The Unitary Fermi Gas:
so simple yet so complex!

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DE-FC02-07ER41457 (SciDAC-UNEDF)

Why would one want to study this system?

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?

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

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

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

Let me consider as an 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 such 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

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 <u>a huge pairing gap</u> !

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

What George Bertsch essentially asked in 1999 is:
What is the value of ξ !

But he wished to know the properties of the system as well:
The system turned out to be superfluid !

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

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

Now these results are a bit unexpected.

- ✓ **The energy looks almost like that of *a non-interacting system*!**
(there are no other dimensional parameters in the problem)
- ✓ **The system has *a huge pairing gap*!**
- ✓ **This system is a very strongly interacting one**
(*the elementary cross section is essentially infinite!*)

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

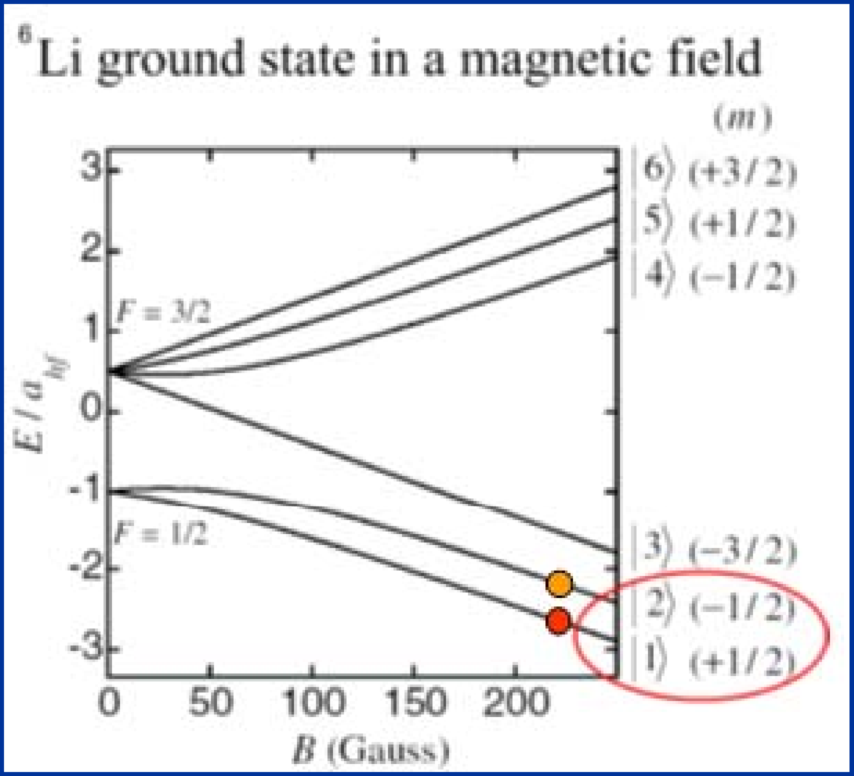
Superconductivity and Superfluidity in Fermi Systems

20 orders of magnitude over a century of (low temperature) physics

✓ 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 ≈ 10^4 K)

In cold old gases one can control the strength of the interaction!



Bartenstein *et al.* Phys. Rev. Lett. 94, 103201 (2005)

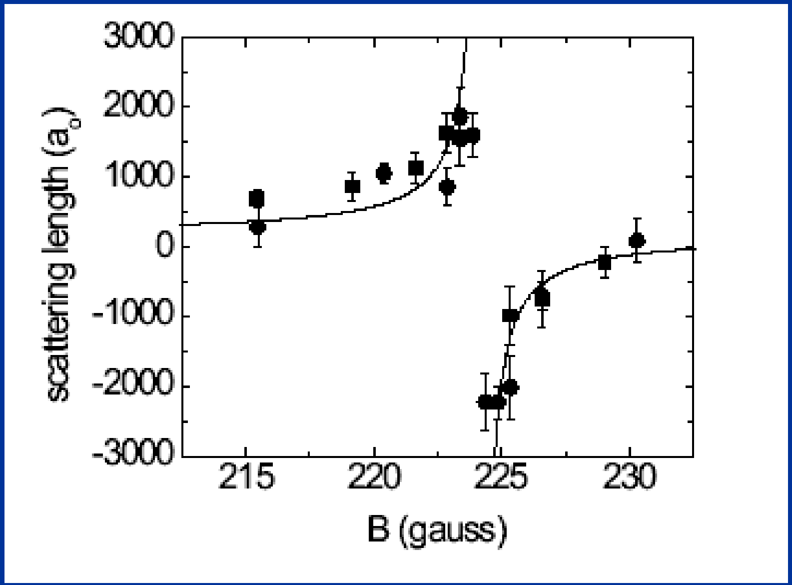
Feshbach resonance

$$H = \frac{\vec{p}^{\,2}}{2\mu_r} + \sum_{i=1}^{2} (V_i^{hf} + V_i^{Z}) + V_0(\vec{r})P_0 + V_1(\vec{r})P_1 + \cancel{V}^{d}$$

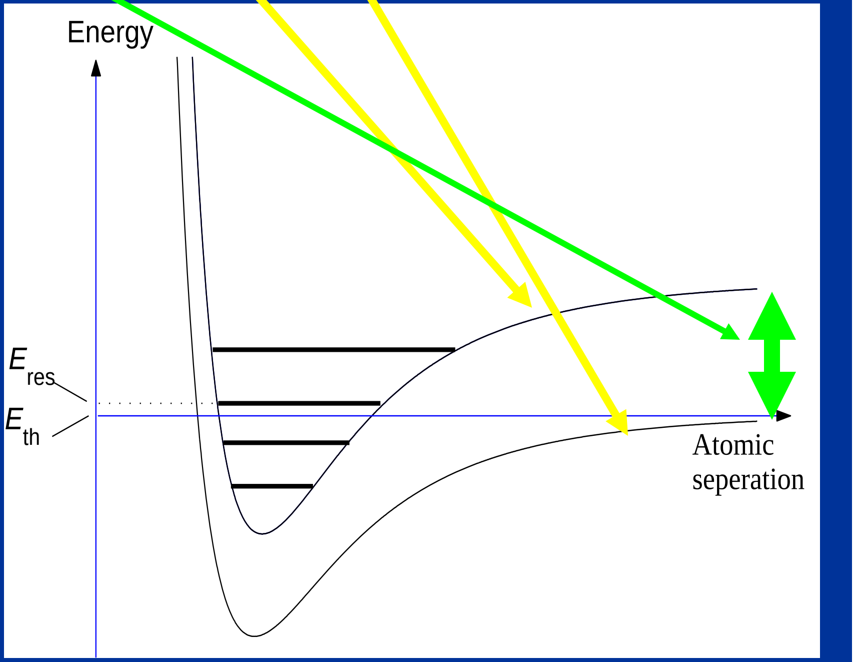
$$V^{hf} = \frac{a_{hf}}{\hbar^2}\vec{S}^{e}\cdot\vec{S}^{n}, \quad V^{Z} = (\gamma_e S_z^{e} - \gamma_n S_z^{n})B$$

Channel coupling

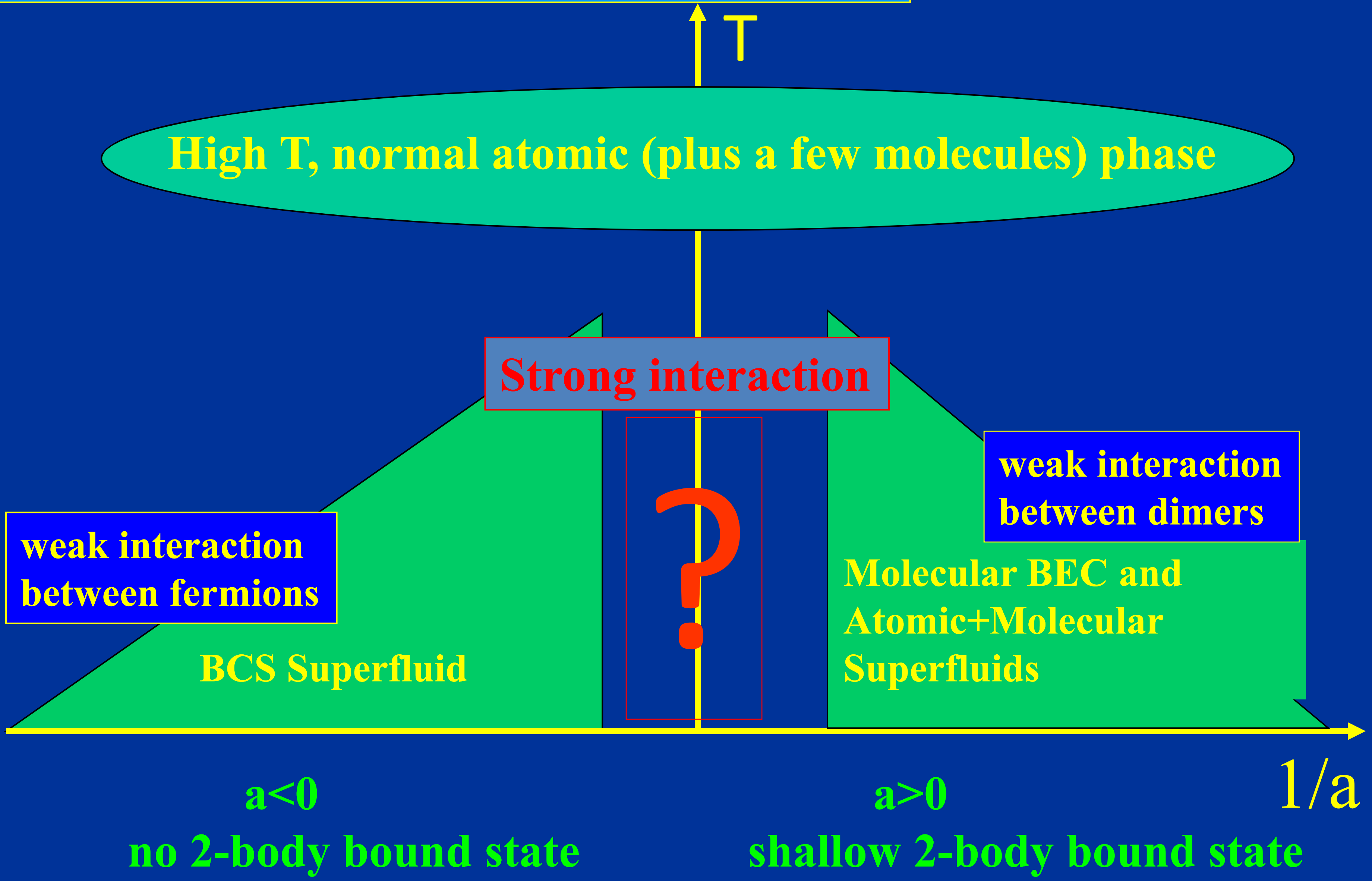
Tiesinga, Verhaar, and Stoof
Phys. Rev. A47, 4114 (1993)



Regal and Jin
Phys. Rev. Lett. 90, 230404 (2003)



Phases of a two species dilute Fermi system in the BCS-BEC crossover



T

High T, normal atomic (plus a few molecules) phase

Strong interaction

?

weak interaction between fermions

BCS Superfluid

weak interaction between dimers

Molecular BEC and Atomic+Molecular Superfluids

1/a

a<0
no 2-body bound state

a>0
shallow 2-body bound state

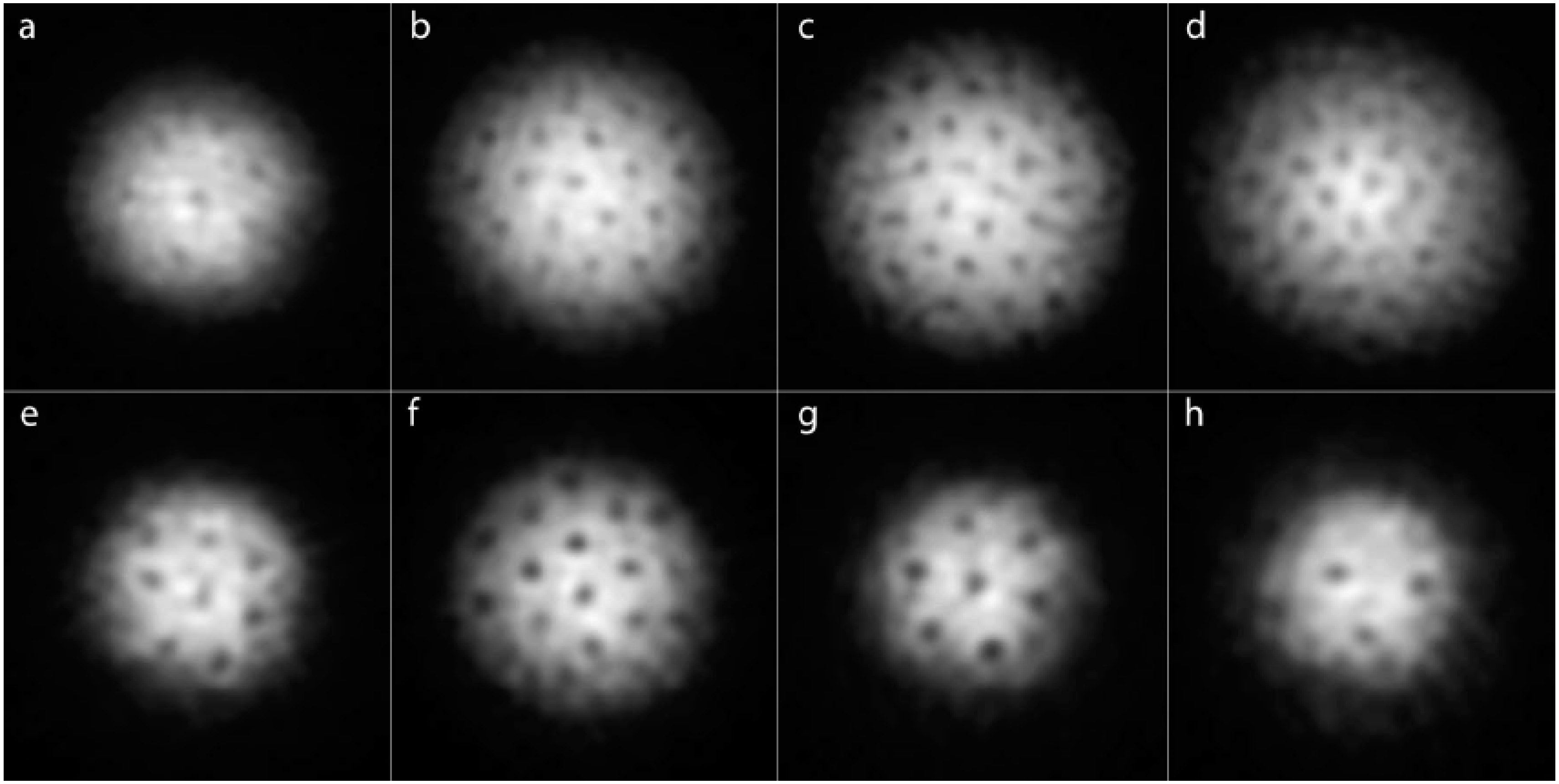


Fig. 2: Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) to 500 ms (b-h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic 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 <u>435</u>, 1047 (2005)

Theoretical tools and features:

- Canonical and Grand Canonical Ensembles
- Hubbard-Stratonovich transformation
- Auxiliary Field Quantum Monte-Carlo
- Absence of Fermion sign problem
- Markov process, Metropolis importance sampling, decorrelation, …
- Renormalization of the two-body interaction
- Spatio- (imaginary) temporal lattice formulation of the problem
- One-particle temperature (Matsubara) propagator, spectral weight function, maximum entropy method/ singular value decomposition method
- Extension of Density Functional Theory to superfluid systems and time-dependent phenomena
- Superfluid to Normal phase transition (second order)
- Off-diagonal long range order, condensate fraction, finite size scaling and extraction of critical temperature
- S- and P-wave superfluidity, induced interactions
  (NB - bare interaction in s-wave only)
- Larkin-Ovchinnikov-Fulde-Ferrell superfluidity (LOFF/FFLO)
- Quantum phase transitions (T=0, first and second order)
- Phase separation
- Pairing gap and pseudo-gap
- Supersolid

Finite Temperatures

Grand Canonical Path-Integral Monte Carlo

$$\hat{H} = \hat{T} + \hat{V} = \int d^3x \left[\psi_\uparrow^\dagger(\vec{x}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \psi_\uparrow(\vec{x}) + \psi_\downarrow^\dagger(\vec{x}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \psi_\downarrow(\vec{x}) \right] - g \int d^3x \, \hat{n}_\uparrow(\vec{x}) \hat{n}_\downarrow(\vec{x})$$

$$\hat{N} = \int d^3x \, \left[\hat{n}_\uparrow(\vec{x}) + \hat{n}_\downarrow(\vec{x}) \right], \qquad \hat{n}_s(\vec{x}) = \psi_s^\dagger(\vec{x}) \psi_s(\vec{x}), \qquad s = \uparrow, \downarrow$$

Trotter expansion (*trotterization* of the propagator)

$$Z(\beta) = \mathrm{Tr} \, \exp\left[-\beta \left(\hat{H} - \mu \hat{N} \right) \right] = \mathrm{Tr} \, \left\{ \exp\left[-\tau \left(\hat{H} - \mu \hat{N} \right) \right] \right\}^{N_\tau}, \qquad \beta = \frac{1}{T} = N_\tau \tau$$

$$E(T) = \frac{1}{Z(T)} \mathrm{Tr} \, \hat{H} \exp\left[-\beta \left(\hat{H} - \mu \hat{N} \right) \right]$$

$$N(T) = \frac{1}{Z(T)} \mathrm{Tr} \, \hat{N} \exp\left[-\beta \left(\hat{H} - \mu \hat{N} \right) \right]$$

No approximations so far, except for the fact that the interaction is not well defined!

Recast the propagator at each time slice and put the system on a 3D-spatial lattice, in a cubic box of side L=N$_s$l, with periodic boundary conditions

$$\exp\left[-\tau\left(\hat{H}-\mu\hat{N}\right)\right]\approx\exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right]\exp(-\tau\hat{V})\exp\left[-\tau\left(\hat{T}-\mu\hat{N}\right)/2\right]+O(\tau^3)$$

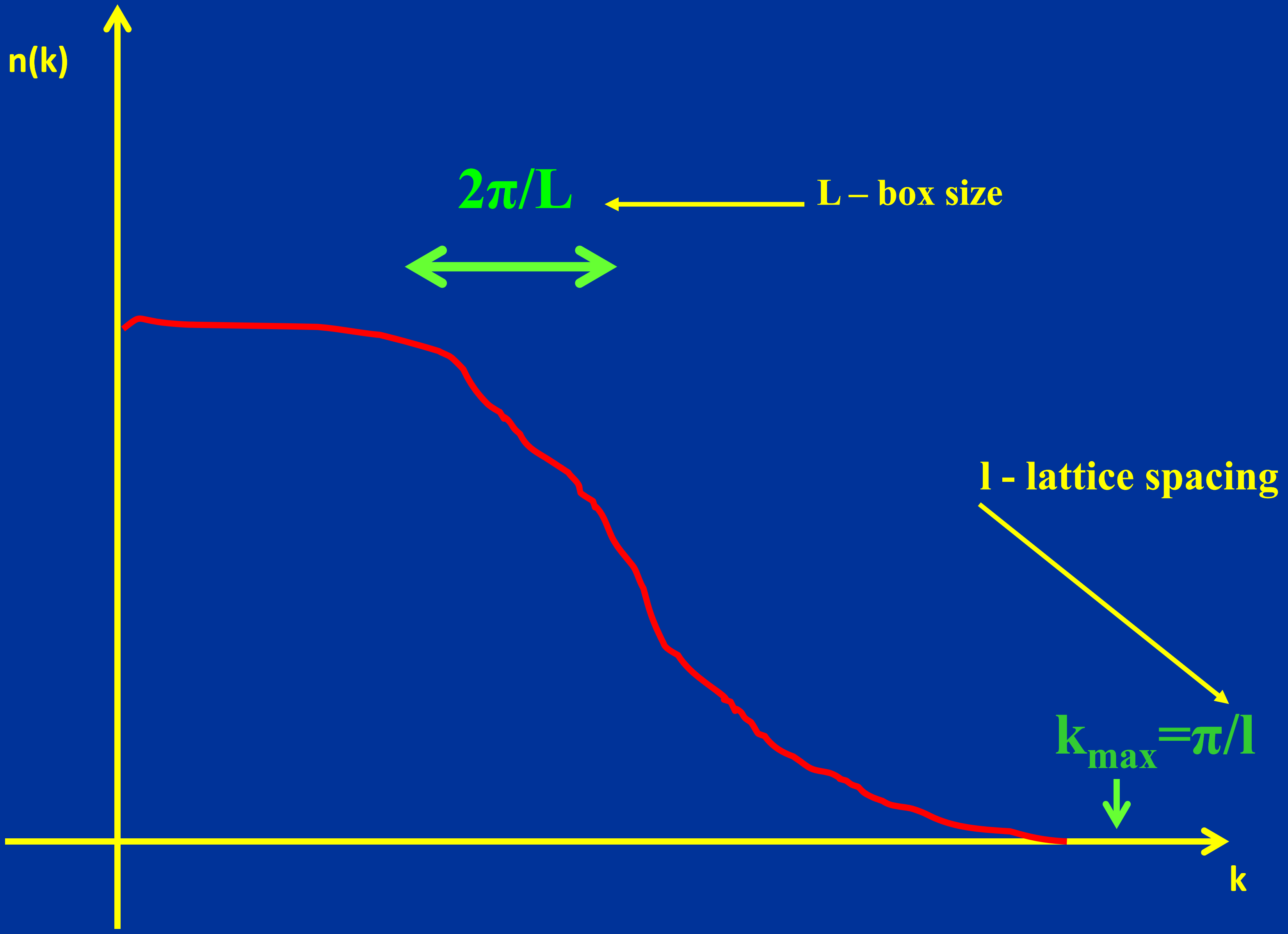
Discrete Hubbard-Stratonovich transformation

$$\exp(-\tau\hat{V})=\prod_{\vec{x}}\sum_{\sigma_\pm(\vec{x})=\pm1}\frac{1}{2}\left[1+\sigma_\pm(\vec{x})A\hat{n}_\uparrow(\vec{x})\right]\left[1+\sigma_\pm(\vec{x})A\hat{n}_\downarrow(\vec{x})\right],\qquad A=\sqrt{\exp(\tau g)-1}$$

σ-fields fluctuate both in space and imaginary time

$$\frac{m}{4\pi\hbar^2 a}=-\frac{1}{g}+\frac{mk_c}{2\pi^2\hbar^2},\qquad k_c<\frac{\pi}{l}$$

Running coupling constant g defined by lattice

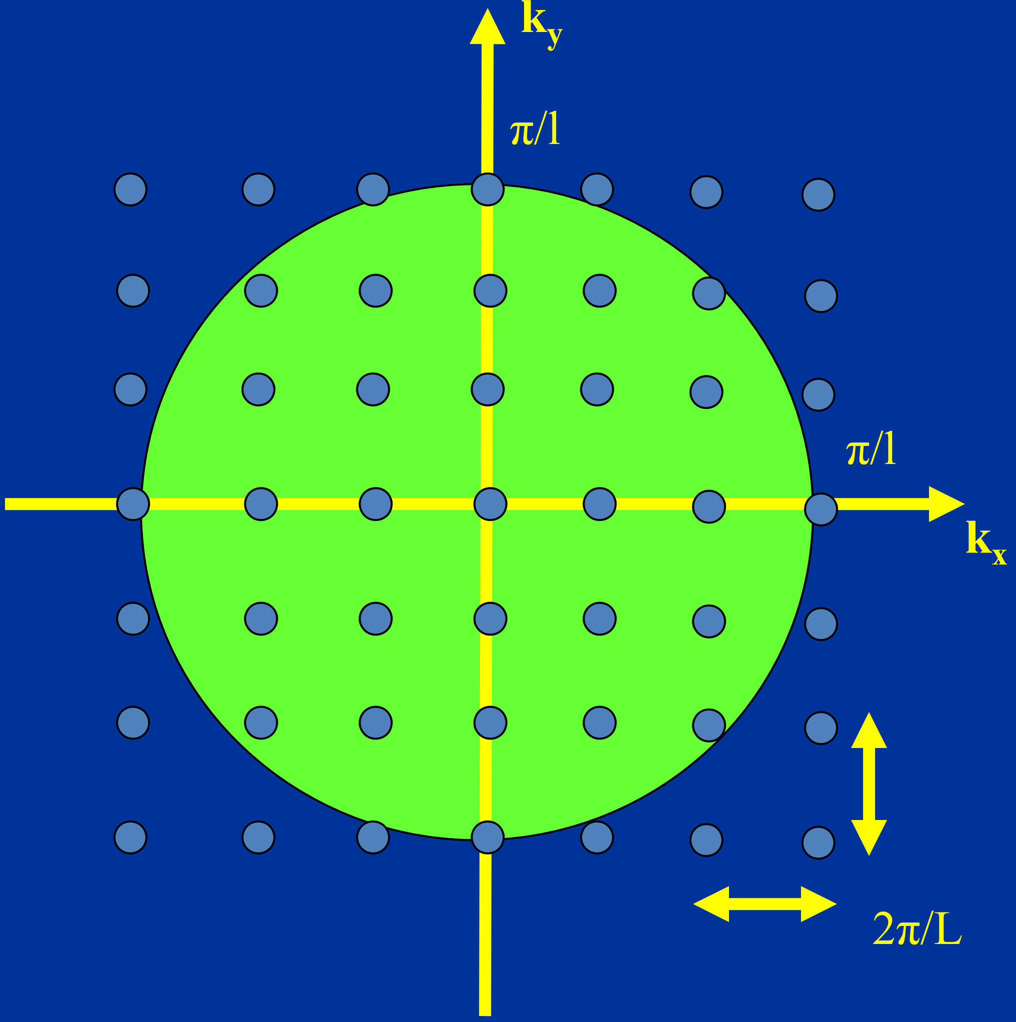


$2\pi/L$ ← **L – box size**

l - lattice spacing

$k_{max}=\pi/l$

How to choose the lattice spacing and the box size?



Momentum space

$$\varepsilon_F,\ \Delta,\ T \ll \frac{\hbar^2\pi^2}{2ml^2}$$

$$\delta\varepsilon > \frac{2\hbar^2\pi^2}{mL^2}$$

$$\varepsilon_F,\ \Delta \gg \frac{2\hbar^2\pi^2}{mL^2}$$

$$\xi \ll L = N_s l$$

$$\delta p > \frac{2\pi\hbar}{L}$$

$$Z(T) = \int \prod_{\vec{x},\tau} D\sigma(\vec{x},\tau)\ \mathrm{Tr}\,\hat{U}(\{\sigma\})$$

$$\hat{U}(\{\sigma\}) = T_{\tau} \prod_{\tau} \exp\{-\tau[\hat{h}(\{\sigma\}) - \mu]\}$$

One-body evolution operator in imaginary time

$$E(T) = \int \frac{\prod_{\vec{x},\tau} D\sigma(\vec{x},\tau)\mathrm{Tr}\,\hat{U}(\{\sigma\})}{Z(T)} \frac{\mathrm{Tr}\left[\hat{H}\hat{U}(\{\sigma\})\right]}{\mathrm{Tr}\,\hat{U}(\{\sigma\})}$$

$$\mathrm{Tr}\,\hat{U}(\{\sigma\}) = \{\det[1 + \hat{U}(\{\sigma\})]\}^2 = \exp[-S(\{\sigma\})] > 0$$

No sign problem!

$$n_{\uparrow}(\vec{x},\vec{y}) = n_{\downarrow}(\vec{x},\vec{y}) = \sum_{k,l<k_c} \varphi_{\vec{k}}(\vec{x}) \left[\frac{\hat{U}(\{\sigma\})}{1 + \hat{U}(\{\sigma\})}\right]_{\vec{k}\,\vec{l}} \varphi^{*}_{\vec{l}}(\vec{y}), \qquad \varphi_{\vec{k}}(\vec{x}) = \frac{\exp(i\vec{k}\cdot\vec{x})}{\sqrt{V}}$$

All traces can be expressed through these single-particle density matrices

More details of the calculations:

- Typical lattice sizes used from $\underline{8^3 \text{ x } 300}$ (high Ts) to $\underline{8^3 \text{ x } 1800}$ (low Ts)

- Effective use of FFT(W) makes all imaginary time propagators diagonal (either in real space or momentum space) and there is no need to store large matrices

- Update field configurations using the Metropolis importance sampling algorithm

- Change randomly at a fraction of all space and time sites the signs the auxiliary fields $\sigma(x,\tau)$ so as to maintain a running average of the acceptance rate between 0.4 and 0.6

- Thermalize for 50,000 – 100,000 MC steps or/and use as a start-up field configuration a $\sigma(x,\tau)$-field configuration from a different T

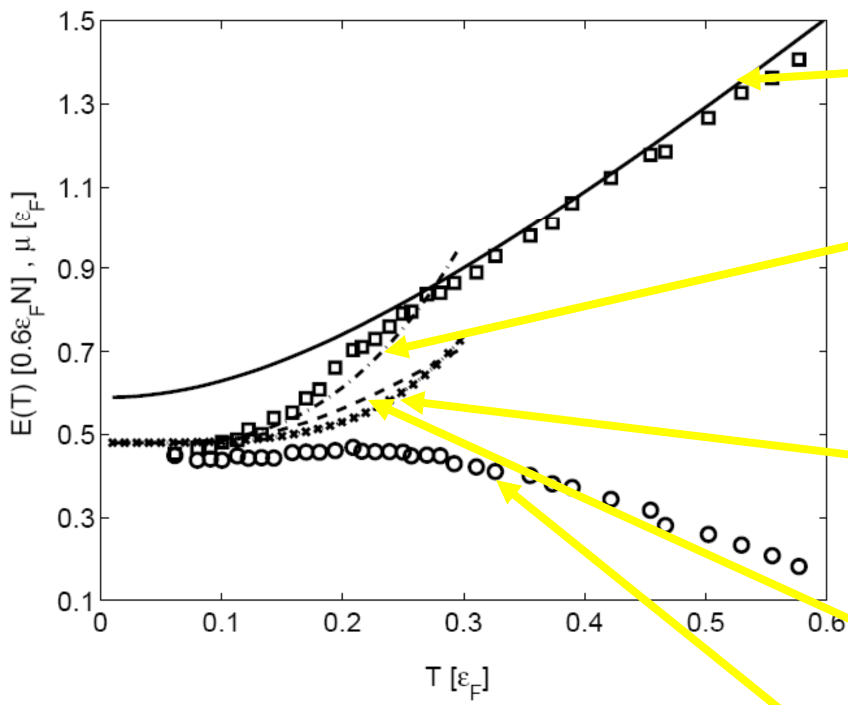
- At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics

- Use 100,000-2,000,000 $\sigma(x,\tau)$- field configurations for calculations

- MC correlation “time” ≈ 250 – 300 time steps at $T \approx T_c$

a = ±∞

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



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)

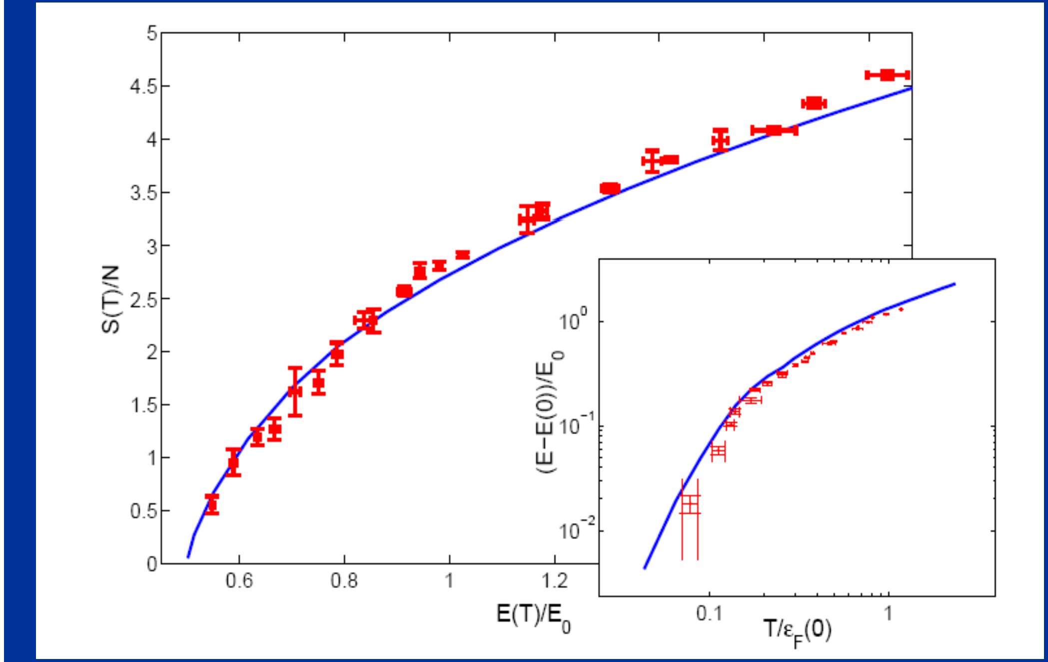
$$E_{\text{phonons}}(T) = \frac{3}{5}\varepsilon_F N \;\frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}}\left(\frac{T}{\varepsilon_F}\right)^4, \qquad \xi_s \approx 0.44$$

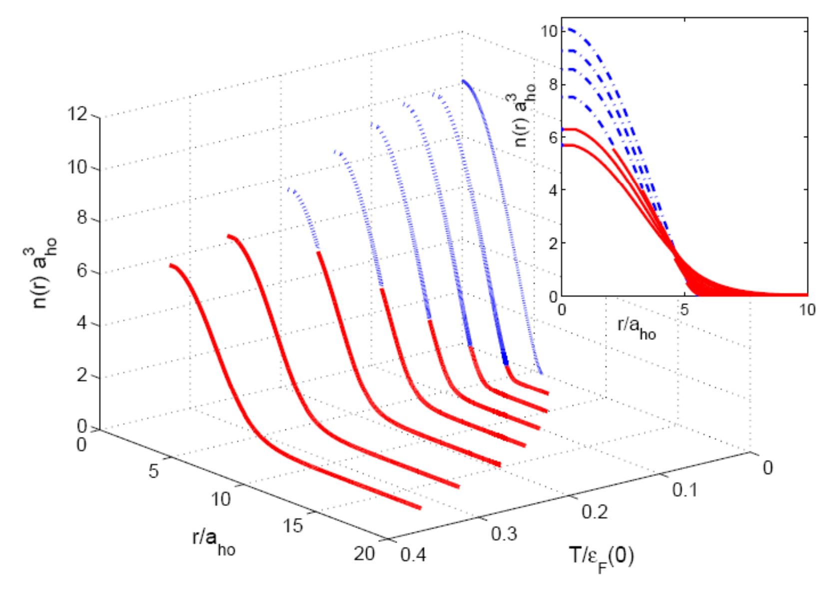
$$E_{\text{quasi-particles}}(T) = \frac{3}{5}\varepsilon_F N \;\frac{5}{2}\sqrt{\frac{2\pi\Delta^3 T}{\varepsilon_F^4}}\exp\left(-\frac{\Delta}{T}\right)$$

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

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)**

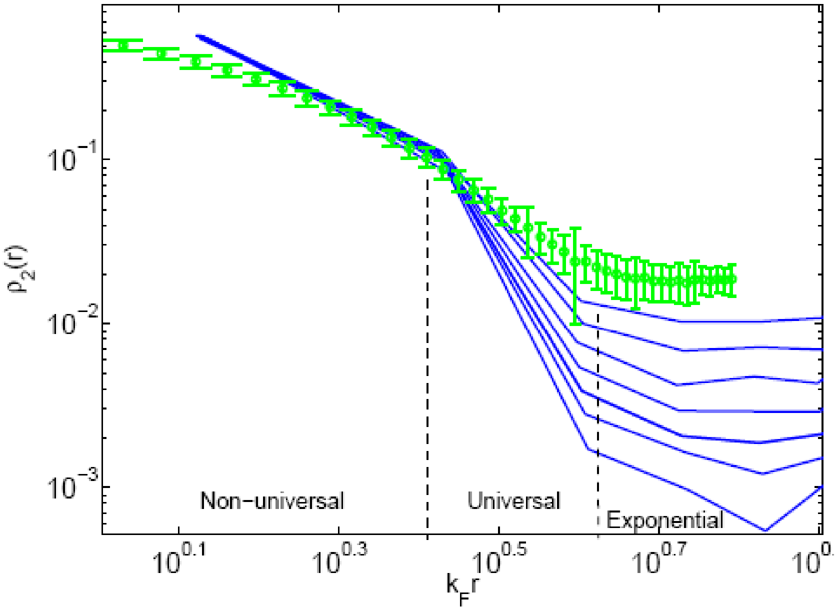


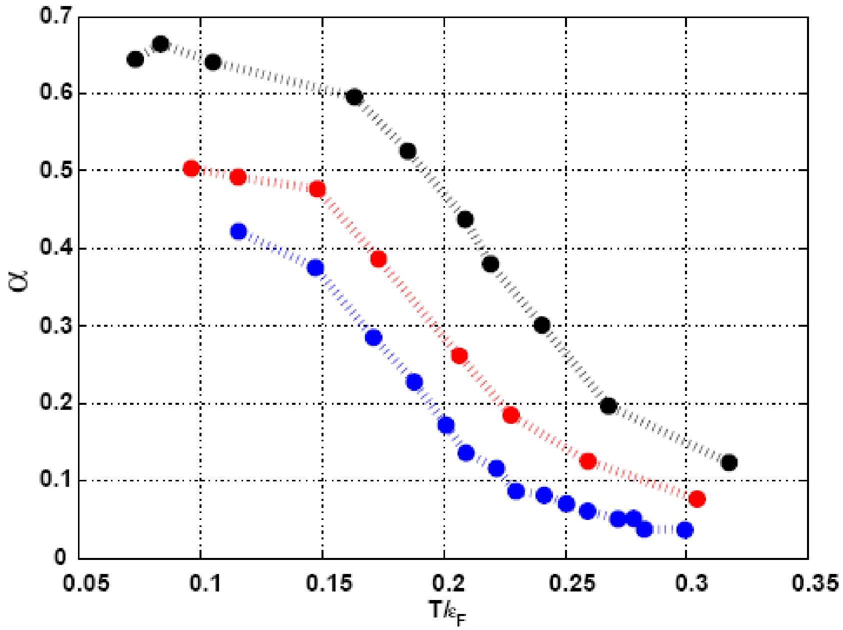


***Ab initio* theory (no free parameters)**

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

Long range order, superfluidity and condensate fraction
O. Penrose (1951), O. Penrose and L. Onsager (1956), C.N. Yang (1962)



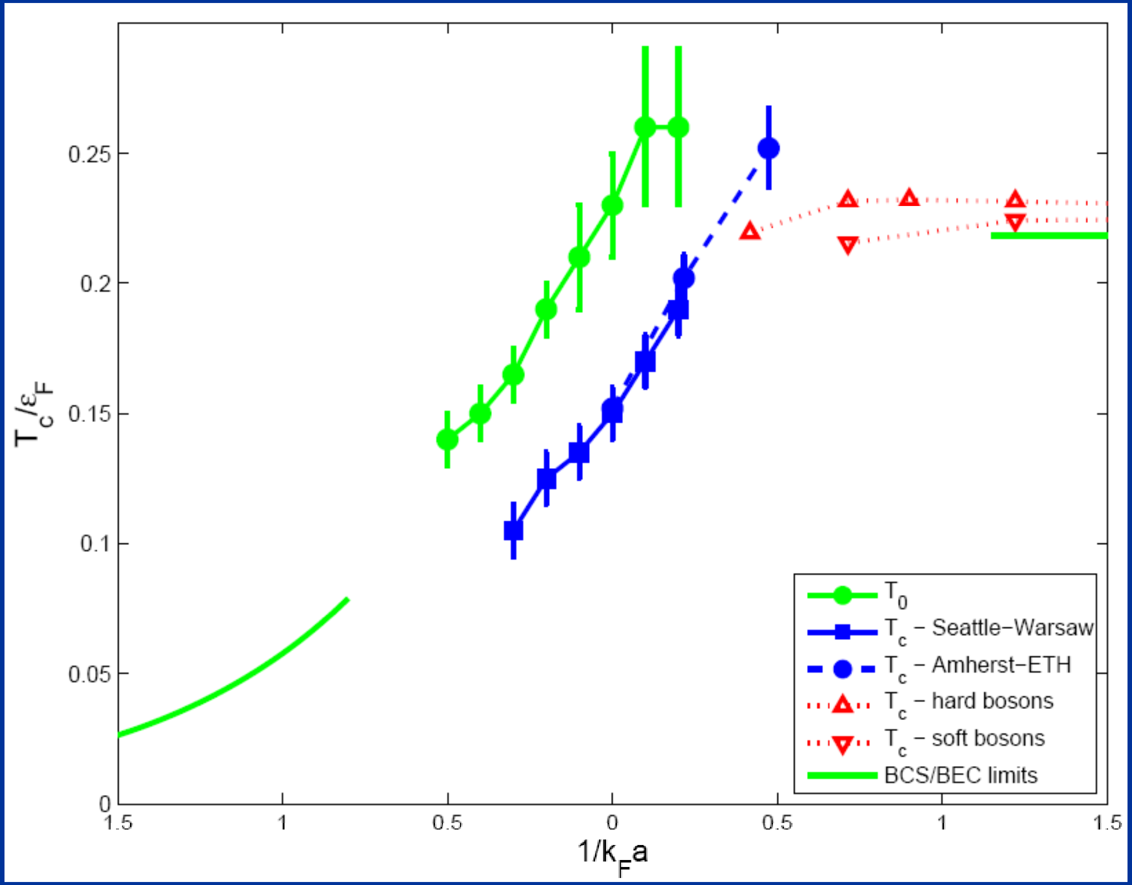


$$g_2(\vec{r}) = \left(\frac{2}{N}\right)^2 \int d^3\vec{r}_1 \int d^3\vec{r}_2 \left\langle \psi_\uparrow^\dagger(\vec{r}_1+\vec{r})\psi_\downarrow^\dagger(\vec{r}_2+\vec{r})\psi_\downarrow(\vec{r}_2)\psi_\uparrow(\vec{r}_2)\right\rangle$$

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

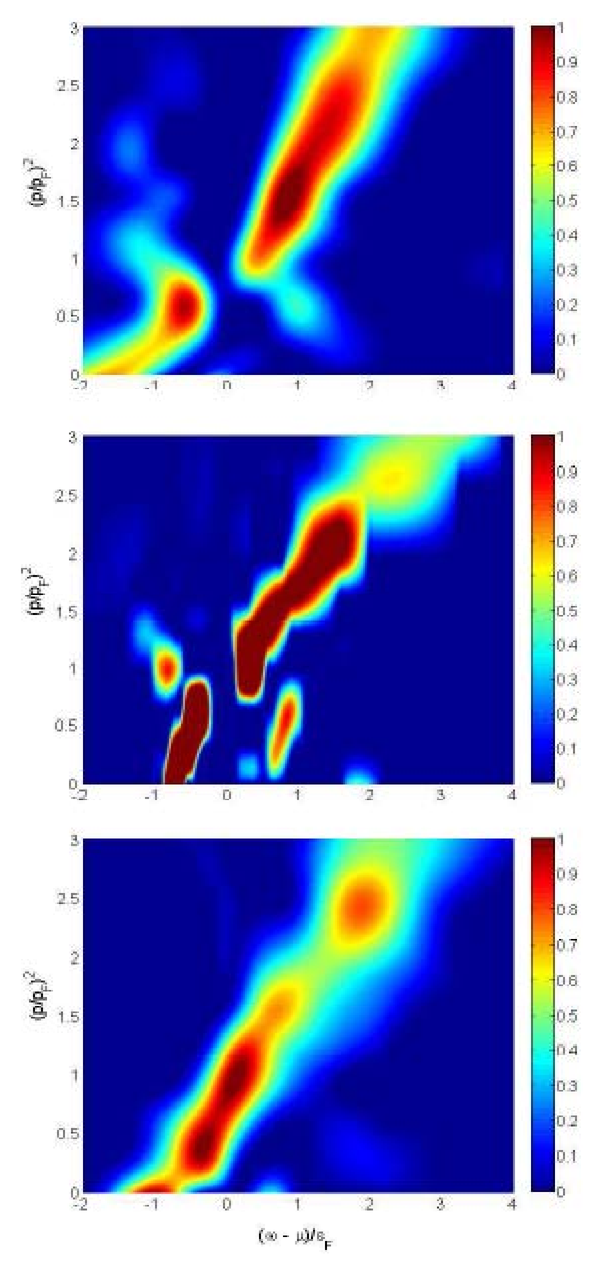
Bulgac, Drut, and Magierski, Phys. Rev. A 78, 023625 (2008)

Critical temperature for superfluid to normal transition

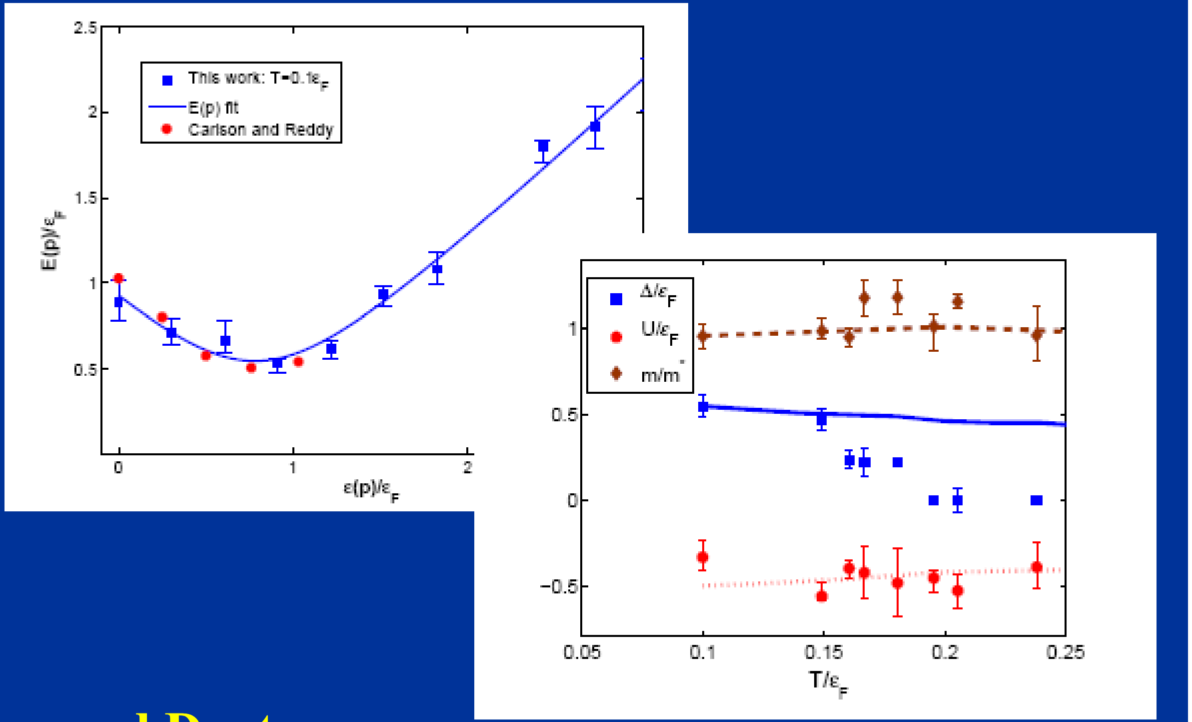


Bulgac, Drut, and Magierski, Phys. Rev. A 78, 023625 (2008)

Amherst-ETH: Burovski et al. Phys. Rev. Lett. 101, 090402 (2008)
Hard and soft bosons: Pilati et al. PRL 100, 140405 (2008)



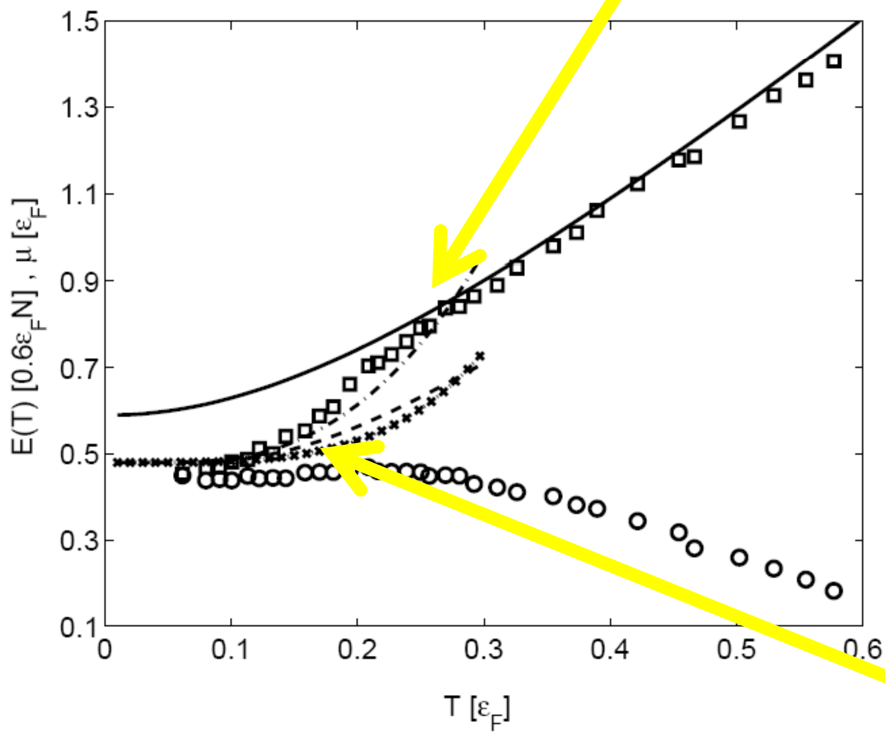
$$G(p,\tau)=\frac{1}{Z}\mathrm{Tr}\left\{\exp\left[-(\beta-\tau)(H-\mu N)\right]\psi^{\dagger}(p)\times\right.$$
$$\left.\exp\left[-\tau(H-\mu N)\right]\psi(p)\right\}$$
$$=-\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega A(p,\omega)\frac{\exp(-\omega\tau)}{1+\exp(-\omega\beta)}$$

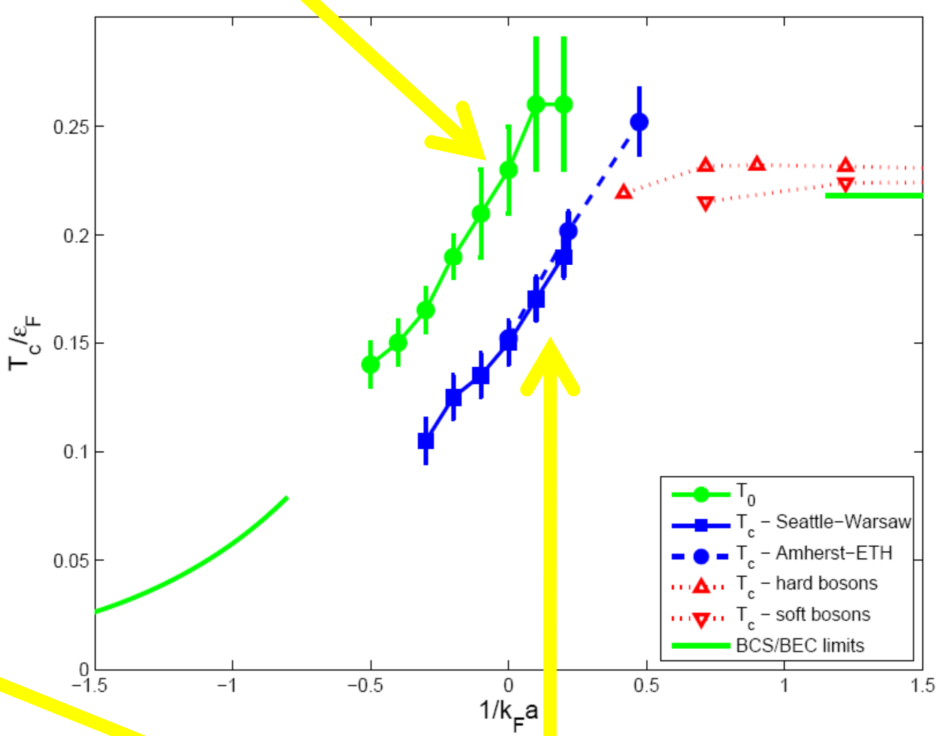


Magierski, Wlazlowski, Bulgac, and Drut
arXiv:0801.1504v3

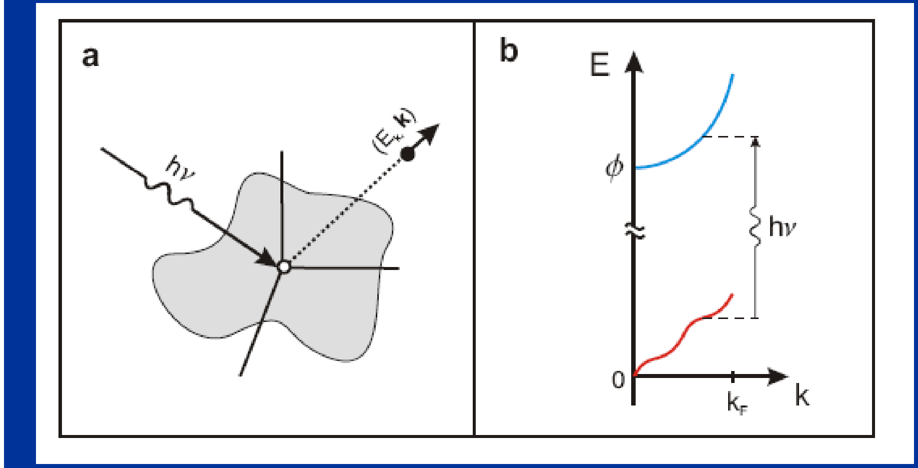
The pseudo-gap vanishes at T_0

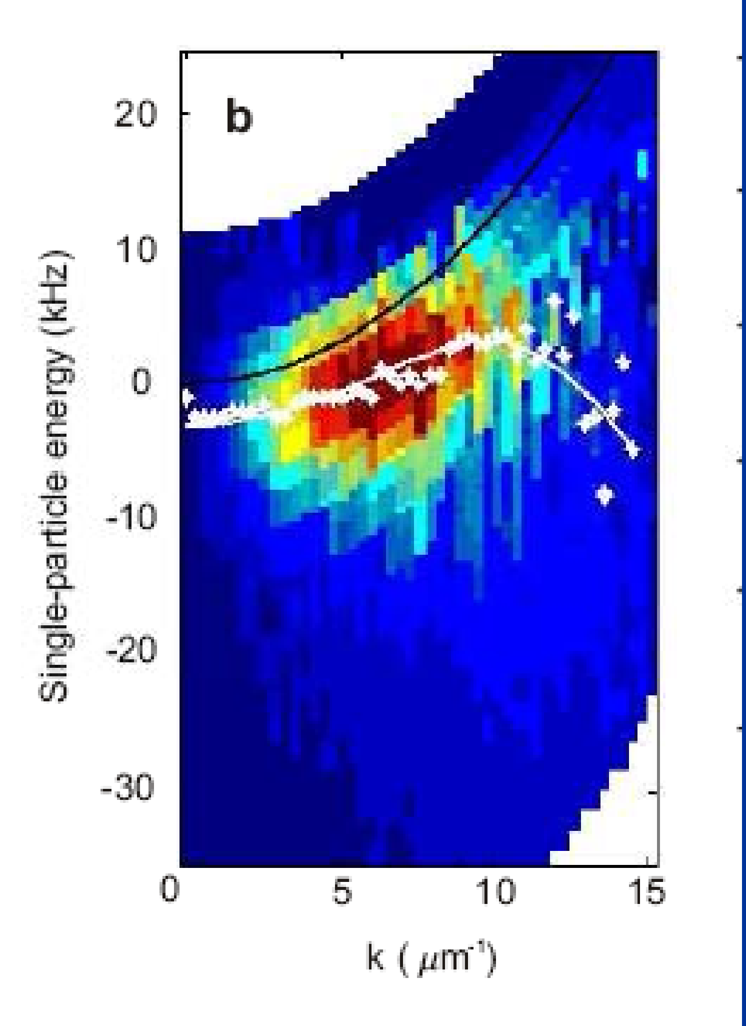
Vanishing of pseudogap





Superfluid to Normal phase transition





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

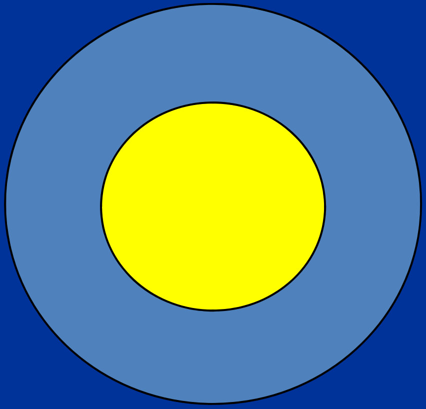
Using photoemission spectroscopy to probe a strongly interacting Fermi gas
Stewart, Gaebler, and Jin, Nature, 454, 744 (2008)

Until now we kept the numbers of spin-up
and spin-down equal.

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

(In particular this is what one expects to happen in color superconductivity, due to a heavier strange quark)

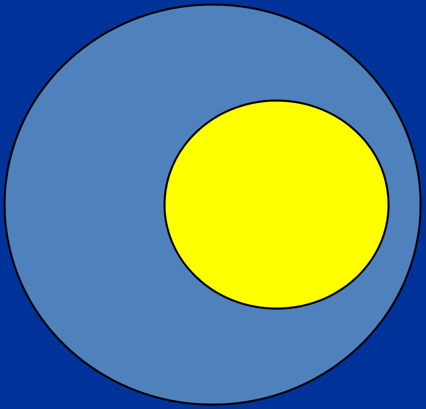
What theory tells us?



Green – Fermi sphere of spin-up fermions

Yellow – Fermi sphere of spin-down fermions

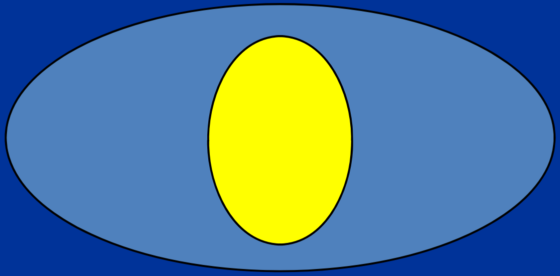
If $\left|\mu_\uparrow - \mu_\downarrow\right| < \dfrac{\Delta}{\sqrt{2}}$ the same solution as for $\mu_\uparrow = \mu_\downarrow$



LOFF/FFLO solution (1964)

Pairing gap becomes a spatially varying function

Translational invariance broken



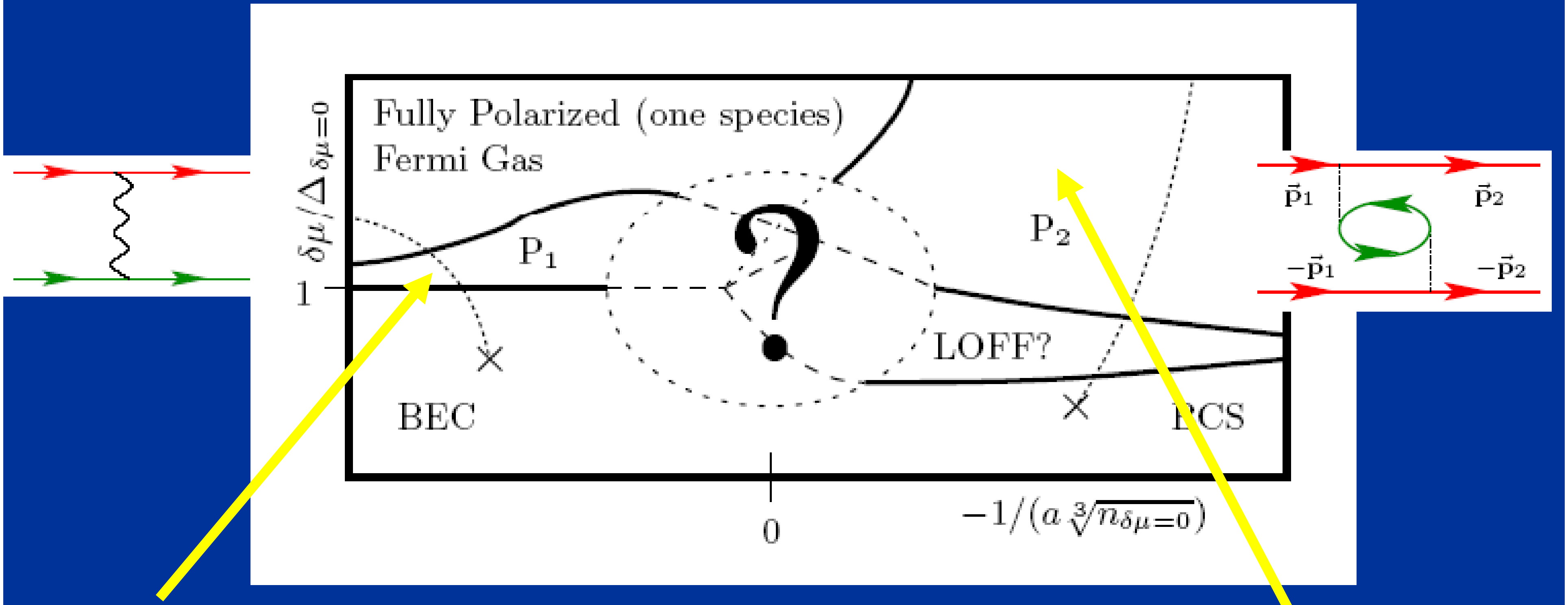
Muether and Sedrakian (2002)

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

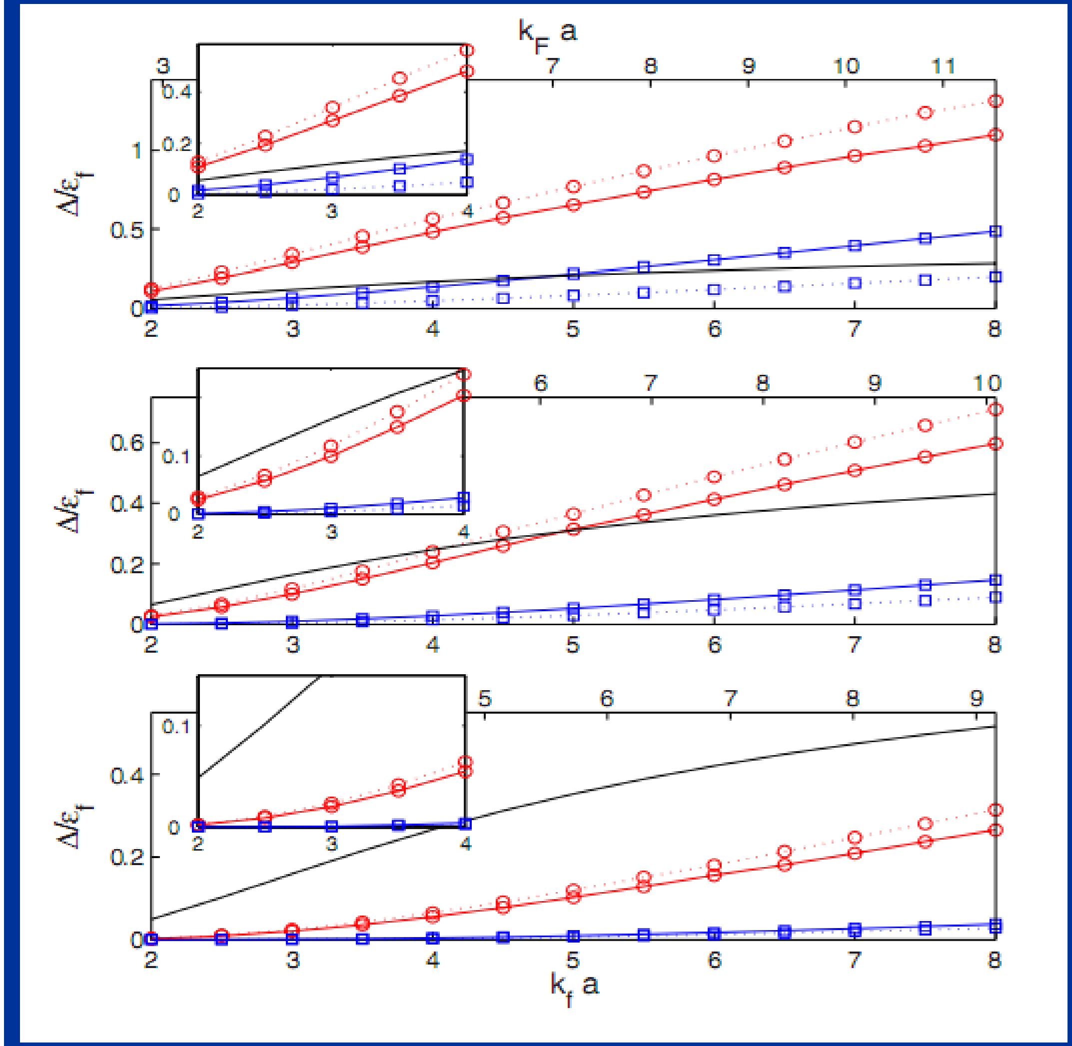


One Bose superfluid coexisting with one P-wave Fermi superfluid

Two coexisting P-wave Fermi superfluids

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

Going beyond the naïve BCS approximation



Eliashberg approx. (red)

BCS approx. (black)

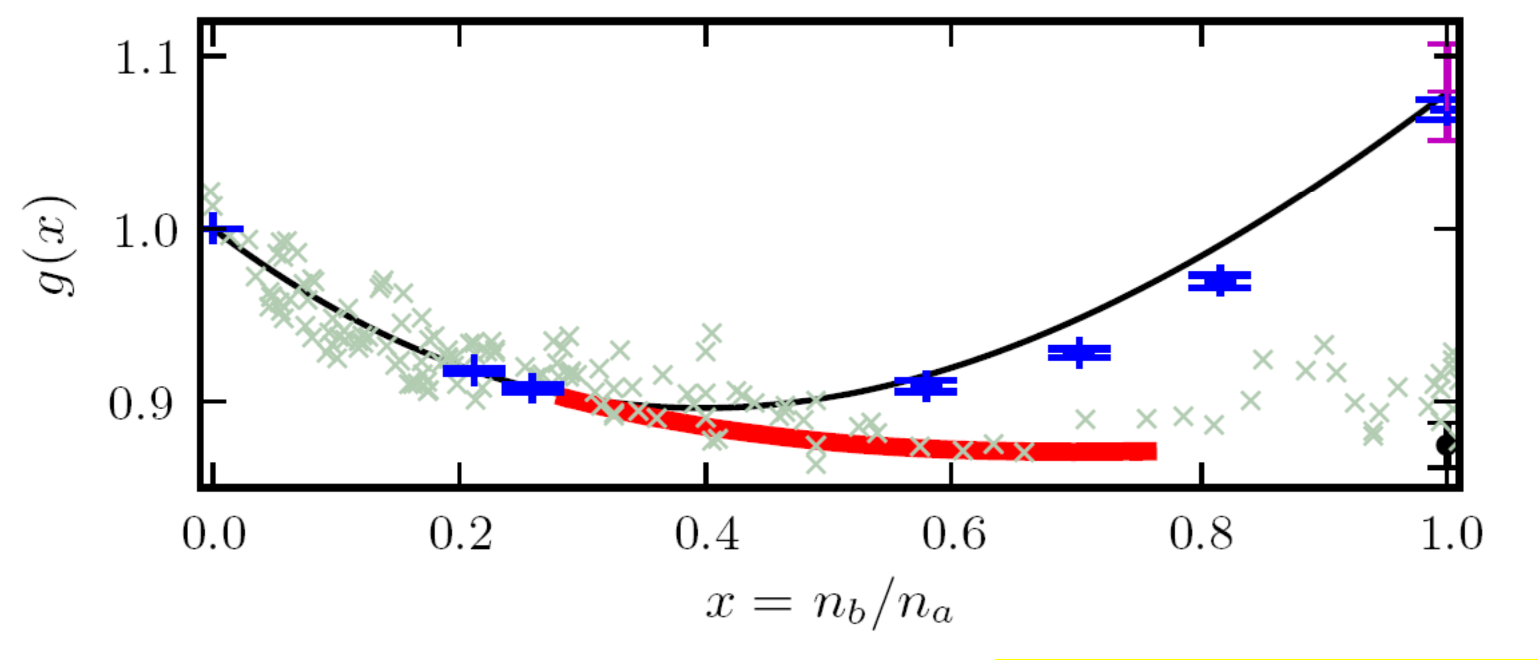
Full momentum and frequency dependence of the self-consistent equations (red)

Bulgac and Yoon, Phys. Rev. A 79, 053625 (2009)

How to treat inhomogeneous systems?

- Monte Carlo
- Density Functional Theory (DFT)
  one needs to find an Energy Density Functional (EDF)

A refined EOS for spin unbalanced systems



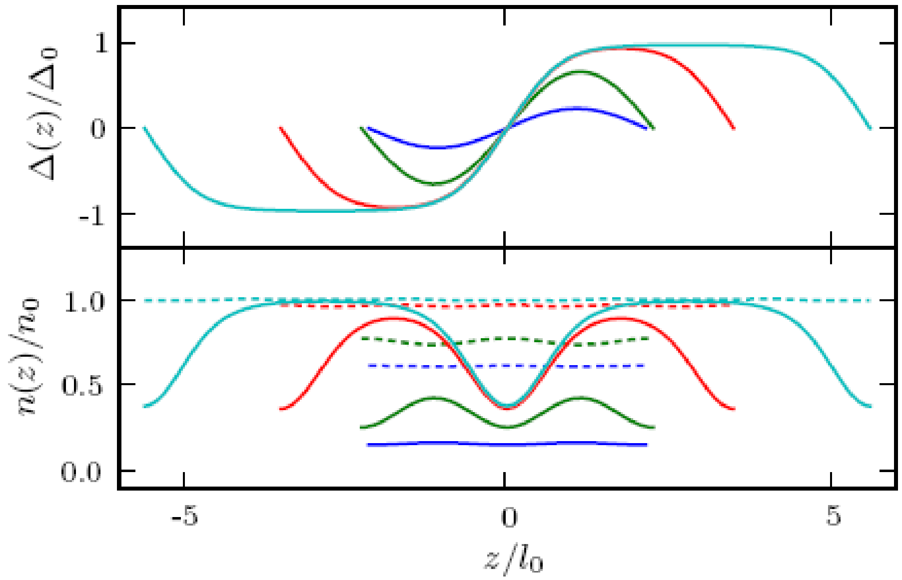
Bulgac and Forbes,
Phys. Rev. Lett. 101, 215301 (2008)

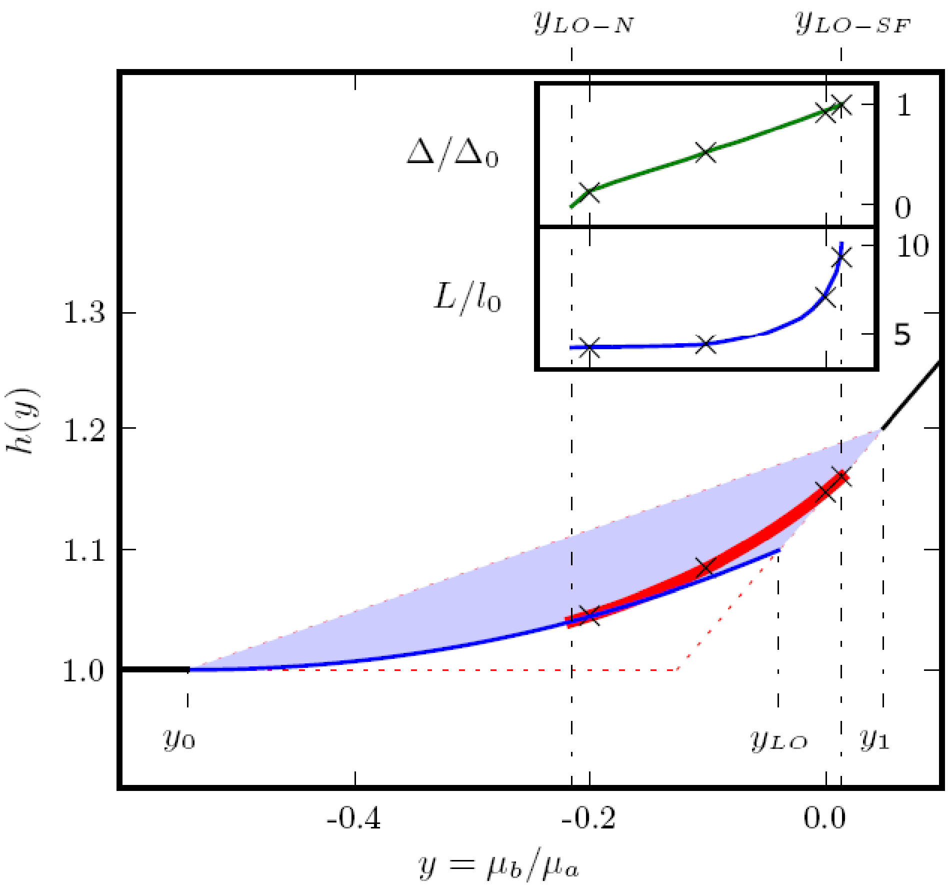
Red line: Larkin-Ovchinnikov phase

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)

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

A Unitary Fermi Supersolid:
the Larkin-Ovchinnikov phase





Bulgac and Forbes
PRL 101, 215301 (2008)

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

Time Dependent Phenomena and Formalism

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 single-particle 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

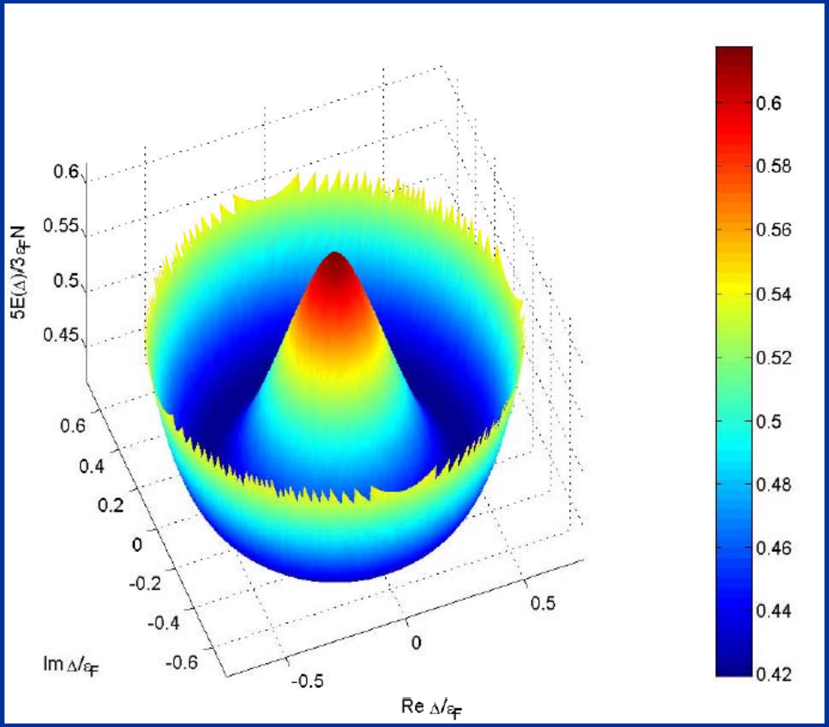
$$E(t) = \int d^3r \ \left[\ \varepsilon(n(\vec{r},t), \tau(\vec{r},t), \nu(\vec{r},t), \underline{\vec{j}(\vec{r},t)}) + V_{ext}(\vec{r},t)n(\vec{r},t) + \ldots \right]$$

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

For time-dependent phenomena one has to add currents.

A very rare excitation mode: the Higgs pairing mode.

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



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

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

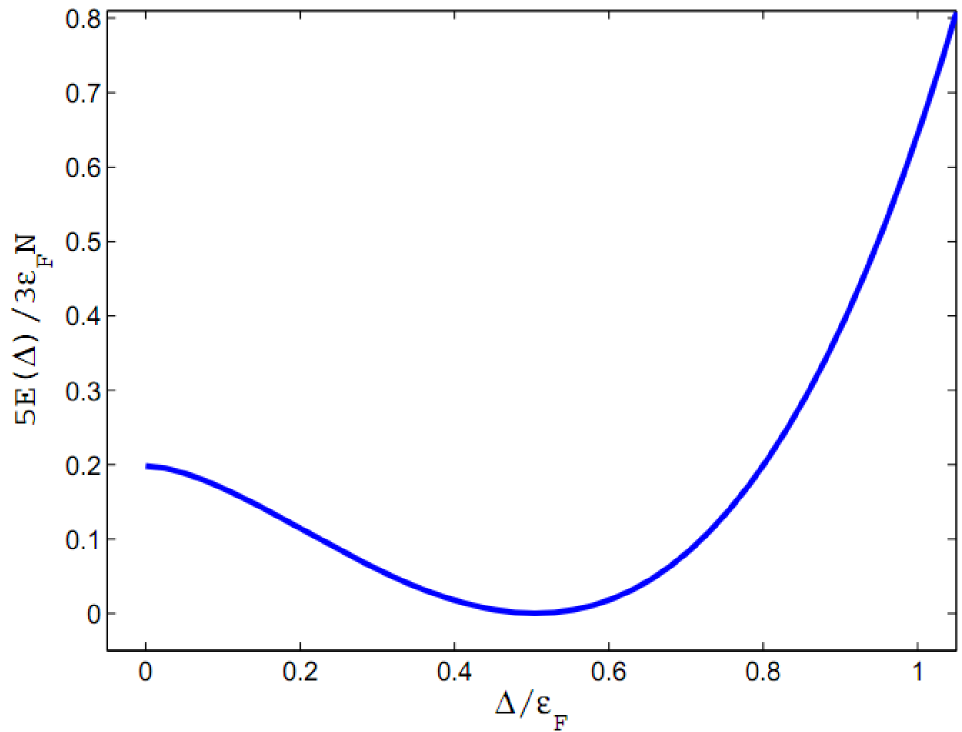
$$i\hbar\dot{\Psi}(\vec{r},t) = -\frac{\hbar^{2}\Delta}{4m}\Psi(\vec{r},t) + U\left(\left|\Psi(\vec{r},t)\right|^{2}\right)\Psi(\vec{r},t)$$

Quantum hydrodynamics

“Landau-Ginzburg” equation

Higgs mode

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

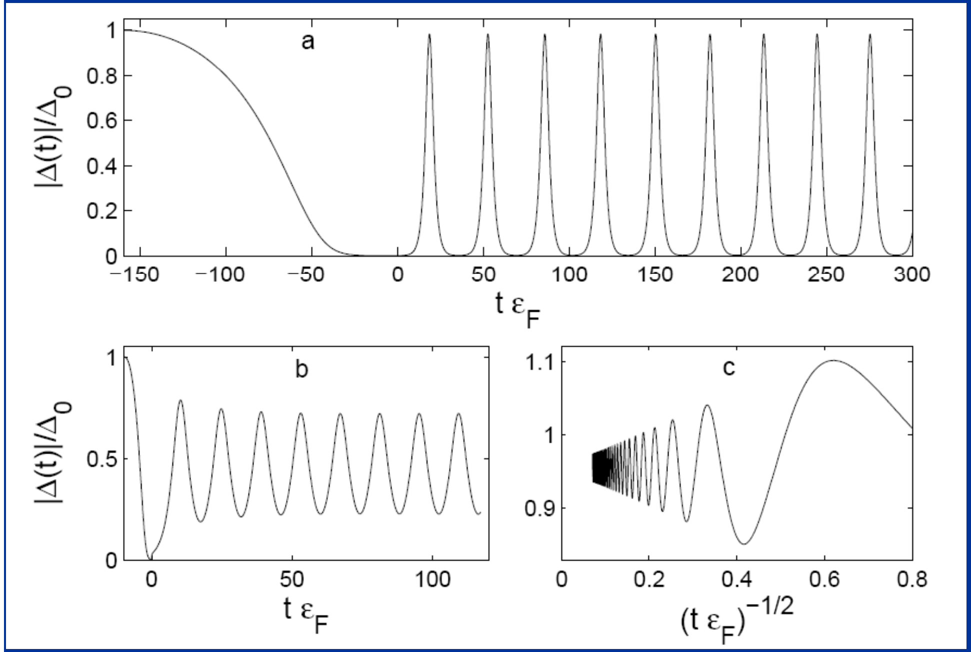


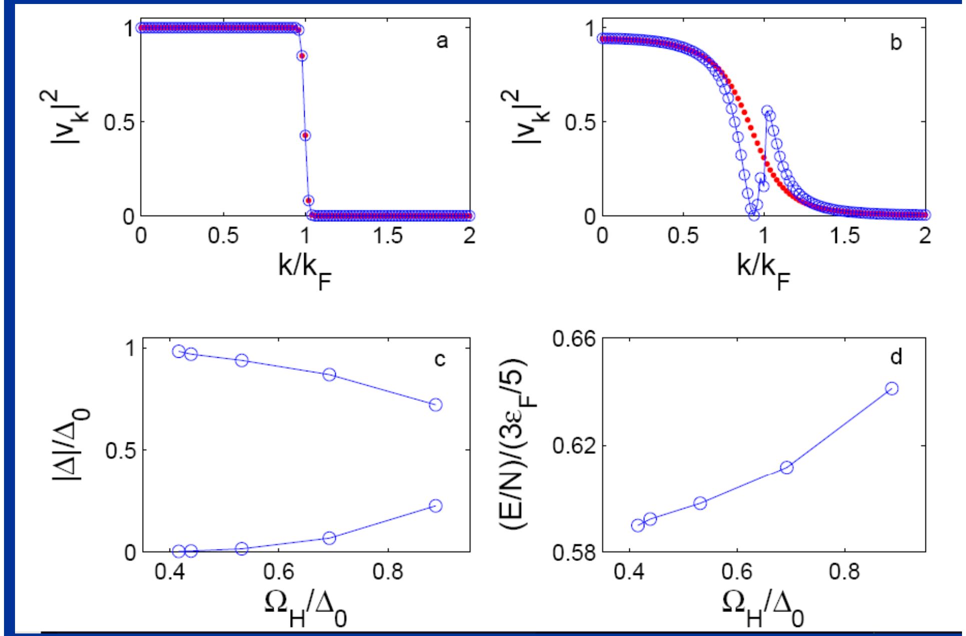
$$\hbar\Omega_H = 2\Delta_0$$

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

Tool: TD DFT extension to superfluid systems (TD-SLDA)





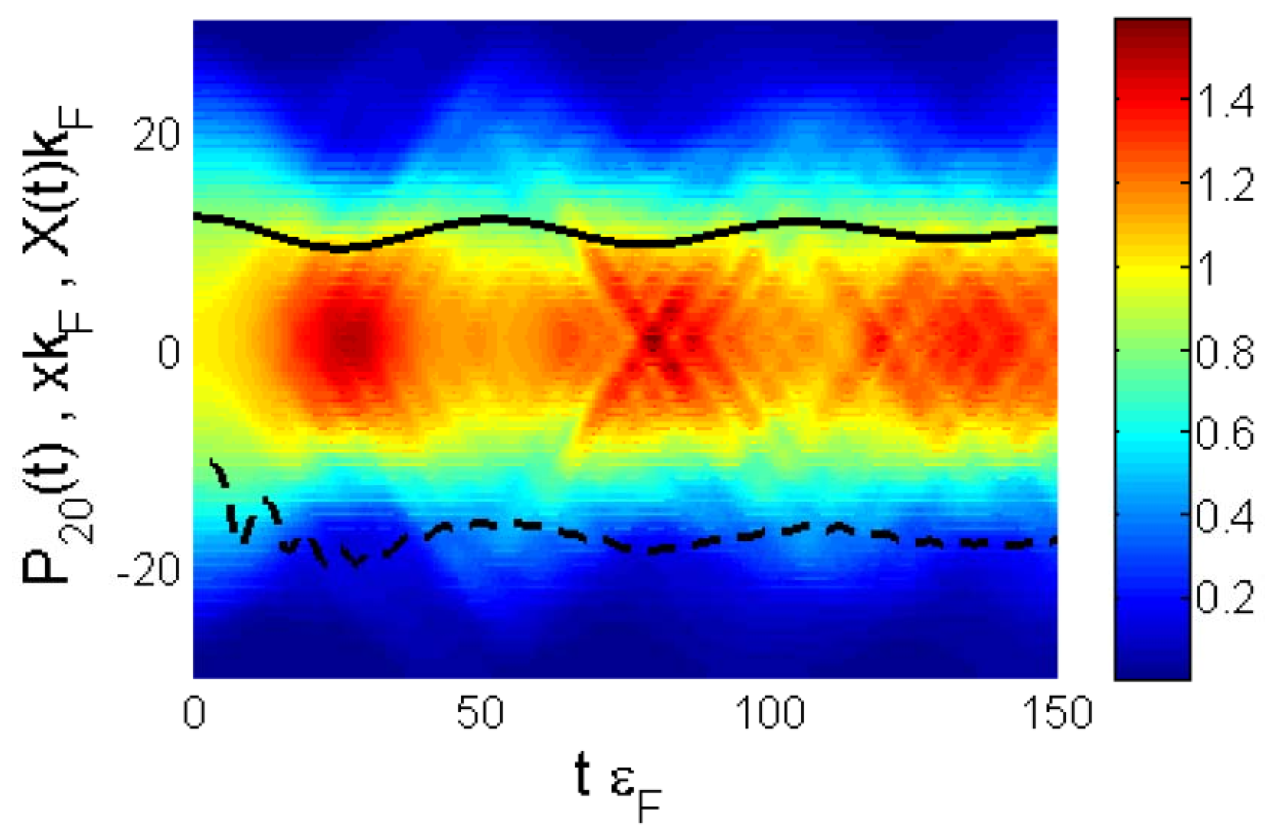
- All these modes have a very low frequency below the pairing gap and a very large amplitude and excitation energy as well

- 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)

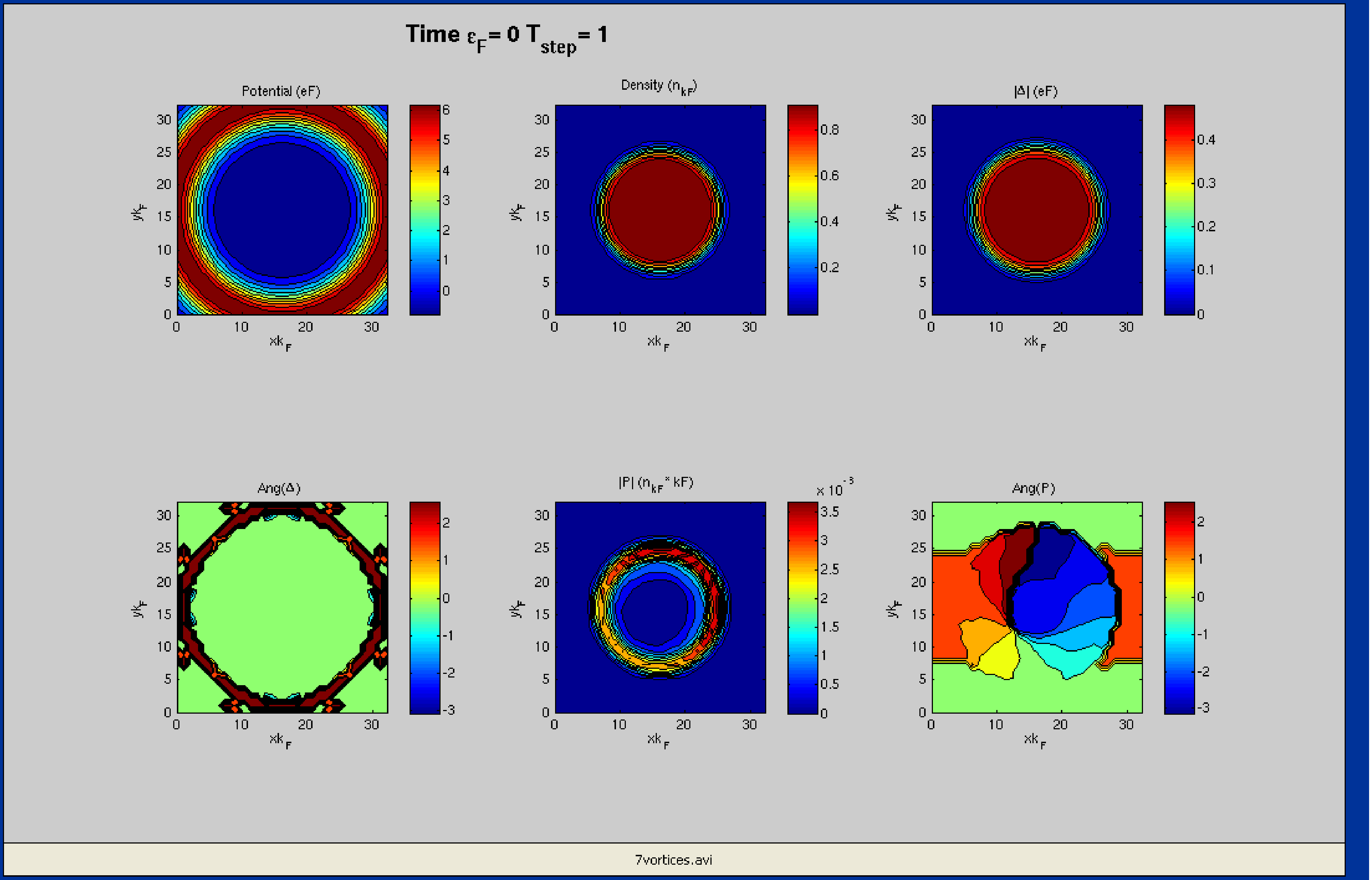
New qualitative excitation mode of a superfluid Fermi system (non-spherical Fermi momentum distribution)



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)



Vortex generation and dynamics, see more movies at
http://www.phys.washington.edu/groups/qmbnt/vortices_movies.html

In case you've got lost: *What did I talk about so far?*

What is a unitary Fermi gas?

Thermodynamic properties, BCS-BEC crossover

Pairing gap and pseudo-gap

EOS for spin imbalanced systems

P-wave pairing, symbiotic superfluids

Unitary Fermi supersolid: the Larkin-Ovchinnikov phase

Time-dependent phenomena, vortex generation, pairing Higgs mode