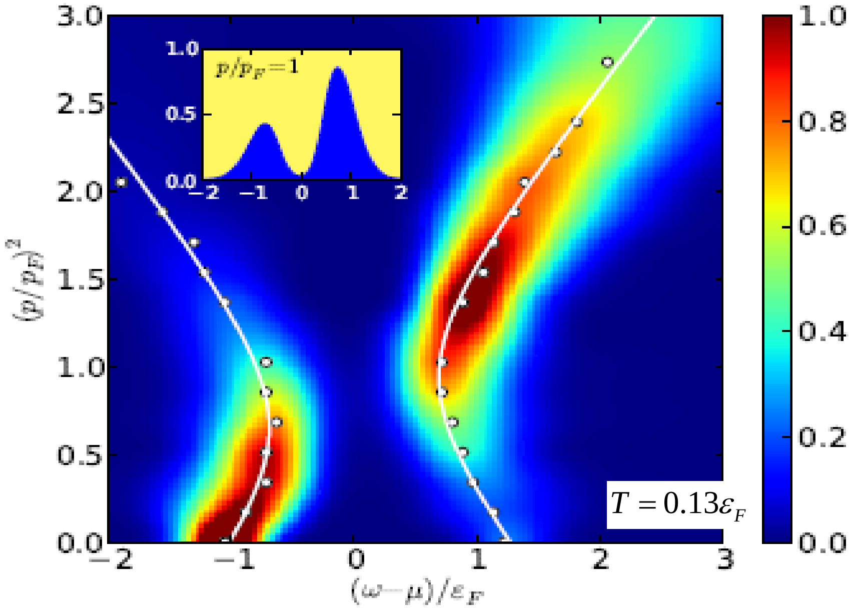
In the limit of independent quasiparticles: $A(\vec{p},\omega)=2\pi\delta(\omega-E(p))$

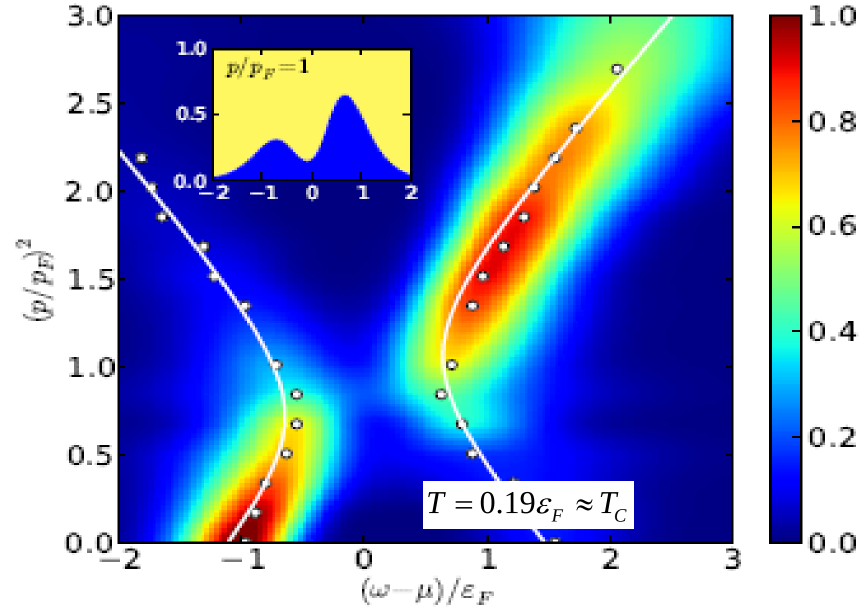
Numerical inversion: Magierski, Wlazłowski, Comp. Phys. Comm. 183 (2012) 2264

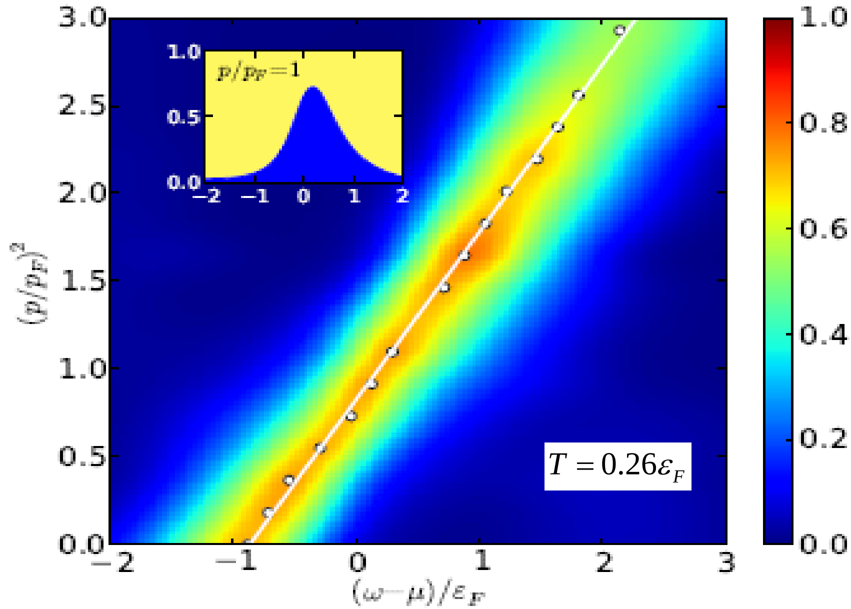
Spectral weight function at unitarity: $(k_F a)^{-1} = 0$



Spectral weight function at the BEC side: $(k_F a)^{-1} = 0.2$







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

$$m^*, U, \Delta$$

Can be used as an input to EDF

Description of the Unitary Fermi Gas within DFT: Local density approximation

$$E_{KS} = \int d^3\mathbf{r}\ \mathscr{E}_{KS}[n(\mathbf{r}), \tau(\mathbf{r}), \nabla n(\mathbf{r}), \ldots] + U(\mathbf{r})n(\mathbf{r}) + \cdots ,$$

$$\Psi_n(\mathbf{r}) = \begin{pmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{pmatrix}$$

$$n_a(\mathbf{r}) = \sum_n |u_n(\mathbf{r})|^2 f_\beta(E_n), \quad n_b(\mathbf{r}) = \sum_n |v_n(\mathbf{r})|^2 f_\beta(-E_n),$$

$$\tau_a(\mathbf{r}) = \sum_n |\nabla u_n(\mathbf{r})|^2 f_\beta(E_n), \quad \tau_b(\mathbf{r}) = \sum_n |\nabla v_n(\mathbf{r})|^2 f_\beta(-E_n),$$

$$\nu(\mathbf{r}) = \frac{1}{2} \sum_n u_n(\mathbf{r}) v_n^*(\mathbf{r}) \left(f_\beta(-E_n) - f_\beta(E_n) \right),$$

$$\mathbf{j}_a(\mathbf{r}) = \frac{\mathrm{i}}{2} \sum_n \left[u_n^*(\mathbf{r}) \nabla u_n(\mathbf{r}) - u_n(\mathbf{r}) \nabla u_n^*(\mathbf{r}) \right] f_\beta(E_n),$$

$$\mathbf{j}_b(\mathbf{r}) = \mathrm{i}2 \sum_n \left[v_n^*(\mathbf{r}) \nabla v_n(\mathbf{r}) - v_n(\mathbf{r}) \nabla v_n^*(\mathbf{r}) \right] f_\beta(-E_n),$$

where $f_\beta(E_n) = 1/(\exp(\beta E_n) + 1)$ is the Fermi distribution and $\beta = 1/T$

Superfluid Local Density Approximation (SLDA)

$$E_{SLDA} = \frac{\hbar^2}{m}\left(\frac{\alpha}{2}\left(\tau_\uparrow + \tau_\downarrow\right) + \beta\frac{3}{10}\left(3\pi^2\right)^{2/3}\left(n_\uparrow + n_\downarrow\right)^{5/3}\right) + g\nu^\dagger\nu + \underbrace{\left(1-\alpha\right)\frac{j^2}{2n}}$$

Bulgac A., Phys.Rev.A76:040502,2007

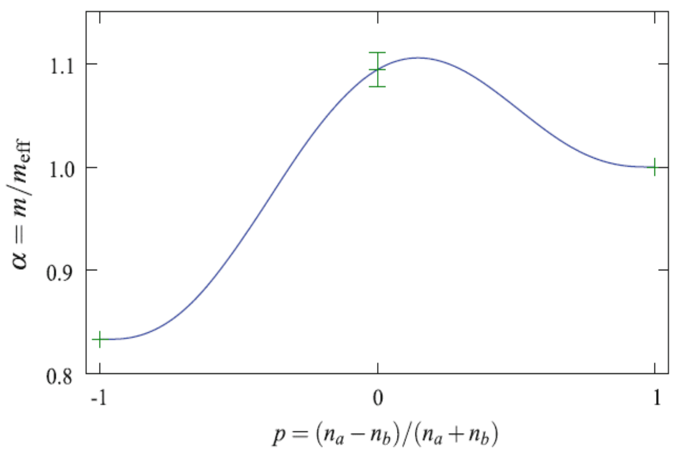
Restoring Galilean invariance

Asymmetric Superfluid Local Density Approximation (ASLDA)

$$E_{ASLDA} = \frac{\hbar^2}{m}\left(\left(\frac{\alpha_\uparrow}{2}\tau_\uparrow + \frac{\alpha_\downarrow}{2}\tau_\downarrow\right) + D\left(n_\uparrow, n_\downarrow\right)\right) + g\nu^\dagger\nu + \underbrace{\left(1-\alpha_\uparrow\right)\frac{j_\uparrow^2}{2n_\uparrow} + \left(1-\alpha_\downarrow\right)\frac{j_\downarrow^2}{2n_\uparrow}}$$

Bulgac, A., Forbes, M.M.: Phys. Rev. A **75**(3), 031605(R) (2007)

Restoring Galilean invariance



$$D\left(n_\uparrow, n_\downarrow\right) \sim \left(n_\uparrow + n_\downarrow\right)^{5/3}\beta(p)$$

$$D(n_a, n_b) = \frac{\left(6\pi^2(n_a + n_b)\right)^{5/3}}{20\pi^2}\left[G(p) - \alpha(p)\left(\frac{1+p}{2}\right)^{5/3} - \alpha(-p)\left(\frac{1-p}{2}\right)^{5/3}\right]$$

$$\alpha(p) = 1.094 + 0.156p\left(1 - \frac{2p^2}{3} + \frac{p^4}{5}\right) - 0.532p^2\left(1 - p^2 + \frac{p^4}{3}\right)$$

Normal State			
(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)
(3,1)	6.6±0.01	6.687	1.3%
(4,1)	8.93±0.01	8.962	0.36%
(5,1)	12.1±0.1	12.22	0.97%
(5,2)	13.3±0.1	13.54	1.8%
(6,1)	15.8±0.1	15.65	0.93%
(7,2)	19.9±0.1	20.11	1.1%
(7,3)	20.8±0.1	21.23	2.1%
(7,4)	21.9±0.1	22.42	2.4%
(8,1)	22.5±0.1	22.53	0.14%
(9,1)	25.9±0.1	25.97	0.27%
(9,2)	26.6±0.1	26.73	0.5%
(9,3)	27.2±0.1	27.55	1.3%
(9,5)	30±0.1	30.77	2.6%
(10,1)	29.4±0.1	29.41	0.034%
(10,2)	29.9±0.1	30.05	0.52%
(10,6)	35±0.1	35.93	2.7%
(20,1)	73.78±0.01	73.83	0.061%
(20,4)	73.79±0.01	74.01	0.3%
(20,10)	81.7±0.1	82.57	1.1%
(20,20)	109.7±0.1	113.8	3.7%
(35,4)	154±0.1	154.1	0.078%
(35,10)	158.2±0.1	158.6	0.27%
(35,20)	178.6±0.1	180.4	1%

Superfluid State			
(N_a, N_b)	E_{FNDMC}	E_{ASLDA}	(error)
(1,1)	2.002±0	2.302	15%
(2,2)	5.051±0.009	5.405	7%
(3,3)	8.639±0.03	8.939	3.5%
(4,4)	12.573±0.03	12.63	0.48%
(5,5)	16.806±0.04	16.19	3.7%
(6,6)	21.278±0.05	21.13	0.69%
(7,7)	25.923±0.05	25.31	2.4%
(8,8)	30.876±0.06	30.49	1.2%
(9,9)	35.971±0.07	34.87	3.1%
(10,10)	41.302±0.08	40.54	1.8%
(11,11)	46.889±0.09	45	4%
(12,12)	52.624±0.2	51.23	2.7%
(13,13)	58.545±0.18	56.25	3.9%
(14,14)	64.388±0.31	62.52	2.9%
(15,15)	70.927±0.3	68.72	3.1%
(1,0)	1.5±0.0	1.5	0%
(2,1)	4.281±0.004	4.417	3.2%
(3,2)	7.61±0.01	7.602	0.1%
(4,3)	11.362±0.02	11.31	0.49%
(7,6)	24.787±0.09	24.04	3%
(11,10)	45.474±0.15	43.98	3.3%
(15,14)	69.126±0.31	62.55	9.5%

Table 9.2 Comparison between the ASLDA density functional as described in this section and the FN-DMC calculations [136, 137] for a harmonically trapped unitary gas at zero temperature. The normal state energies are obtained by fixing $\Delta = 0$ in the functional: In the FN-DMC calculations, this is obtained by choosing a nodal ansatz without any pairing. In the case of small asymmetry, the resulting "normal states" may be a somewhat artificial construct as there is no clear way of preparing a physical system in this "normal state" when the ground state is superfluid.

From A. Bulgac, M.M. Forbes, P. Magierski, Lecture Notes in Physics, vol. 836, p.305 (2012)

Challenge for DFT:

How to distinguish the existence of superfluid phase from the existence of the gap in the single-particle spectrum?

Superfluidity = existence of the long range order

$$\lim_{r\to\infty} g_2(r) \neq 0$$

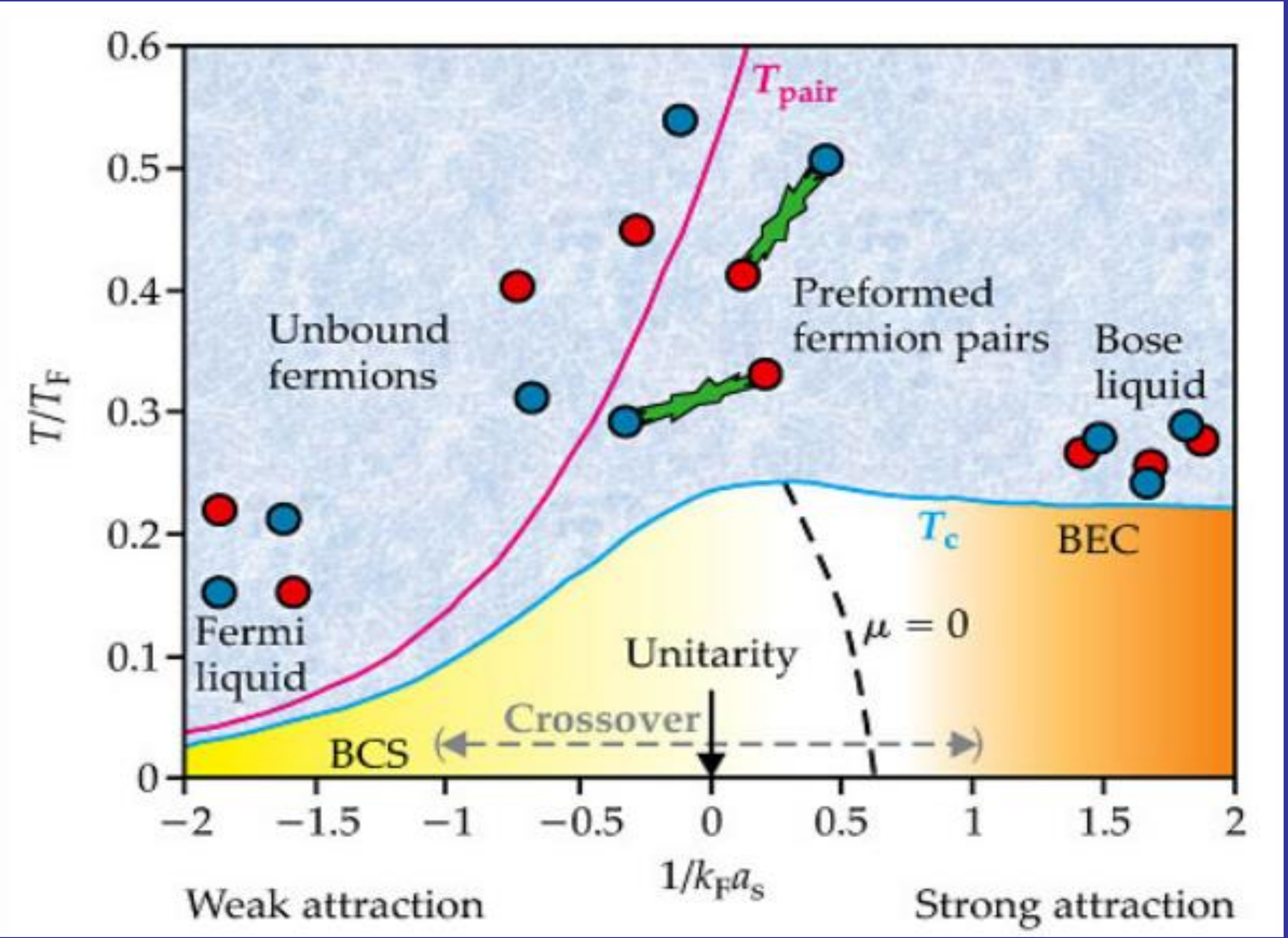
$$g_2(r) = \left(\frac{2}{N}\right)^2 \int \langle \psi_\uparrow^\dagger(r_1+r)\psi_\downarrow^\dagger(r_2+r)\psi_\uparrow(r_2)\psi_\uparrow(r_1)\rangle d^3r_1 d^3r_2; \quad g_2(0)=1$$

On the other hand the pairing gap is extracted from odd-even energy difference or equivalently from the gap in the spectral function.

One may have however: $\lim_{r\to\infty} g_2(r) = 0 \ \text{ and } \Delta \neq 0$

However in EDF both quantities: g_2 and Δ are expressed through anomalous density which implies that either:

$\lim_{r\to\infty} g_2(r) = 0 \ \text{ and } \Delta = 0$ or $\lim_{r\to\infty} g_2(r) \neq 0 \ \text{ and } \Delta \neq 0$



From Sa de Melo, Physics Today (2008)

Pairing pseudogap: suppression of low-energy spectral weight function due to incoherent pairing in the normal state ($T > T_c$)

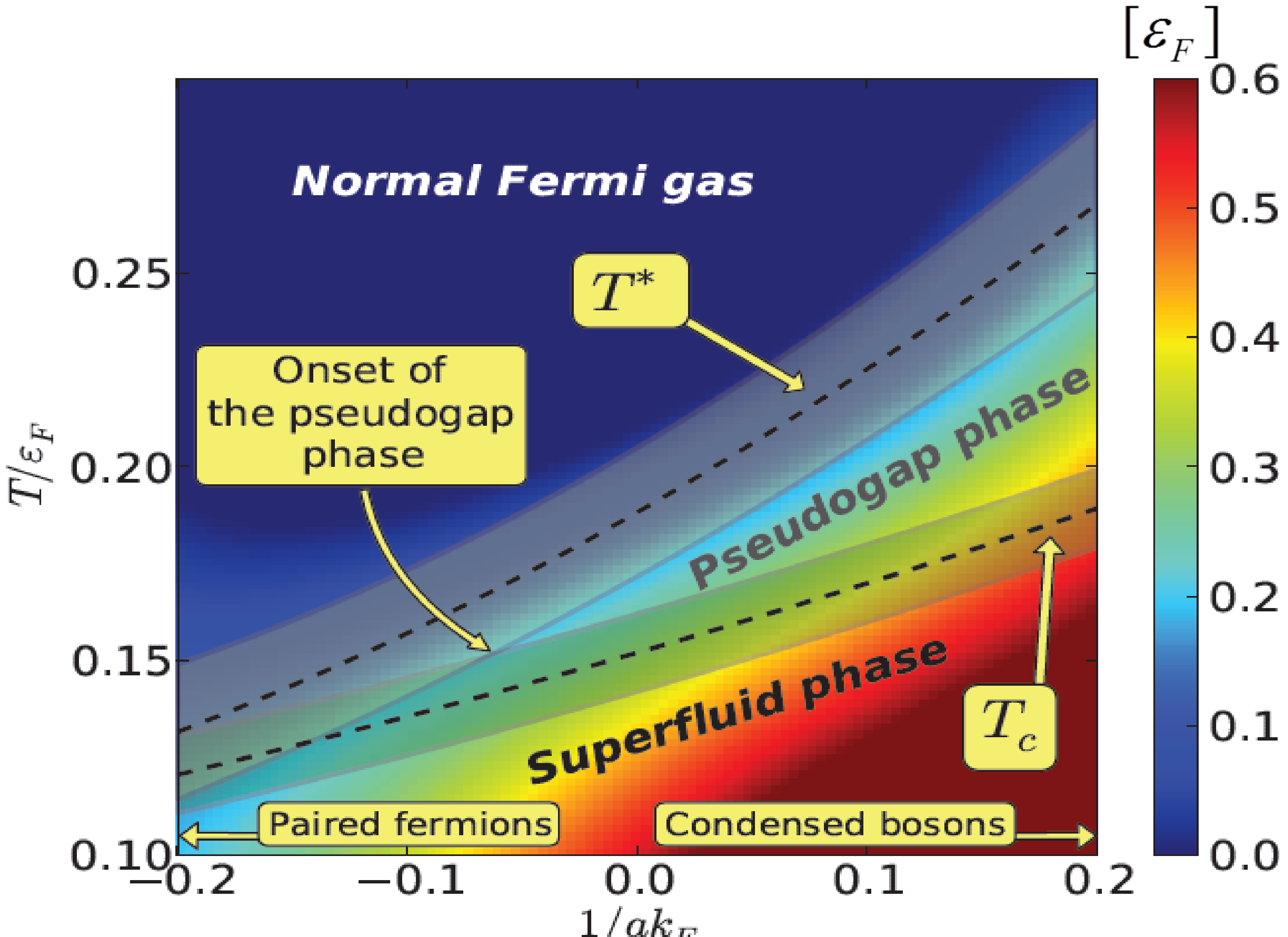
Important issue related to pairing pseudogap:

- Are there sharp gapless quasiparticles in a normal Fermi liquid

YES: Landau's Fermi liquid theory;

NO: breakdown of Fermi liquid paradigm

Gap in the single particle fermionic spectrum - theory



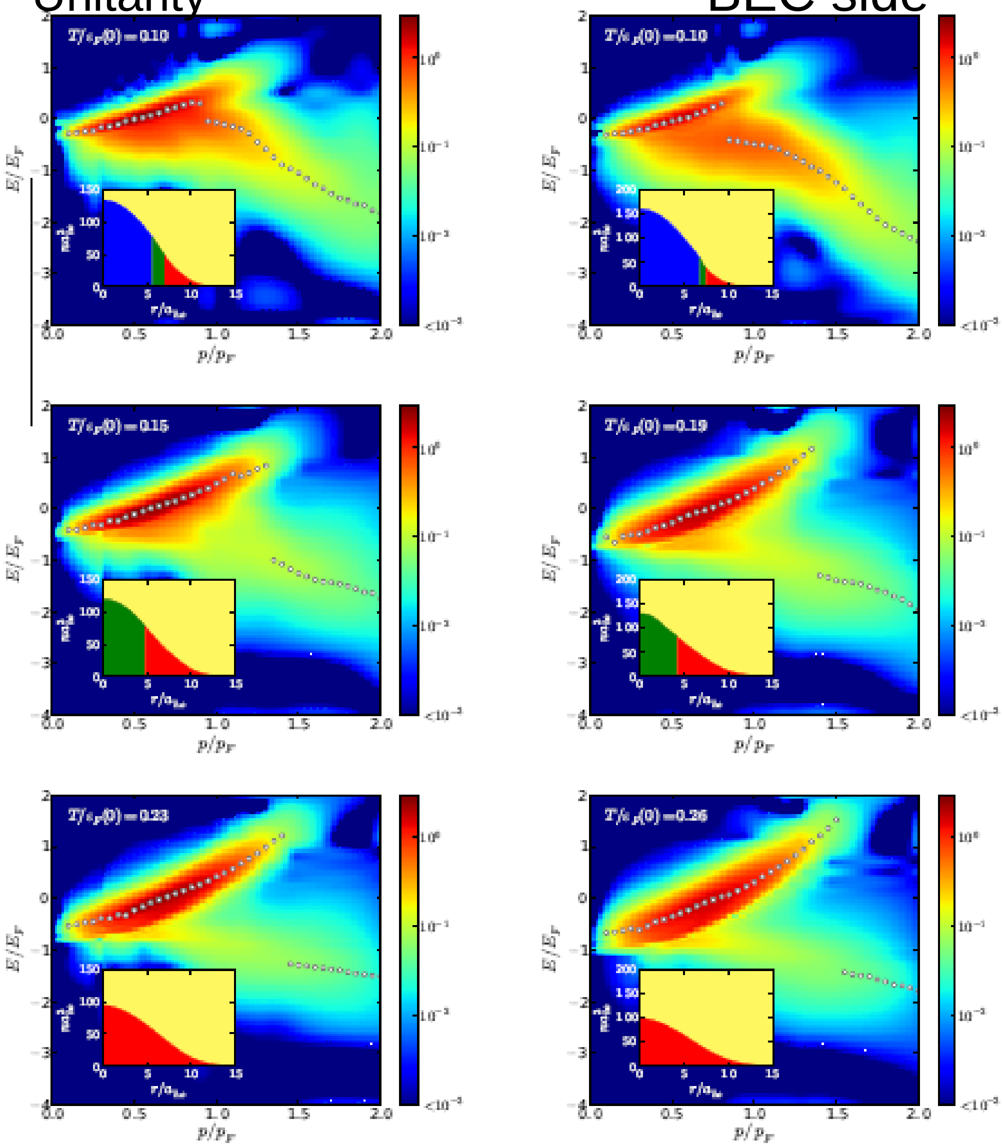
Ab initio **result: The onset of pseudogap phase at $1/ak_F \approx -0.05$.**

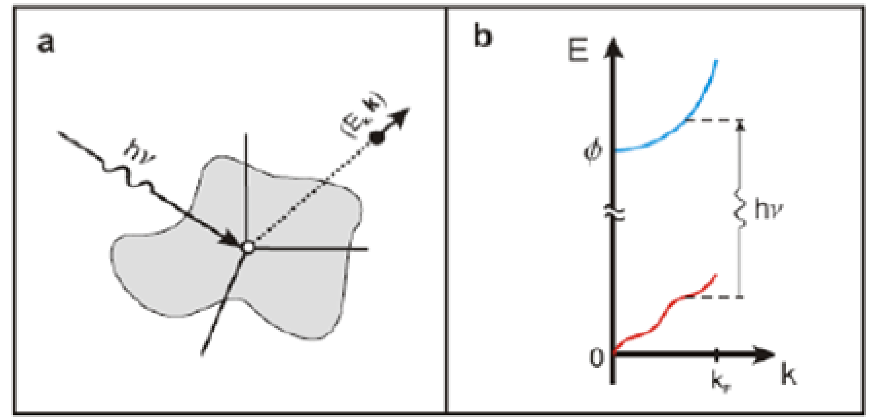
Magierski, Wlazłowski, Bulgac, *Phys. Rev. Lett.* 107,145304(2011)
Magierski, Wlazłowski, Bulgac, Drut, *Phys. Rev. Lett.* 103,210403(2009)

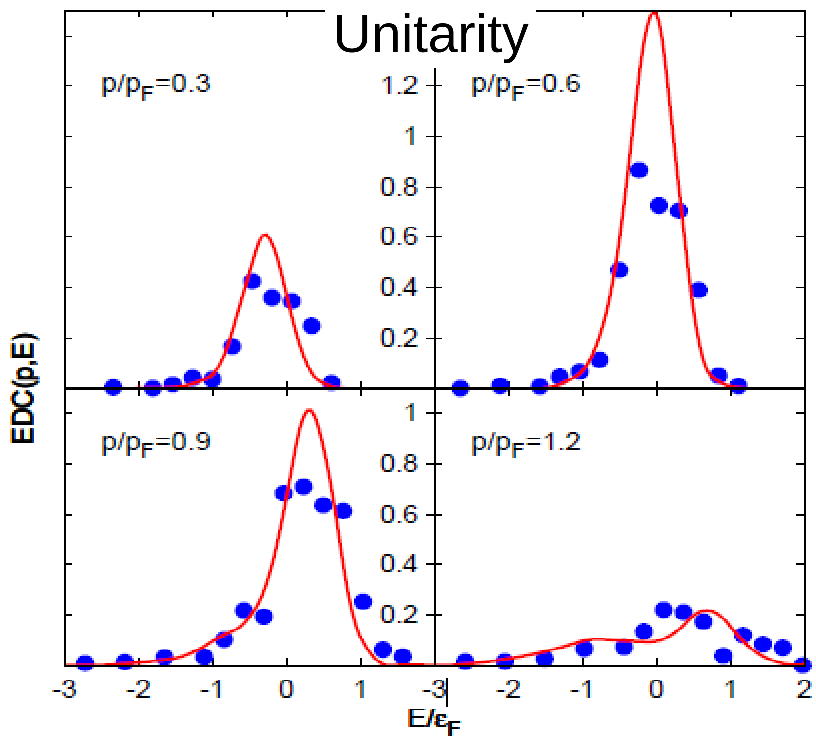
Energy distribution curves (EDC) from the spectral weight function

$$\mathrm{EDC}(p,E,T)=\mathcal{C}p^2\int_0^\infty dr\, r^2\frac{1}{\varepsilon_F(r)}A\left[\frac{p}{p_F(r)},\frac{E-\mu(r)}{\varepsilon_F(r)},\frac{T}{\varepsilon_F(r)}\right]f(E-\mu(r)),$$

Unitarity | BEC side







Experiment (blue dots): Gaebler et al. *Nature Physics 6, 569(2010)*
QMC (red line): Magierski, Wlazłowski, Bulgac, Phys. Rev. Lett. 107, 145304 (2011)

Spin susceptibility and spin drag rate

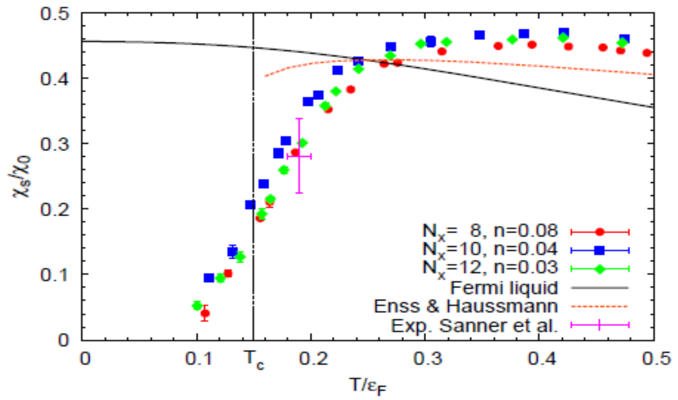


FIG. 2: (Color online) The static spin susceptibility as a function of temperature for an 8^3 lattice solid (red) circles, 10^3 lattice (blue) squares and 12^3 lattice (green) diamonds. Vertical black dotted line indicates the critical temperature of superfluid to normal phase transition $T_c = 0.15\,\varepsilon_F$. For comparison Fermi liquid theory prediction and recent results of the T-matrix theory produced by Enss and Haussmann [25] are plotted with solid and dashed (brown) lines, respectively. The experimental data point from Ref. [15] is also shown.

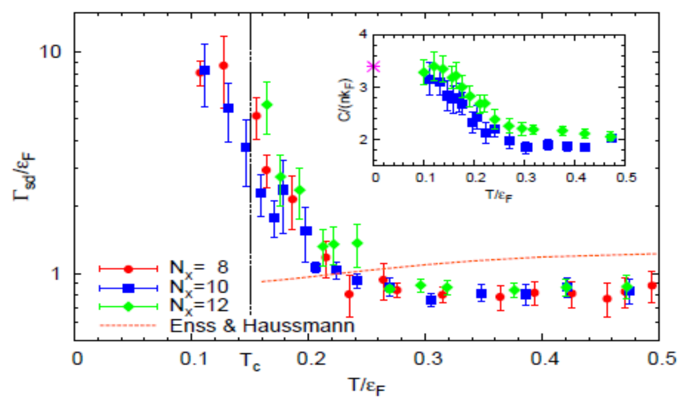


FIG. 3: (Color online) The spin drag rate $\Gamma_{sd} = n/\sigma_s$ in units of Fermi energy as a function of temperature for an 8^3 lattice solid (red) circles, 10^3 lattice (blue) squares and 12^3 lattice (green) diamonds. Vertical black dotted line locates the critical temperature of superfluid to normal phase transition. Results of the T-matrix theory are plotted by dashed (brown) line [25]. The inset shows extracted value of the contact density as function of the temperature. The (purple) asterisk shows the contact density from the QMC calculations of Ref. [29] at $T = 0$.

$$\Gamma = \frac{n}{\sigma_s}$$ - spin drag rate

$$\sigma_s(\omega) = \pi\rho_s(q=0,\omega)/\omega$$ - spin conductivity

$$G_s(q,\tau) = \frac{1}{V}\left\langle \left(\hat{j}^z_{q\uparrow}(\tau) - \hat{j}^z_{q\downarrow}(\tau)\right)\left(\hat{j}^z_{-q\uparrow}(0) - \hat{j}^z_{-q\downarrow}(0)\right)\right\rangle$$

$$G_s(q,\tau) = \int_0^\infty \rho_s(q,\omega)\frac{\cosh\left[\omega(\tau-\beta/2)\right]}{\sinh\left[\omega\beta/2\right]}d\omega$$

Wlazłowski, Magierski, Bulgac, Drut, Roche,
Phys. Rev. Lett. 110, 090401,(2013)

$$D_s = \frac{\sigma_s}{\chi_s}$$

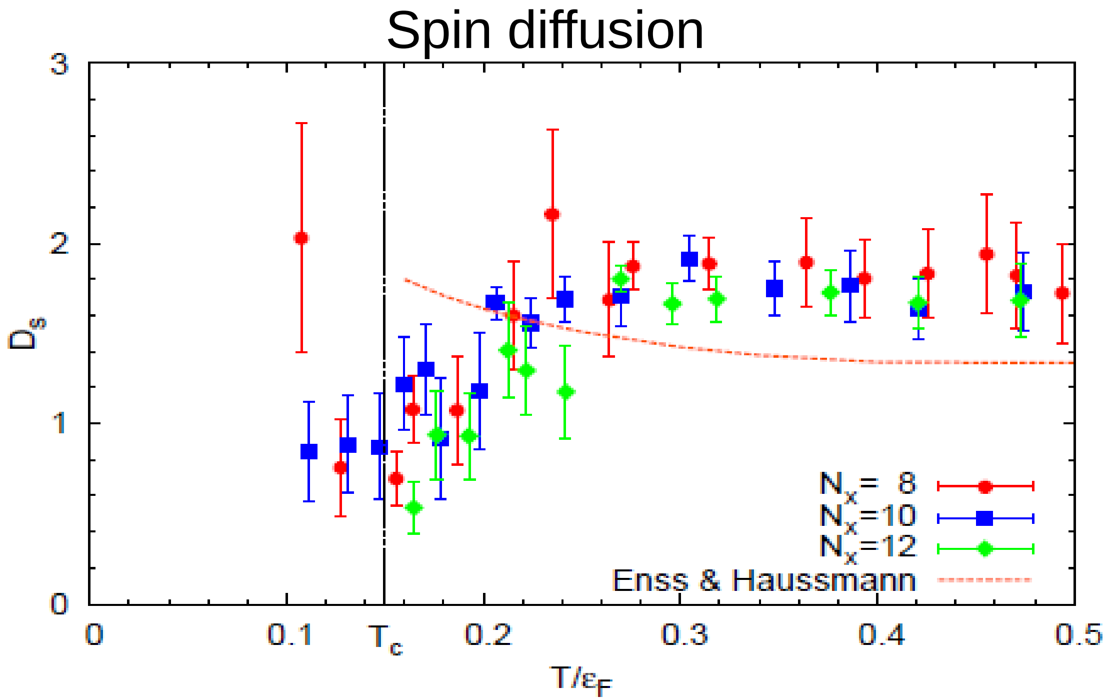


FIG. 4: (Color online) The spin diffusion coefficient obtained by the Einstein relation $D_s = \sigma_s/\chi_s$ as function of temperature. The notation is identical to Fig. 3.

No minimum is seen in QMC down to 0.1 of Fermi energy

Estimate from kinetic theory at low T:	$D_s \sim p_F l \sim n^{1/3} n^{-1/3} \sim 1$

Wlazłowski, Magierski, Bulgac, Drut, Roche, Phys. Rev. Lett. 110, 090401,(2013)

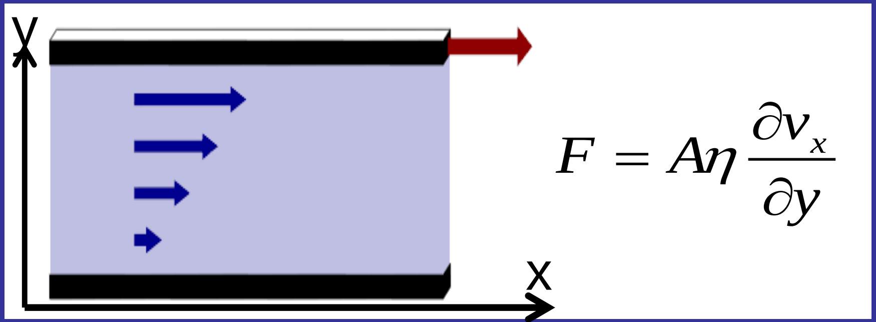
Hydrodynamics at unitarity

Scaling: $\psi_i(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) \to \frac{1}{\lambda^{3N/2}} \psi_i\left(\vec{r}_1/\lambda, \vec{r}_2/\lambda, \ldots, \vec{r}_N/\lambda\right); E_i \to E_i/\lambda^2$

No intrinsic length scale ➡ Uniform expansion keeps the unitary gas in equilibrium

Consequence:
uniform expansion does not produce entropy = bulk viscosity is zero!

Shear viscosity:



For any physical fluid:

$$\frac{\eta}{S} \geq \frac{\hbar}{4\pi k_B}$$ **KSS conjecture**

Kovtun,Son,Starinets, (2005) from AdS/CFT correspondence

Maxwell classical estimate: $\eta \sim$ mean free path

Perfect fluid $\frac{\eta}{S} = \frac{\hbar}{4\pi k_B}$ - strongly interacting quantum system = No well defined quasiparticles

Candidates: unitary Fermi gas, QGP

Shear viscosity

$$\eta(\omega) = \pi\rho_{xyxy}(q=0,\omega)/\omega$$

$$G_{xyxy}(q,\tau) = \int d^3r \left\langle \hat{\Pi}_{xy}(r,\tau)\hat{\Pi}_{xy}(0,0)\right\rangle e^{iqr}$$

$$G_{xyxy}(q,\tau) = \int_0^\infty \rho_{xyxy}(q,\omega)\frac{\cosh\left[\omega(\tau-\beta/2)\right]}{\sinh\left[\omega\beta/2\right]}d\omega$$

$$i\left[\hat{j}_k(r),\hat{H}\right] = \partial_l\hat{\Pi}_{kl}(r)$$

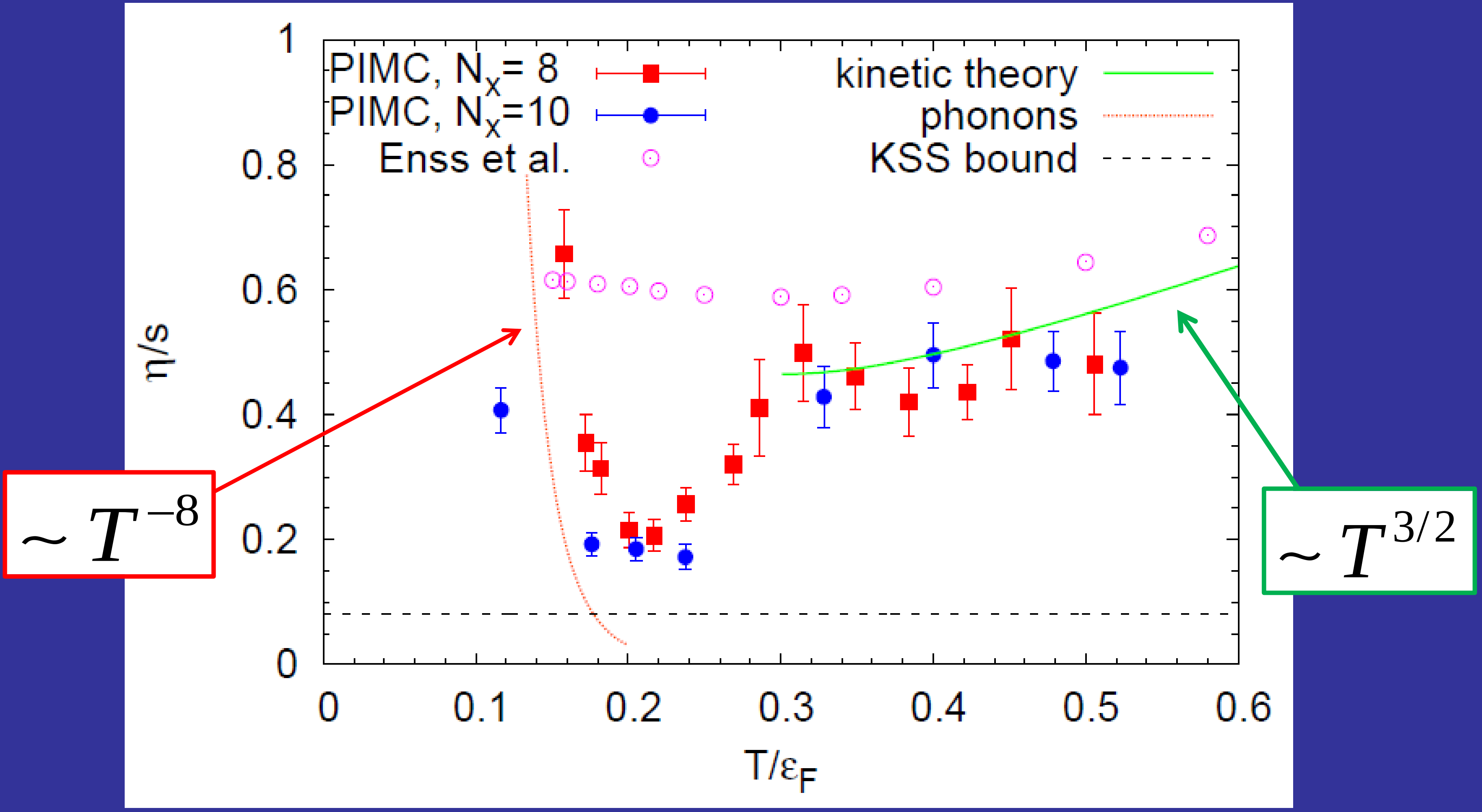
Additional symmetries and sum rules:

$$G(\tau) = G(\beta-\tau)$$

$$\frac{1}{\pi}\int_0^\infty d\omega\left[\eta(\omega) - \frac{C}{15\pi\sqrt{m\omega}}\right] = \frac{\varepsilon}{3},$$ ε – *energy density*

$$\eta(\omega\to\infty) \simeq \frac{C}{15\pi\sqrt{m\omega}}.$$

Shear viscosity to entropy density ratio



G.Wlazłowski, P.Magierski,J.E.Drut,
Phys. Rev. Lett. 109, 020406 (2012)

Foundations of time dependent DFT: Runge Gross mapping

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle, \quad \left|\psi_0\right\rangle = \left|\psi(t_0)\right\rangle$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0$$

$$\left.\begin{array}{l}\rho(\vec{r},t)\\ \left|\psi(t_0)\right\rangle\end{array}\right\} \leftrightarrow e^{i\alpha(t)}\left|\psi(t)\right\rangle$$

Up to an arbitrary function α(t)

and consequently the functional exists:

$$F[\psi_0,\rho] = \int_{t_0}^{t_1}\left\langle\psi[\rho]\right|\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\left|\psi[\rho]\right\rangle dt$$

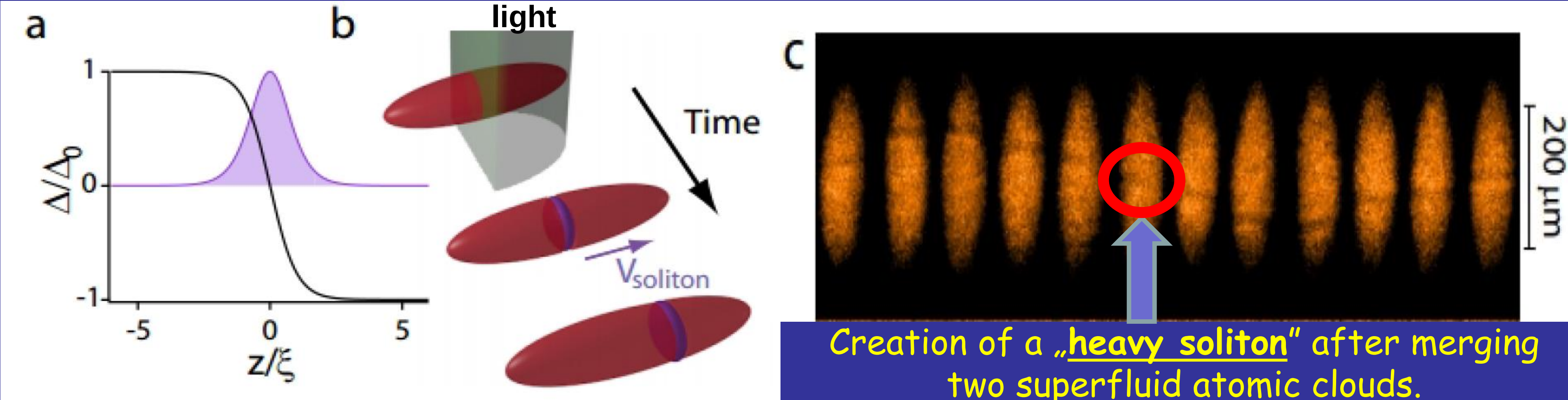
E. Runge, E.K.U Gross, PRL 52, 997 (1984)
B.-X. Xu, A.K. Rajagopal, PRA 31, 2682 (1985)
G. Vignale, PRA77, 062511 (2008)

The simplest realization of TDDFT

- Local in time (no memory effects) and no dissipation, except the one-body dissipation.
- Only one body observables can be reliably evaluated within standard DFT.

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow,\uparrow}(\mathbf{r},t) & h_{\uparrow,\downarrow}(\mathbf{r},t) & 0 & \Delta(\mathbf{r},t) \\ h_{\downarrow,\uparrow}(\mathbf{r},t) & h_{\downarrow,\downarrow}(\mathbf{r},t) & -\Delta(\mathbf{r},t) & 0 \\ 0 & -\Delta^*(\mathbf{r},t) & -h^*_{\uparrow,\uparrow}(\mathbf{r},t) & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) \\ \Delta^*(\mathbf{r},t) & 0 & -h^*_{\uparrow,\downarrow}(\mathbf{r},t) & -h^*_{\downarrow,\downarrow}(\mathbf{r},t) \end{pmatrix}\begin{pmatrix} u_{k\uparrow}(\mathbf{r},t) \\ u_{k\downarrow}(\mathbf{r},t) \\ v_{k\uparrow}(\mathbf{r},t) \\ v_{k\downarrow}(\mathbf{r},t) \end{pmatrix}$$

Still works impressively well...



Creation of a „**heavy soliton**" after merging two superfluid atomic clouds.
T. Yefsah et al., Nature 499, 426 (2013).

Experimental results – Cascade of Solitary Waves

Figures taken from: M. Zwierlein talk, (http://en.sif.it/activities/fermi_school/mmxiv)
School of Physics E. Fermi – Quantum Matter at Ultralow Temperatures Varenna, July 9th , 2014
See also: Mark J.H. Ku, et al., Phys. Rev. Lett. 116, 045304 (2016)

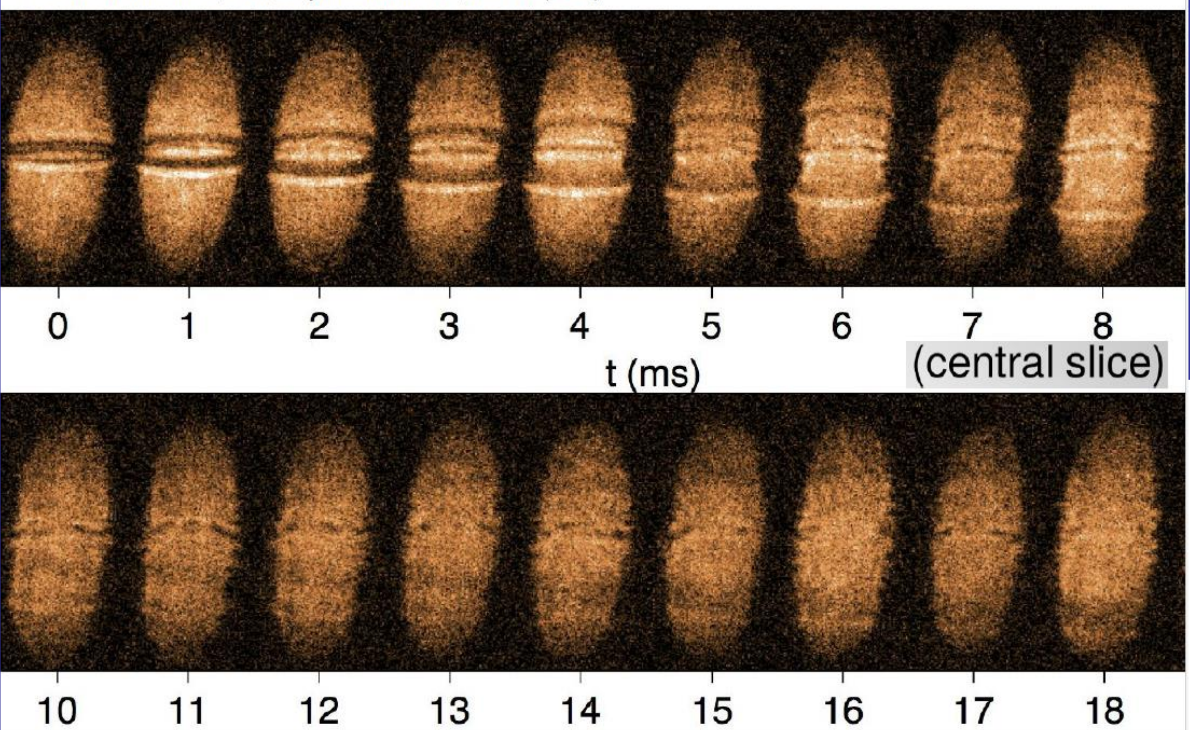
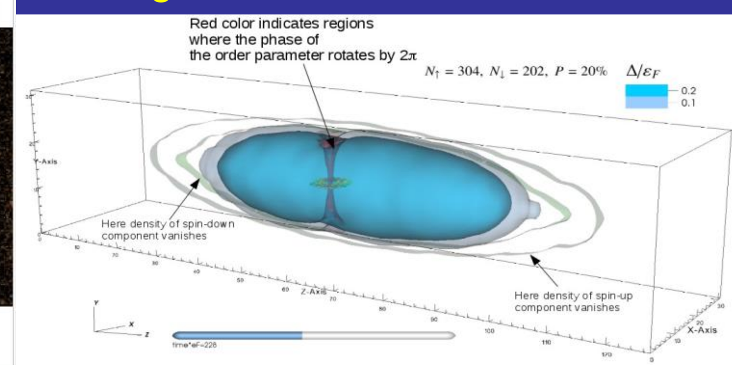
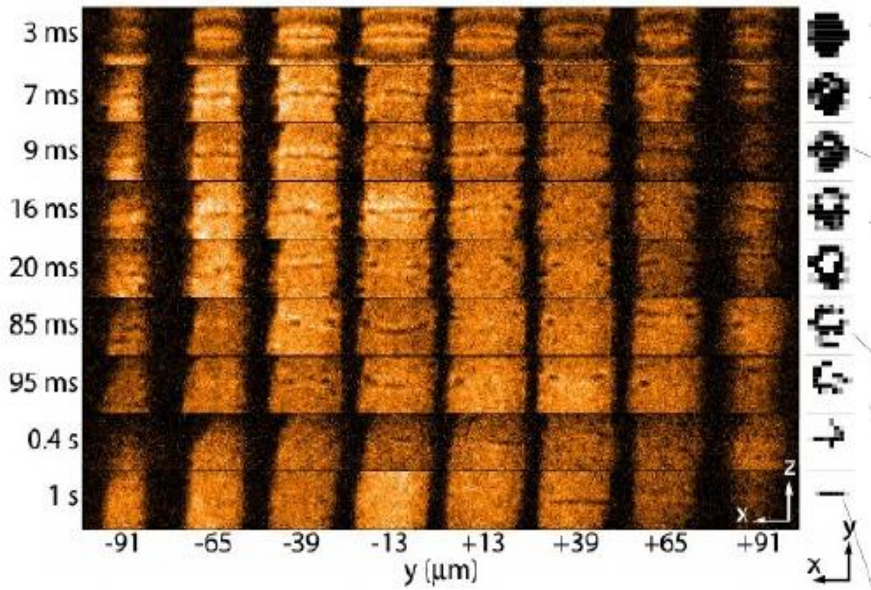
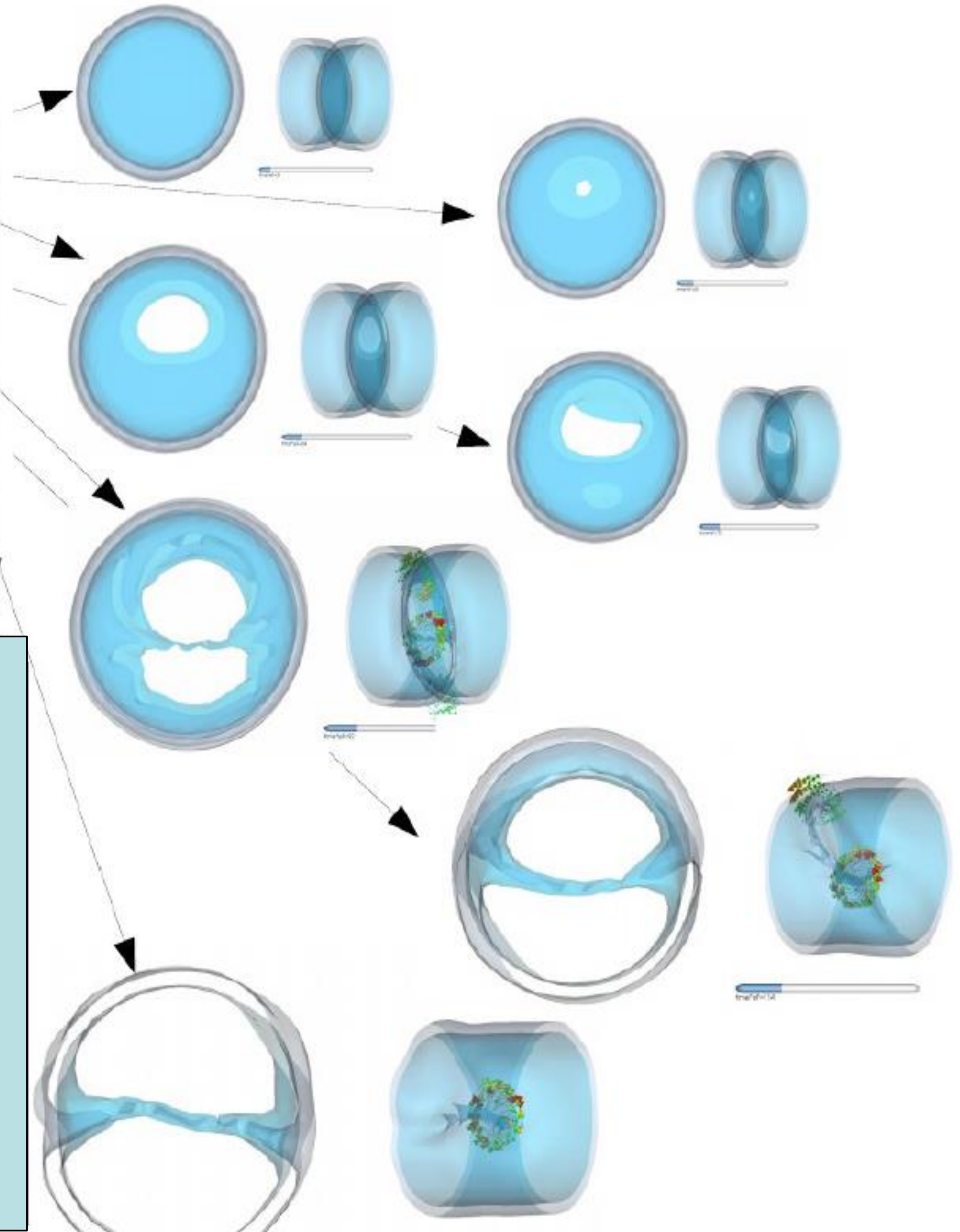


Image from TDDFT simulation





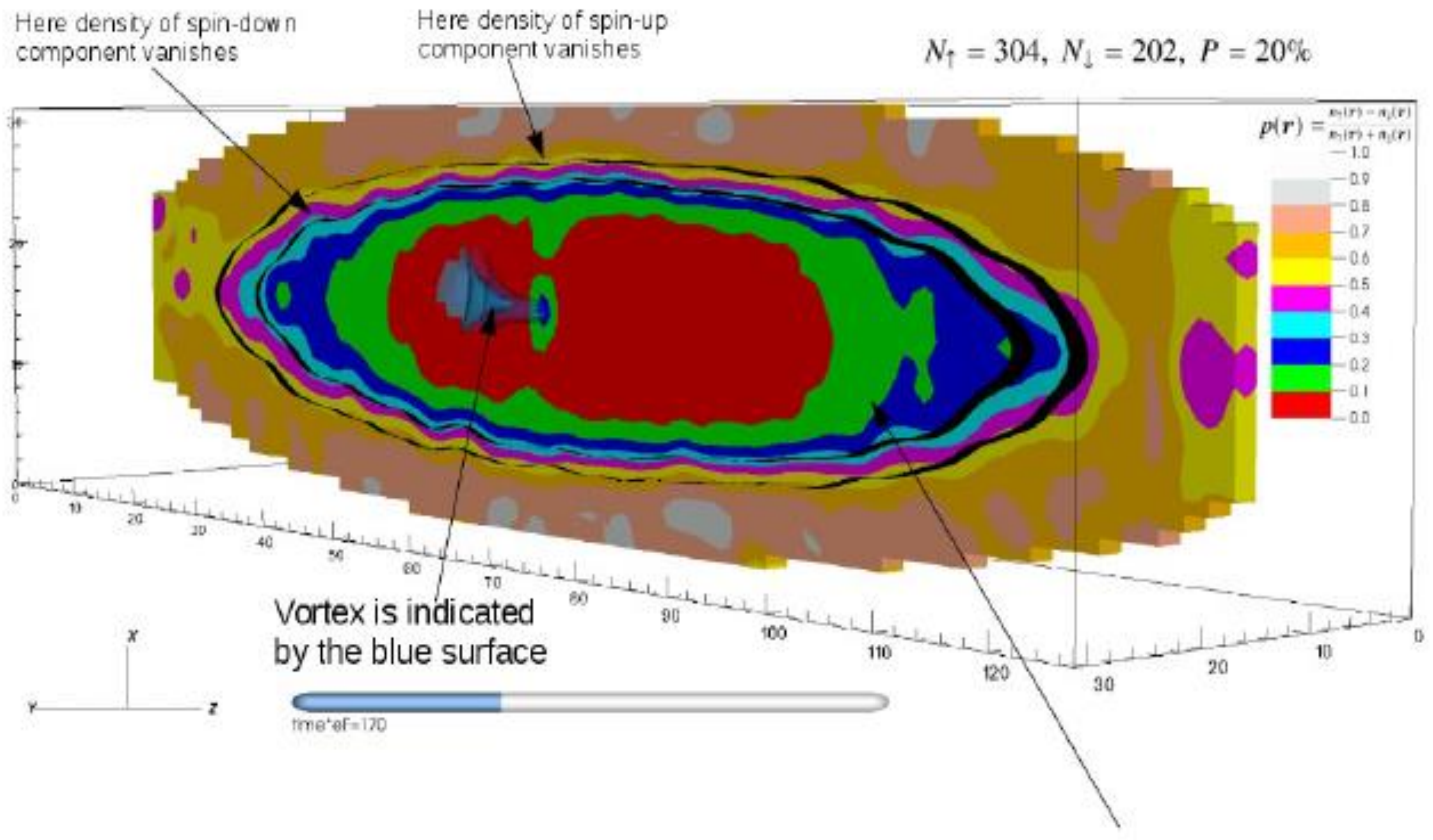


We can reproduce all stages of the experimentally observed solitonic cascade within time dependent SLDA.

From Gabriel Wlazłowski talk

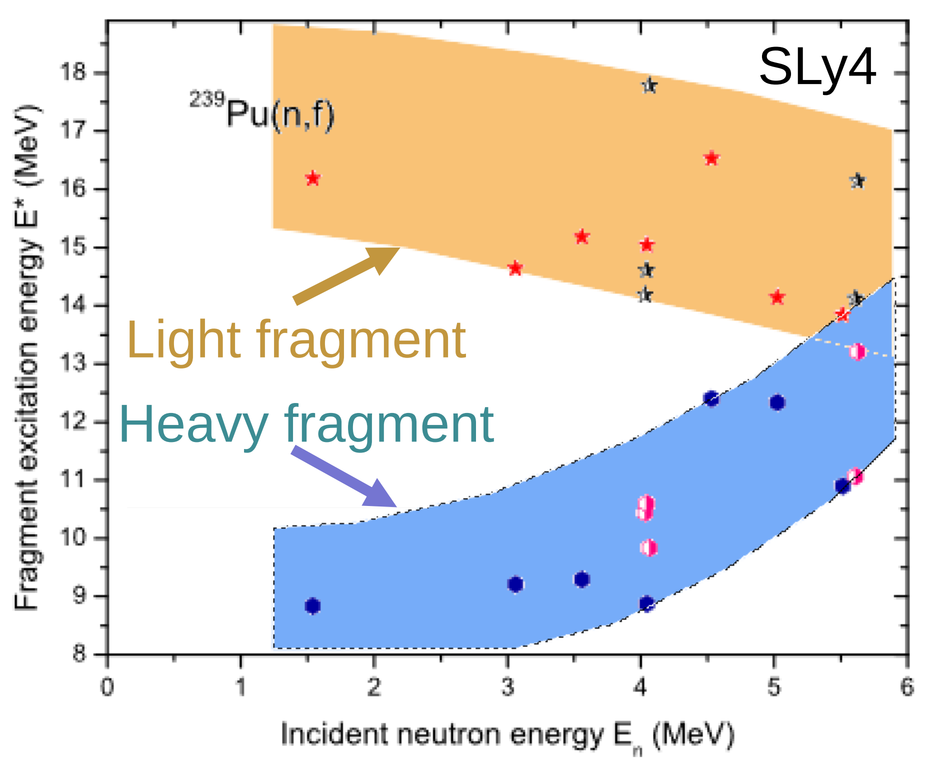
Wlazłowski, Sekizawa, Magierski (in preparation)

Vortex in spin-imbalanced unitary Fermi gas within TD ASLDA



From Gabriel Wlazłowski talk

Note that the core of the vortex is polarized – dynamics of vortices is affected



E^* (MeV)	E_n (MeV)	$t_{fission}$ (fm/c)	TKE (MeV)	Z_L	N_L
8.08	1.542	8517	173.81	40.825	62.246
9.60	3.063	9215	174.73	40.500	61.536
10.10	3.560	9287	179.09	41.625	62.783
10.57	4.032	7243	173.67	40.092	61.256
10.58	4.043	7287	173.39	40.146	61.388
10.58	4.047	7134	175.11	40.313	61.475
10.60	4.065	7737	174.75	40.904	62.611
11.07	4.534	6444	176.46	41.495	63.134
11.56	5.024	6261	175.15	40.565	61.894
12.05	5.515	5898	176.75	40.412	61.809
12.15	5.610	6100	176.36	40.355	61.695
12.16	5.626	7404	176.10	41.386	62.764

Induced fission of 240Pu

The lighter fragment is more excited (and strongly deformed) than the heavier one.

Energies are not shared proportionally to mass numbers of the fragments!

$$\mathrm{TKE} = 177.80 - 0.3489 E_n \quad [\text{in MeV}],$$

Nuclear data evaluation, Madland (2006)

Calculated TKEs slightly underestimate the observed values by no more than: 1 - 3 MeV !

J. Grineviciute, et al. (in preparation)

see also:

A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu, Phys. Rev. Lett. 116, 122504 (2016)

Conclusions/questions:

- How to extend DFT to finite temperatures with right Tc and pseudogap?

- Why TDDFT works so well even if it is constructed within so simplified framework (local in time and space)?