

What do we know about the unitary Fermi gas?

Aurel Bulgac

University of Washington, Seattle, WA

Collaborators: **Joaquin E. Drut** (Seattle, now at OSU, Columbus)
Michael McNeil Forbes (Seattle, now at LANL)
Yuan Lung (Alan) Luo (Seattle)
Piotr Magierski (Warsaw/Seattle)
Kenneth J. Roche (ORNL, now at PNNL-Seattle)
Achim Schwenk (Seattle, now at TRIUMF)
Gabriel Wlazlowski (Warsaw)
Sukjin Yoon (Seattle)

Funding: DOE grants No. DE-FG02-97ER41014 (UW NT Group)
DE-FC02-07ER41457 (SciDAC-UNEDF)

Slides to be posted at: <http://www.phys.washington.edu/users/bulgac/>

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 $1/2$ fermions interacting via a zero-range, infinite scattering-length contact interaction.

What are the scattering length and the effective range?

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

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

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

Let us consider a very old 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 1/2 requires some hard work.

Let us turn now to dilute fermion matter

The ground state energy is given by a function:

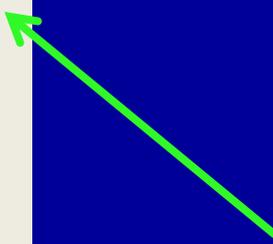
$$E_{gs} = f(N, V, \hbar, m, a, r_0)$$

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

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

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

Pure number
(dimensionless)



What are the ground state properties of the many-body system composed of spin $1/2$ 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 !
- **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 !

$$E_{gs} = \frac{3}{5} \varepsilon_F N \times \xi \quad \Delta = \varepsilon_F \times \zeta$$
$$\xi = 0.40(1), \quad \zeta = 0.50(1)$$

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!

$$n r_0^3 \ll 1$$

$$n |a|^3 \gg 1$$

n - number density

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

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 $T_c \approx 10^{-12} - 10^{-9} \text{ eV}$
- ✓ Liquid ^3He $T_c \approx 10^{-7} \text{ eV}$
- ✓ Metals, composite materials $T_c \approx 10^{-3} - 10^{-2} \text{ eV}$
- ✓ Nuclei, neutron stars $T_c \approx 10^5 - 10^6 \text{ eV}$
- QCD color superconductivity $T_c \approx 10^7 - 10^8 \text{ eV}$

units ($1 \text{ eV} \approx 10^4 \text{ K}$)

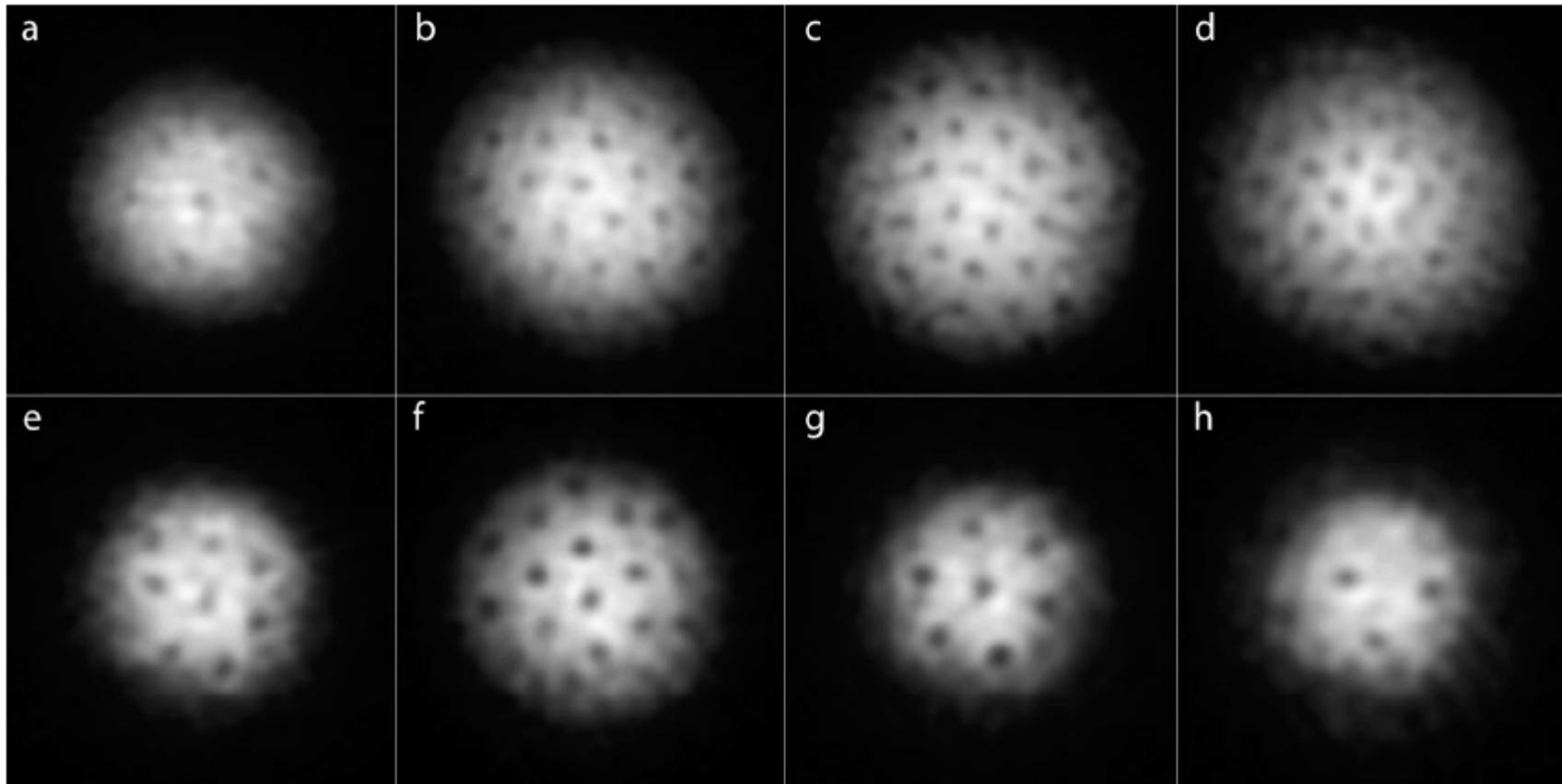


Fig. 2: Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) to 500 ms (b-h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic 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 $880 \mu\text{m} \times 880 \mu\text{m}$.

How we handle Finite Temperatures?

Grand Canonical Path-Integral Monte Carlo

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

Trotter expansion

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

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

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

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

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

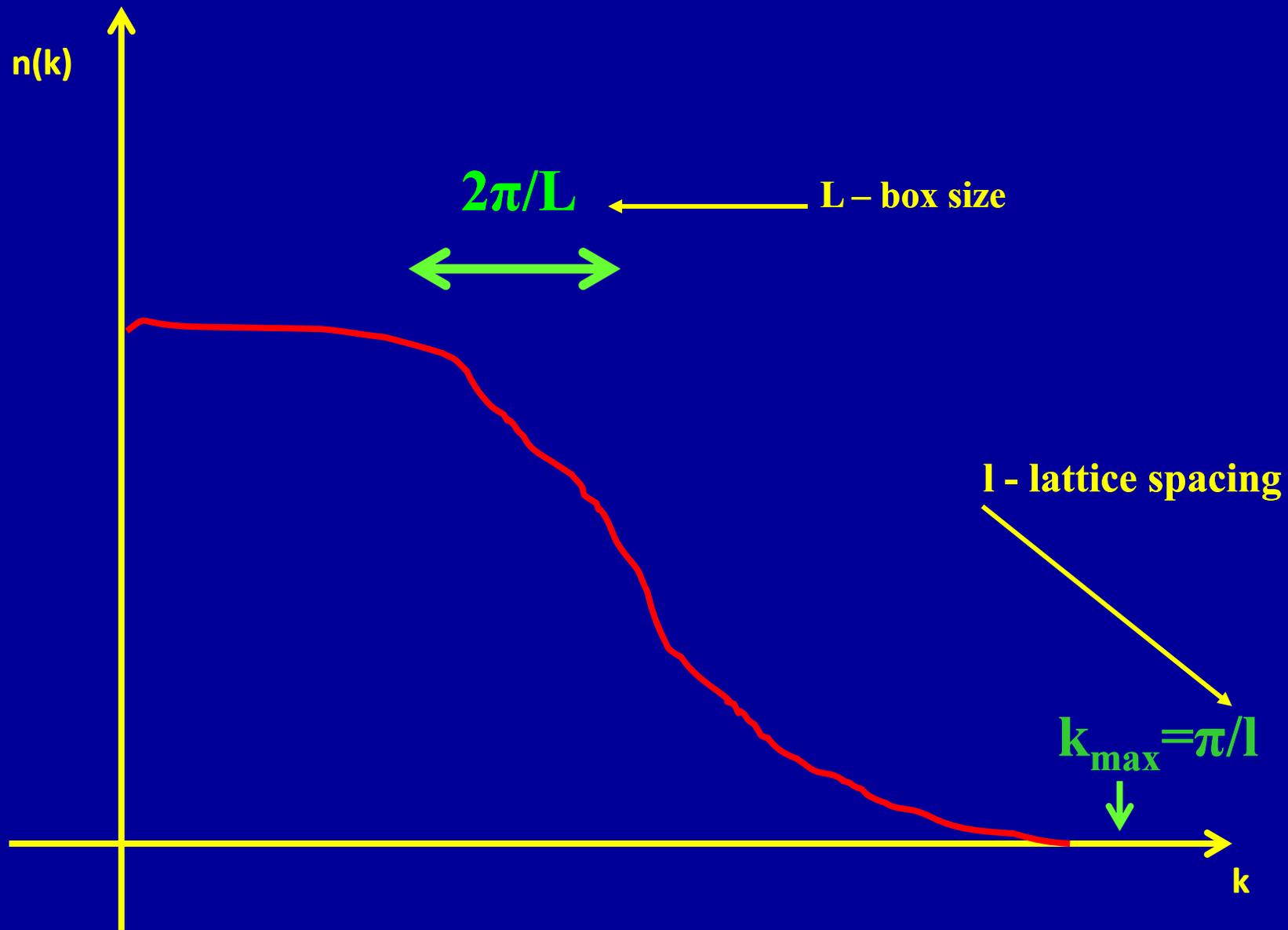
Discrete Hubbard-Stratonovich transformation

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

σ -fields fluctuate both in space and imaginary time

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

Running coupling constant g defined by lattice



How to choose the lattice spacing and the box size?

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

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

One-body evolution operator in imaginary time

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

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

No sign problem!

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

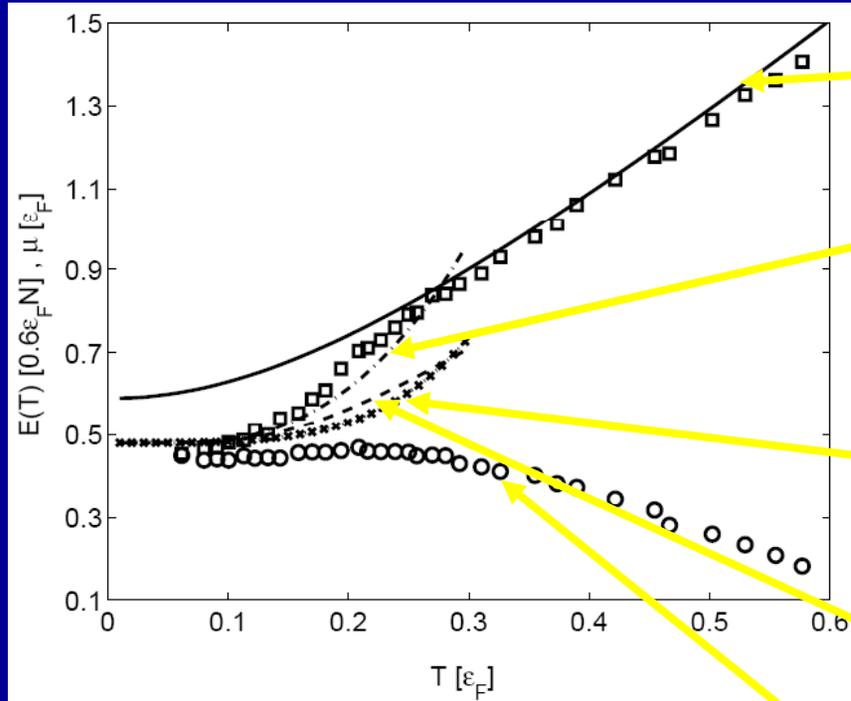
All traces can be expressed through these single-particle density matrices

One can thus determine as a function of T , V and chemical potential:

- ✓ **Total Energy**
- ✓ **Particle number**
- ✓ **Entropy of the system**
- ✓ **Pressure**
- ✓ **Spectrum of fermionic elementary excitations**
(pairing gap, pseudogap, effective mass, self-energy)
- ✓ **Long range order, condensate fraction**
(onset of phase transition, critical temperature)

$$a = \pm\infty$$

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)

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

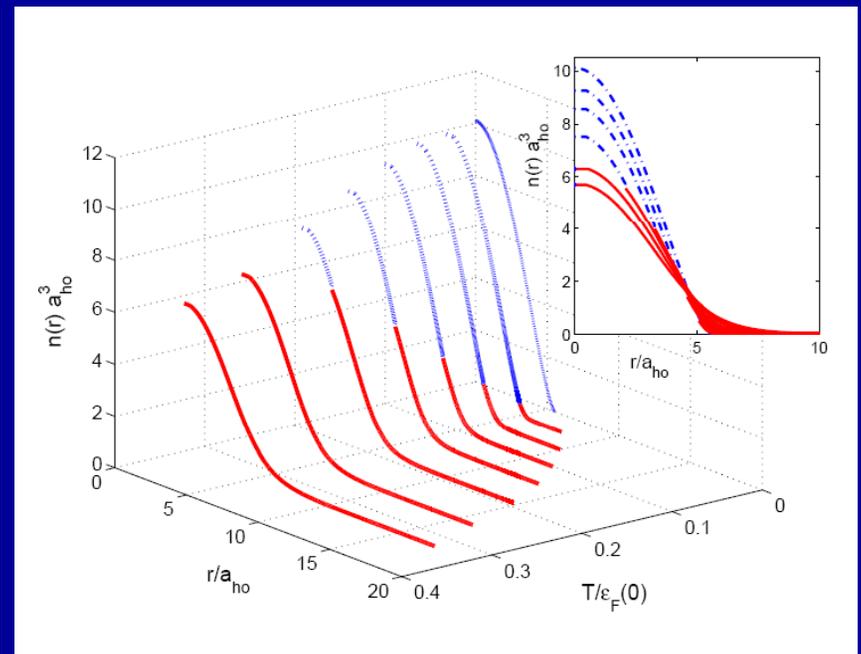
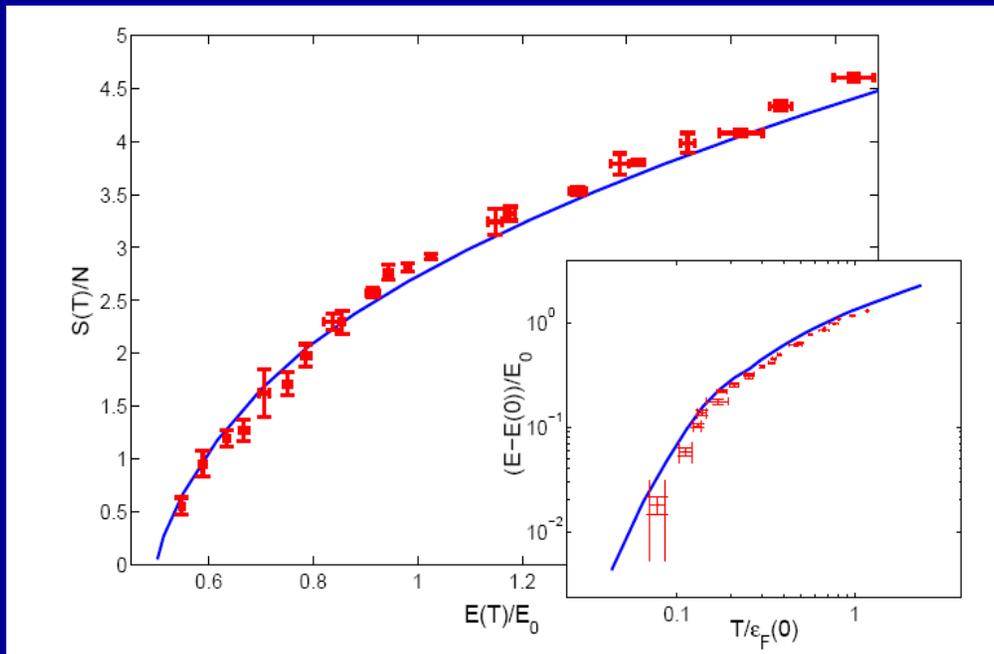
$$E_{\text{quasi-particles}}(T) = \frac{3}{5} \varepsilon_F N \frac{5}{2} \sqrt{\frac{2\pi\Delta^3 T}{\varepsilon_F^4}} \exp\left(-\frac{\Delta}{T}\right)$$

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

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. 98, 080402 (2007)

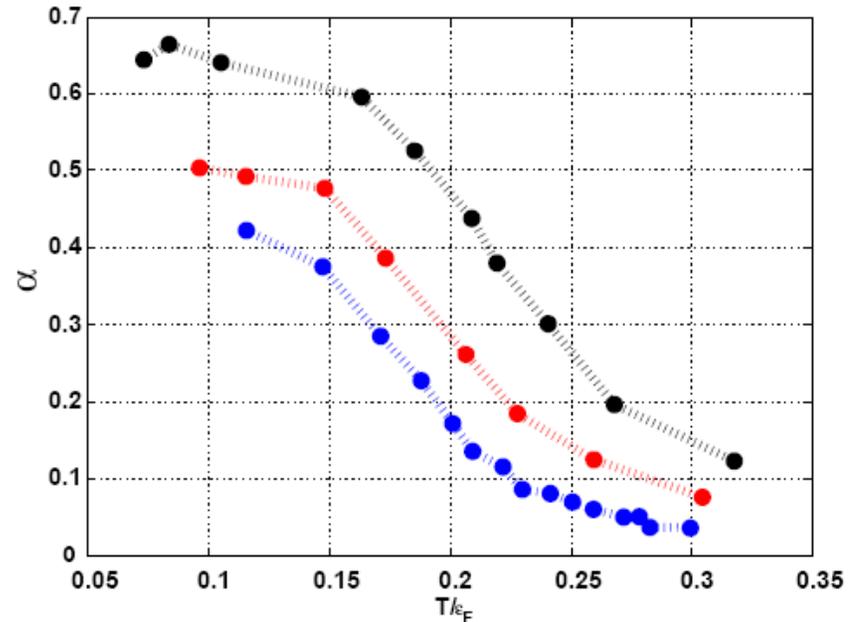
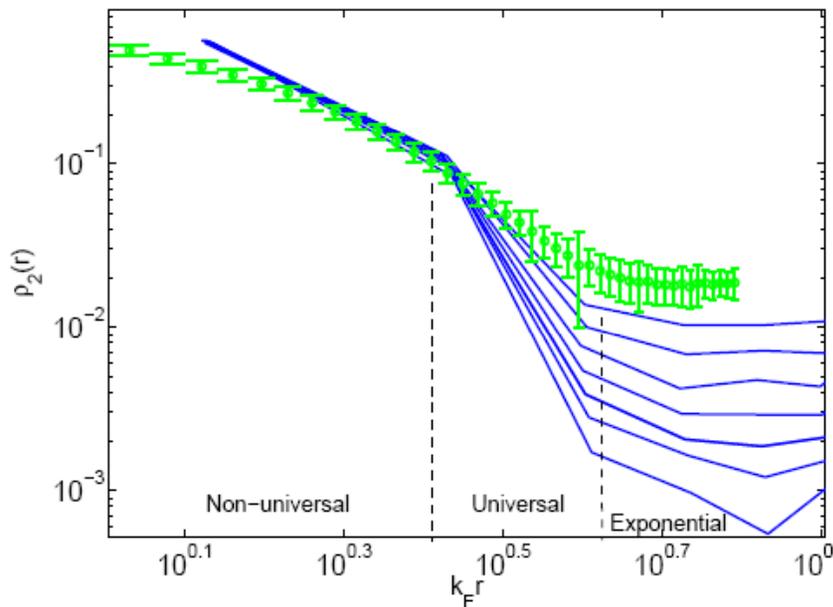


Full *ab initio* theory (no free parameters)

Bulgac, Drut, and Magierski, Phys. Rev. Lett. 99, 120401 (2007)

Long range order, superfluidity and condensate fraction

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

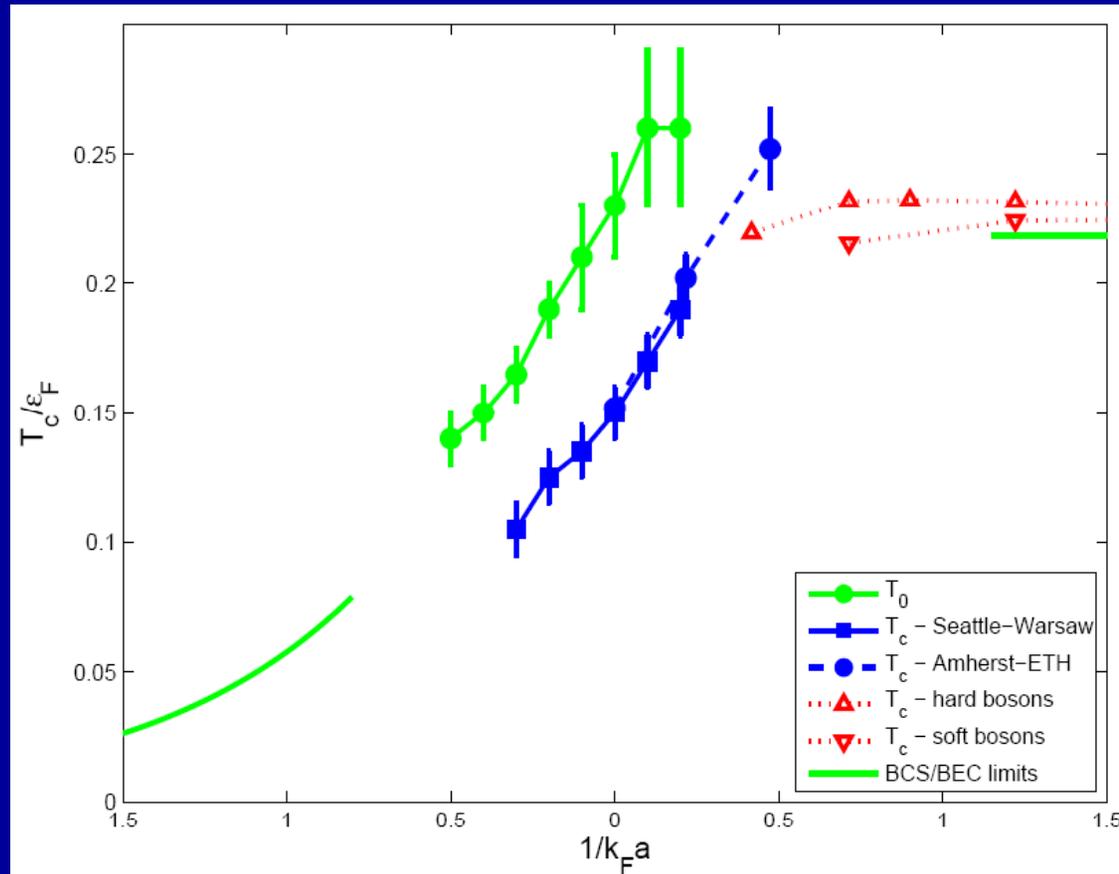


$$g_2(\vec{r}) = \left(\frac{2}{N}\right)^2 \int d^3\vec{r}_1 \int d^3\vec{r}_2 \langle \psi_{\uparrow}^{\dagger}(\vec{r}_1 + \vec{r}) \psi_{\downarrow}^{\dagger}(\vec{r}_2 + \vec{r}) \psi_{\downarrow}(\vec{r}_2) \psi_{\uparrow}(\vec{r}_2) \rangle$$

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

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

Critical temperature for superfluid to normal transition



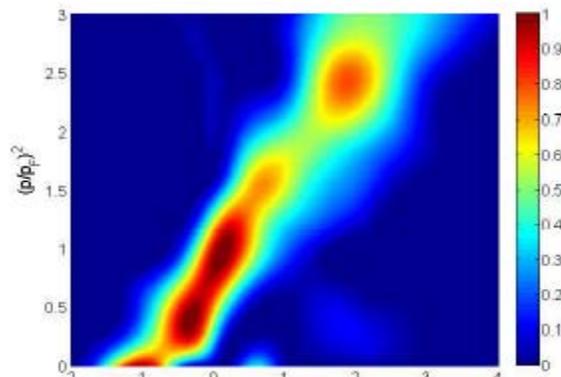
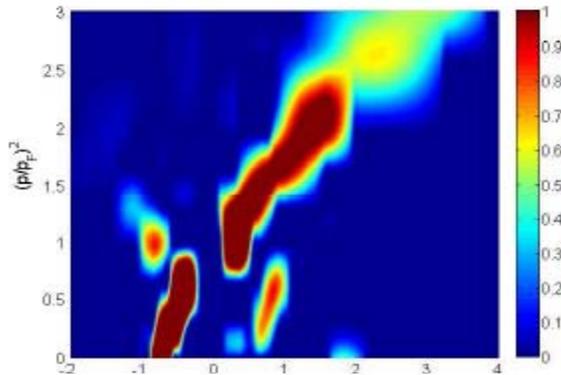
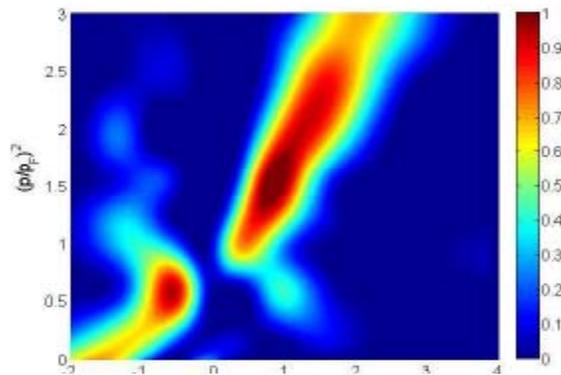
Bulgac, Drut, and Magierski, Phys. Rev. A 78, 023625 (2008)

Amherst-ETH:

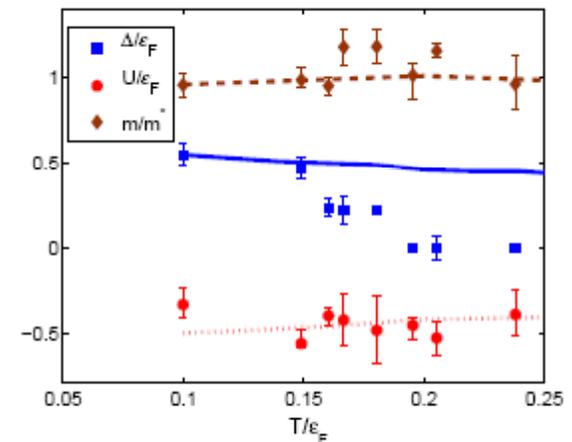
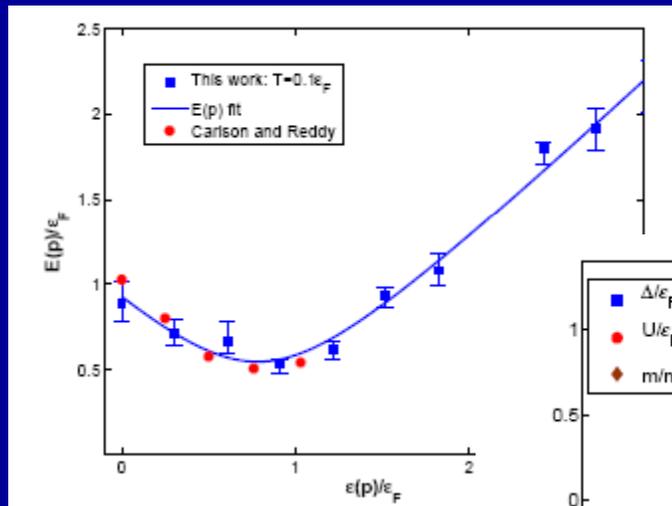
Burovski et al. Phys. Rev. Lett. 101, 090402 (2008)

Hard and soft bosons:

Pilati et al. PRL 100, 140405 (2008)



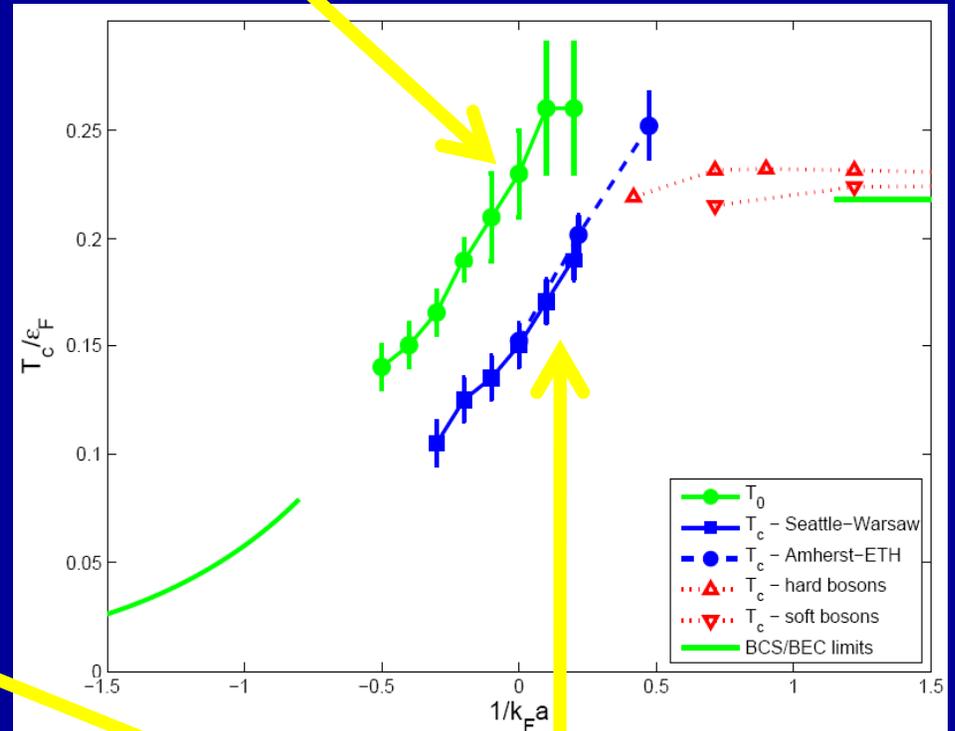
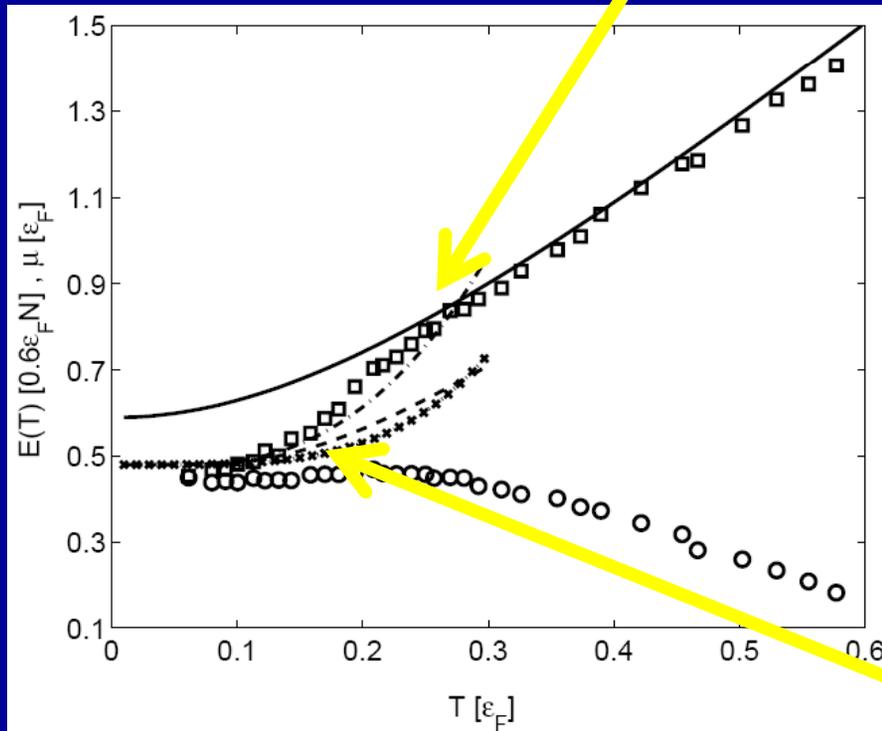
$$G(p, \tau) = \frac{1}{Z} \text{Tr} \left\{ \exp \left[-(\beta - \tau)(H - \mu N) \right] \psi^\dagger(p) \times \right. \\ \left. \exp \left[-\tau(H - \mu N) \right] \psi(p) \right\} \\ = -\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A(p, \omega) \frac{\exp(-\omega\tau)}{1 + \exp(-\omega\beta)}$$



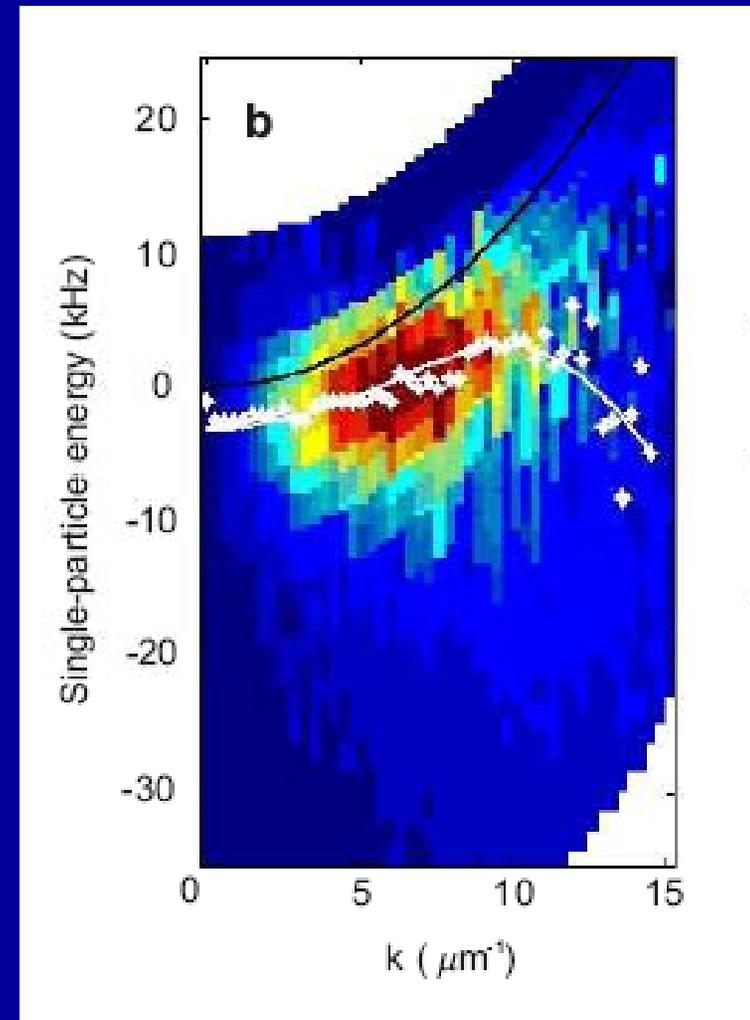
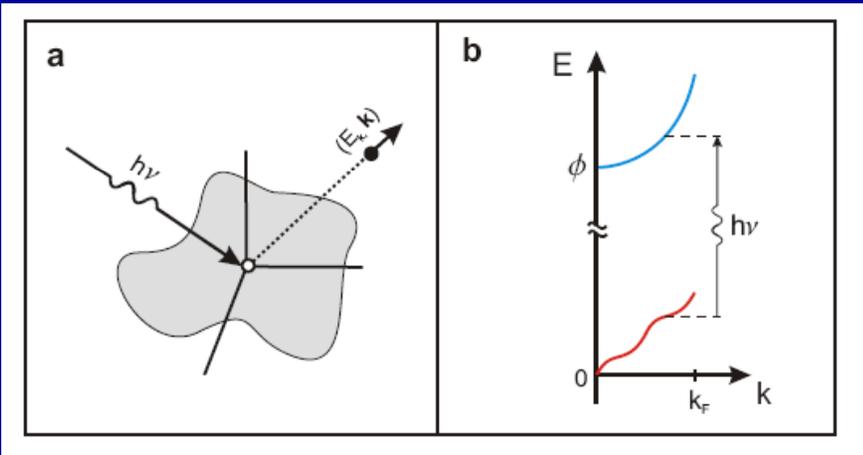
Magierski, Wlazlowski, Bulgac, and Drut
 Phys. Rev. Lett. 103, 210403 (2009)

The pseudo-gap vanishes at T_0

Vanishing of pseudogap

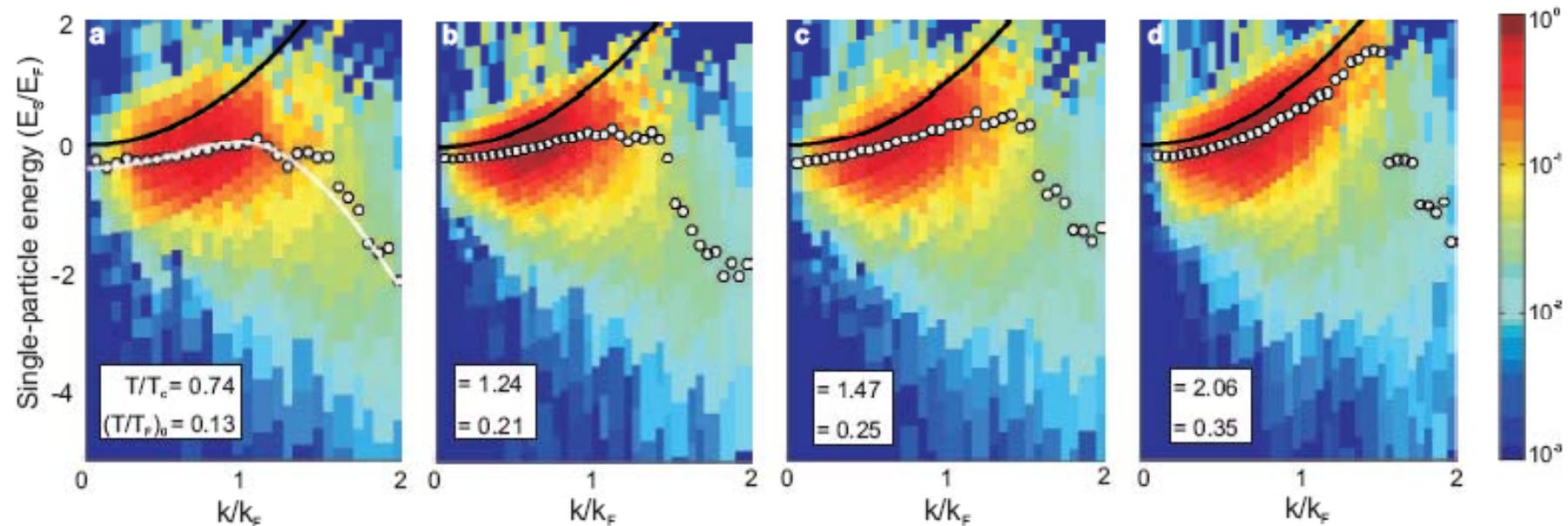


Superfluid to Normal phase transition



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

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



Observation of pseudogap behavior in a strongly interacting Fermi gas

Gaebler, Stewart, Drake, Jin, Perali, Pieri, and Strinati, arXiv::1003.1147v1

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

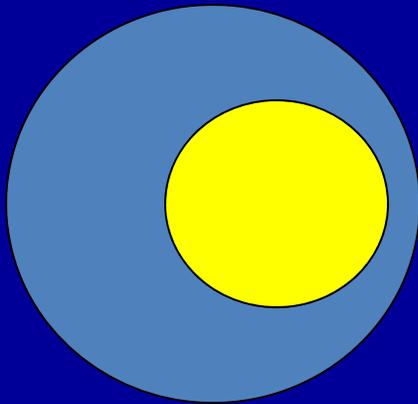
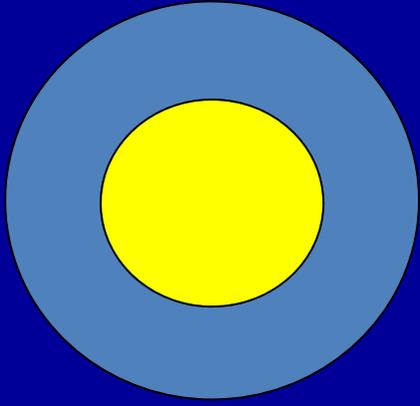
What happens when there are not enough partners for everyone to pair with?

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

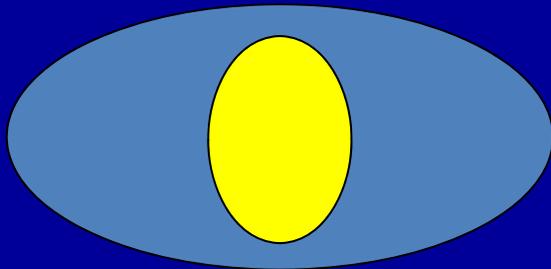
What theory tells us?

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

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



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

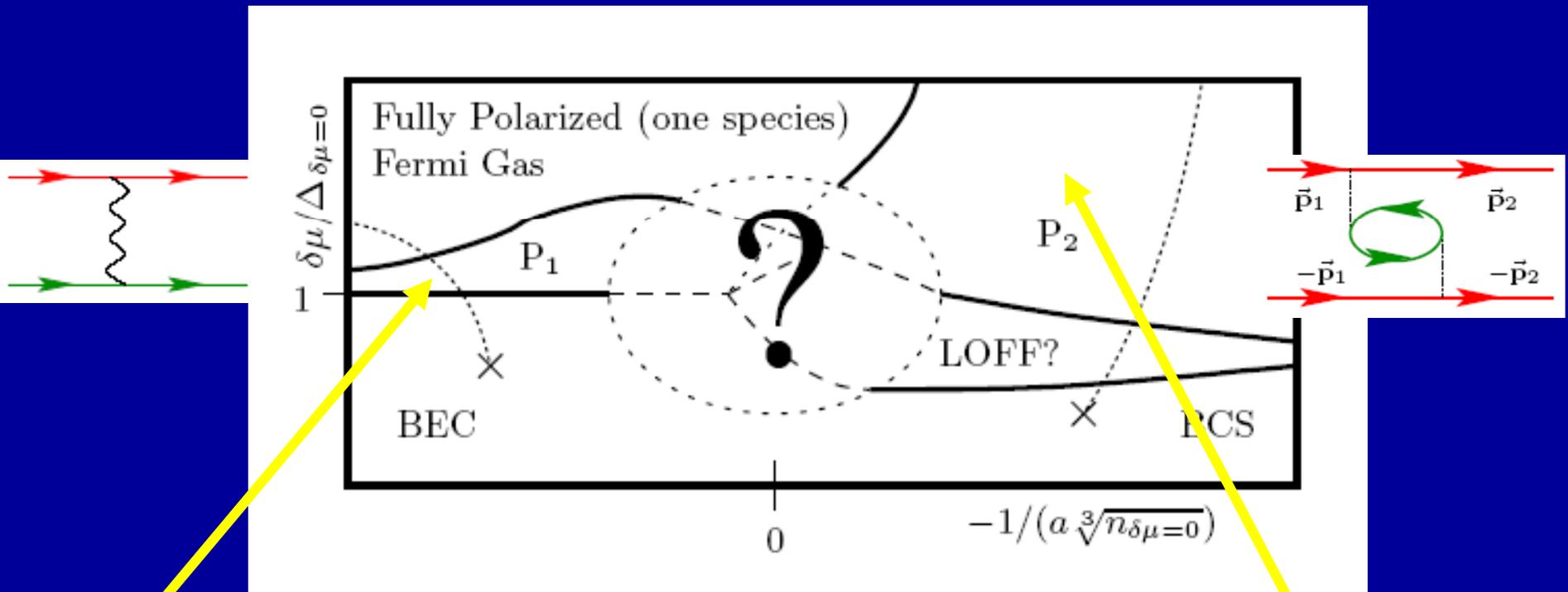


Muether and Sedrakian (2002)
Translational invariant solution
Rotational invariance broken

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)

We have to also treat inhomogeneous systems!

- **Monte Carlo (small particle numbers only feasible)**
- **Density Functional Theory (arbitrary particle numbers)**

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

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

Only this combination is cutoff independent

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

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

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

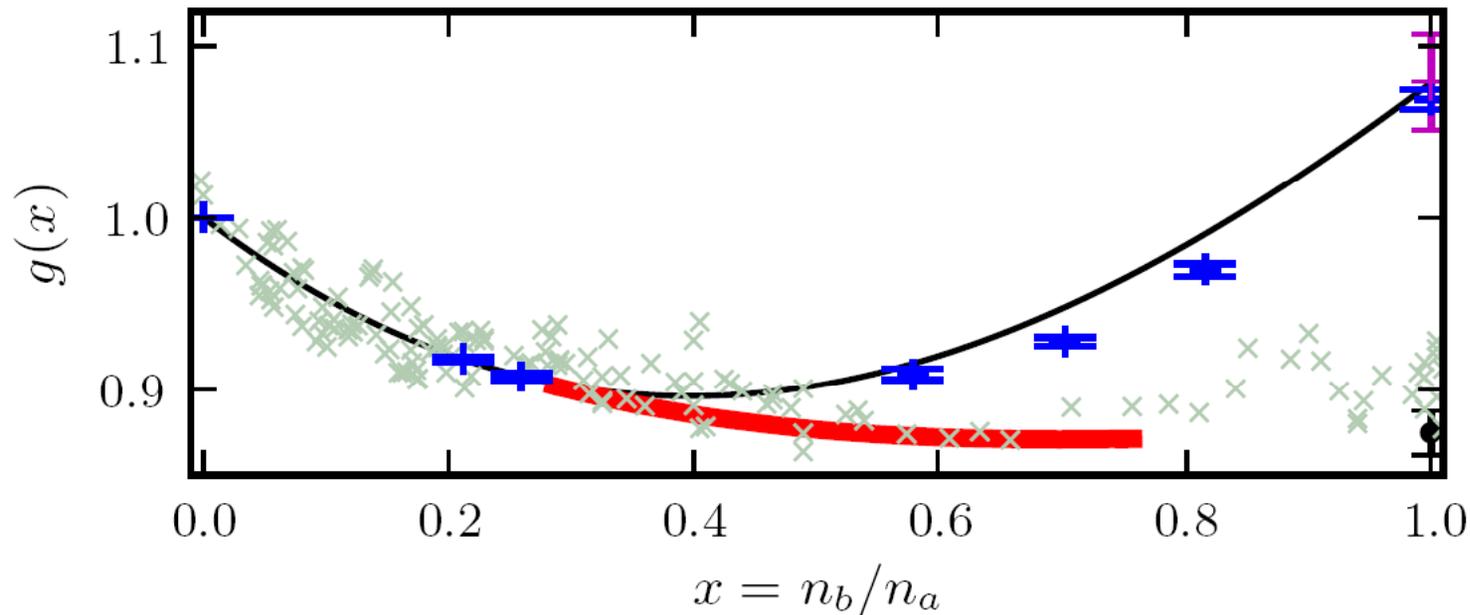
$$U(\vec{r}) = \beta \frac{(3\pi^2)^{2/3} n^{2/3}(\vec{r})}{2} - \frac{|\Delta(\vec{r})|^2}{3\gamma n^{2/3}(\vec{r})} + V_{ext}(\vec{r}) + \text{small correction}$$

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

α can take any positive value,

but the best results are obtained when α is fixed by the qp-spectrum

A refined EOS for spin unbalanced systems



Red line: Larkin-Ovchinnikov phase

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

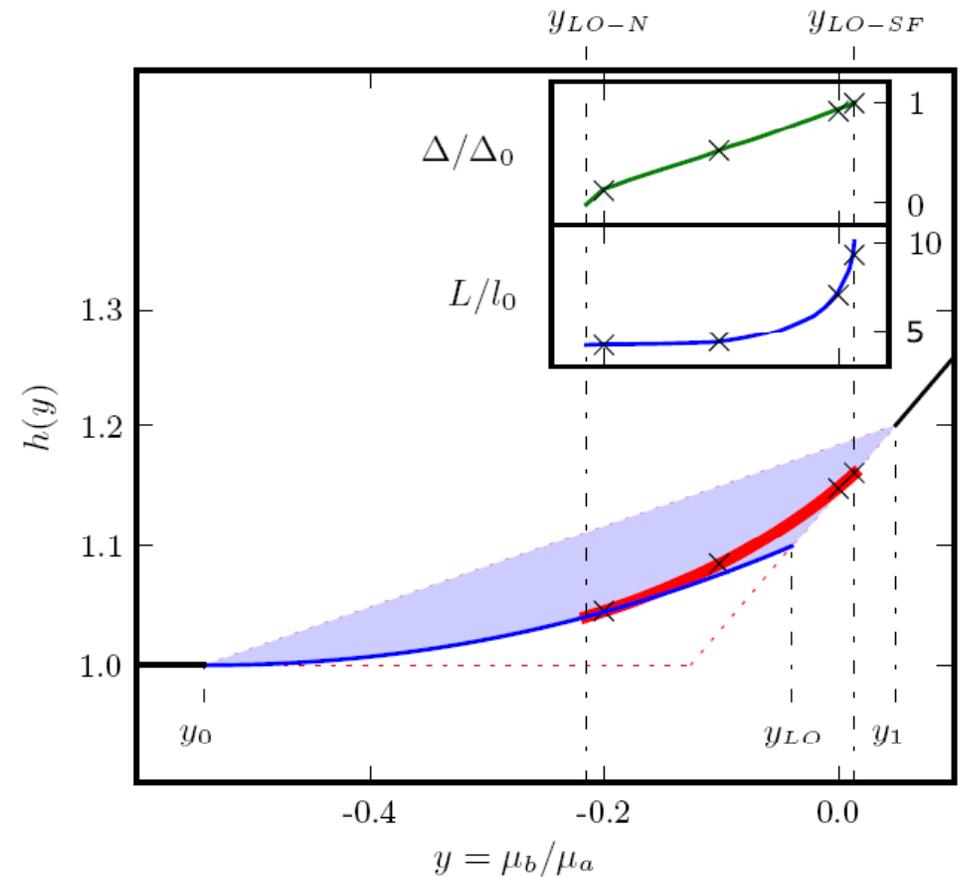
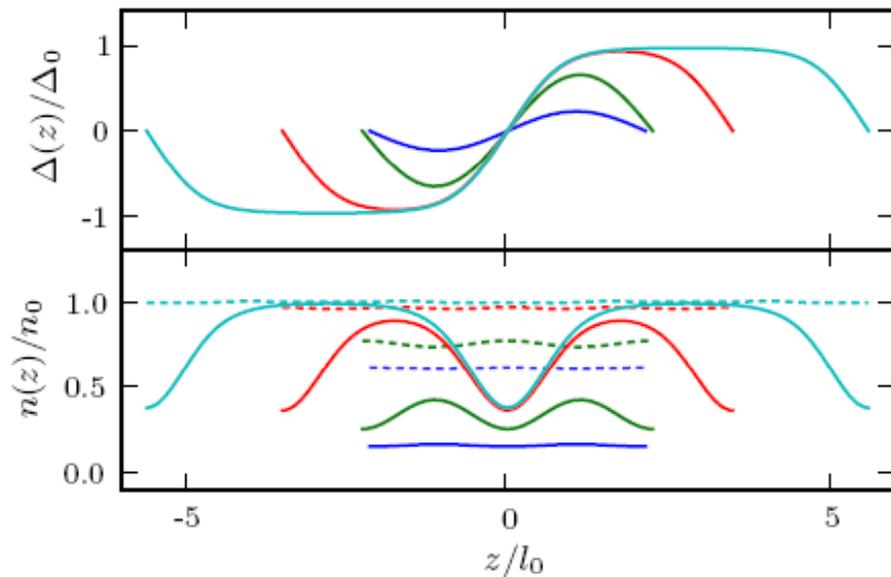
Black line: normal part of the energy density

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

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.

TDDFT for normal systems:

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>

TDSLDA

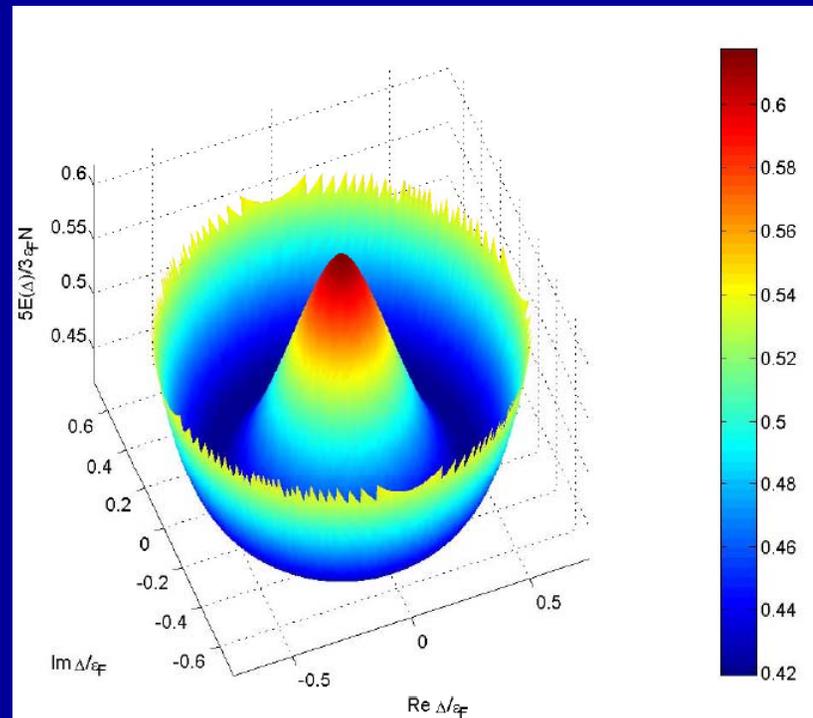
$$E(t) = \int d^3r \left[\varepsilon(n(\vec{r},t), \tau(\vec{r},t), \nu(\vec{r},t), \vec{j}(\vec{r},t)) + V_{ext}(\vec{r},t)n(\vec{r},t) + \dots \right]$$

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

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



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

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

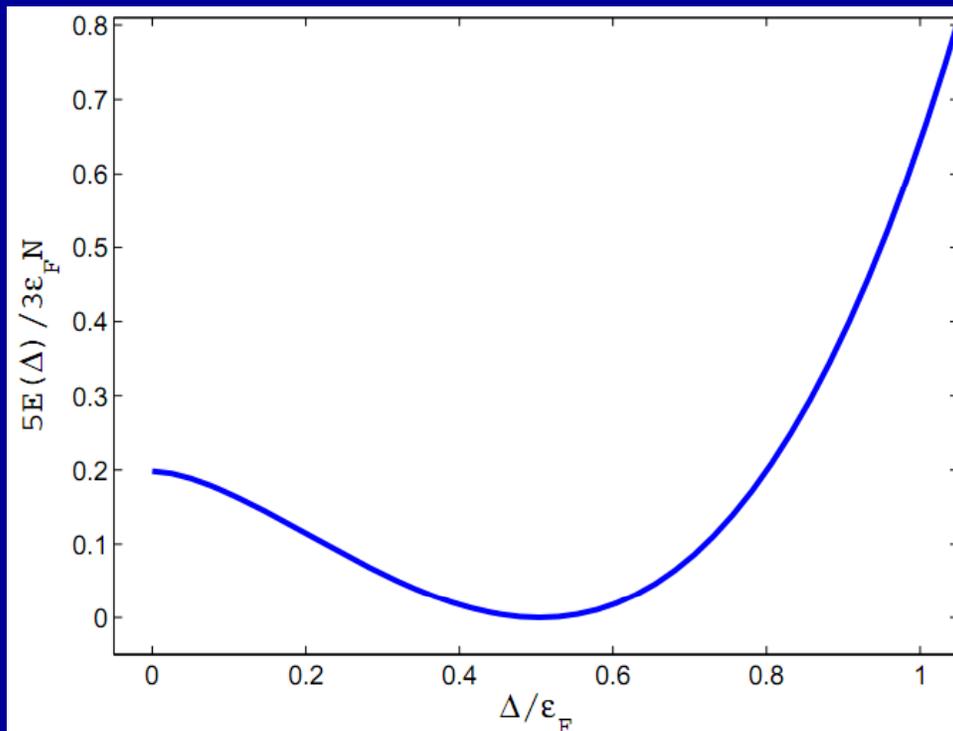
$$i\hbar\dot{\Psi}(\vec{r},t) = -\frac{\hbar^2\Delta}{4m}\Psi(\vec{r},t) + U(|\Psi(\vec{r},t)|^2)\Psi(\vec{r},t)$$

Quantum hydrodynamics

“Landau-Ginzburg” equation

Higgs mode

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

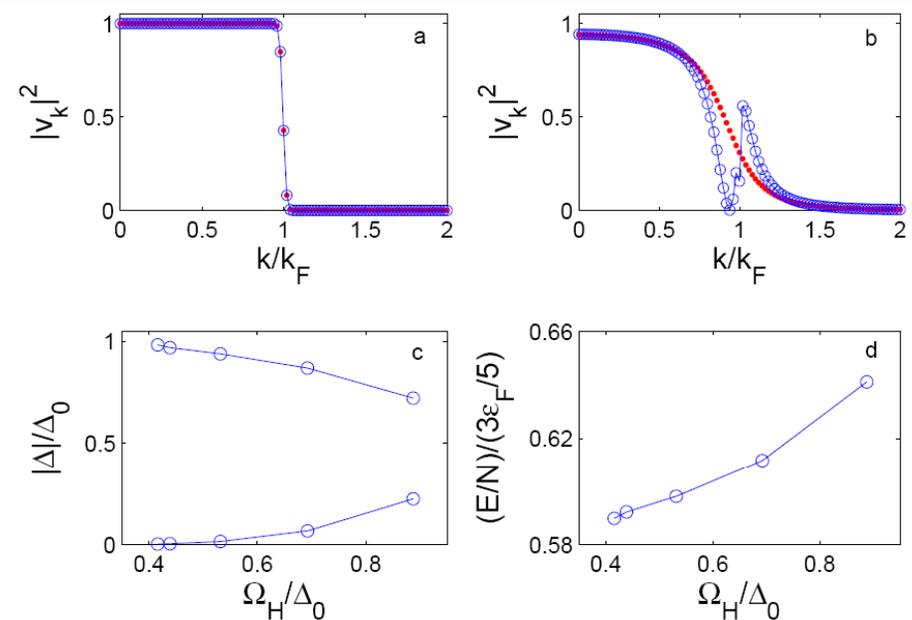
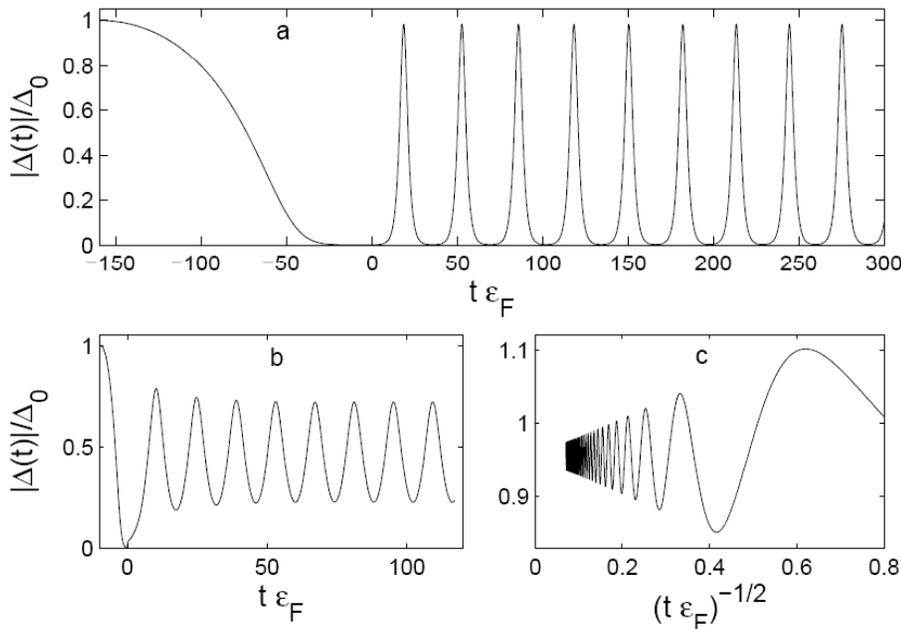
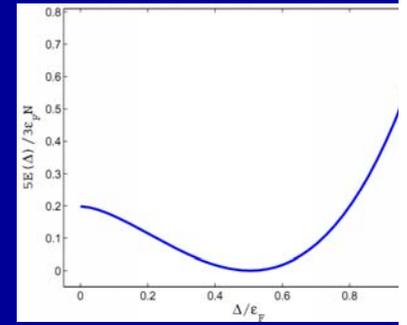


$$\hbar\Omega_H = 2\Delta_0$$

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

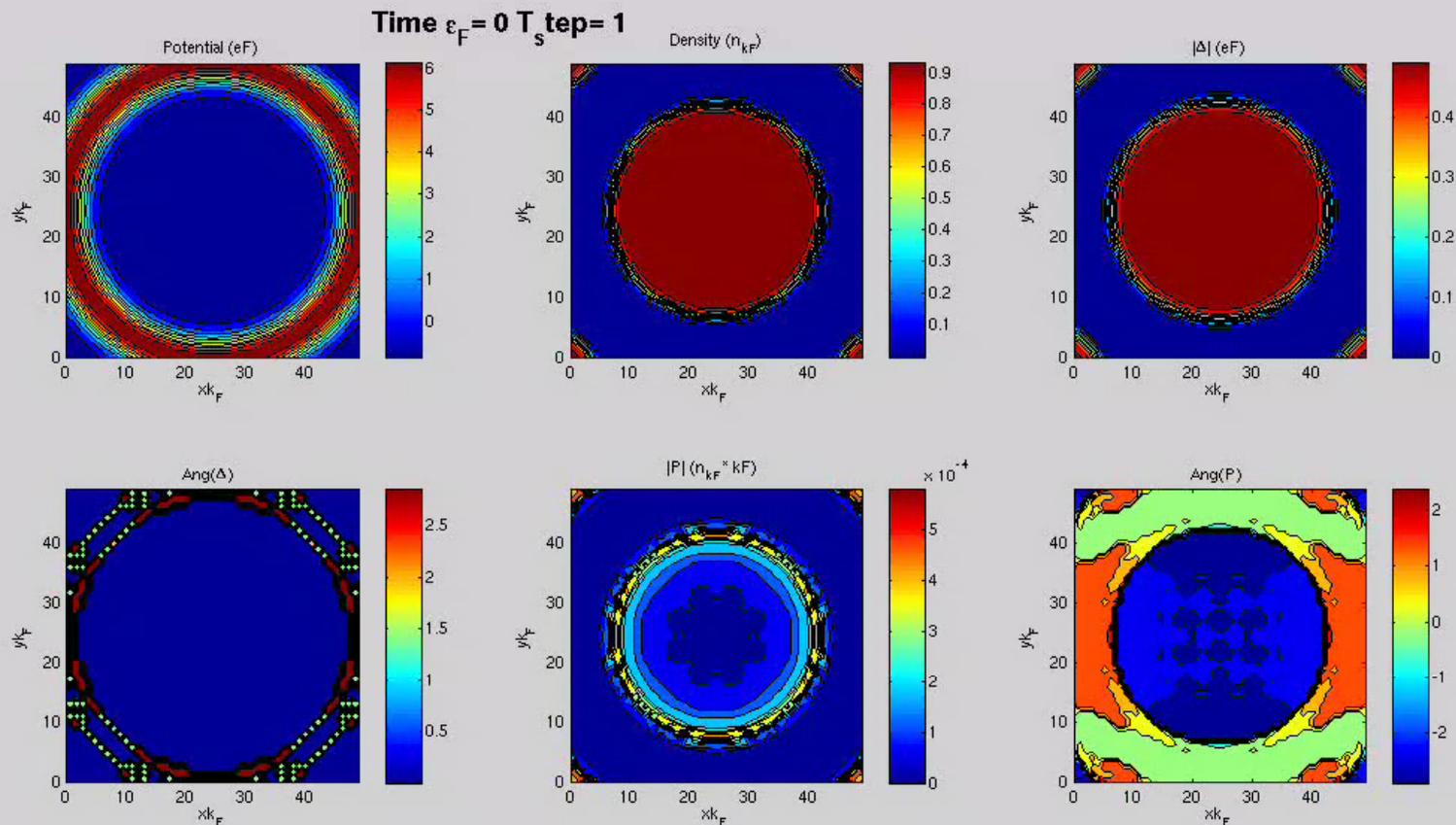
Response of a unitary Fermi system to changing the scattering length with time

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)



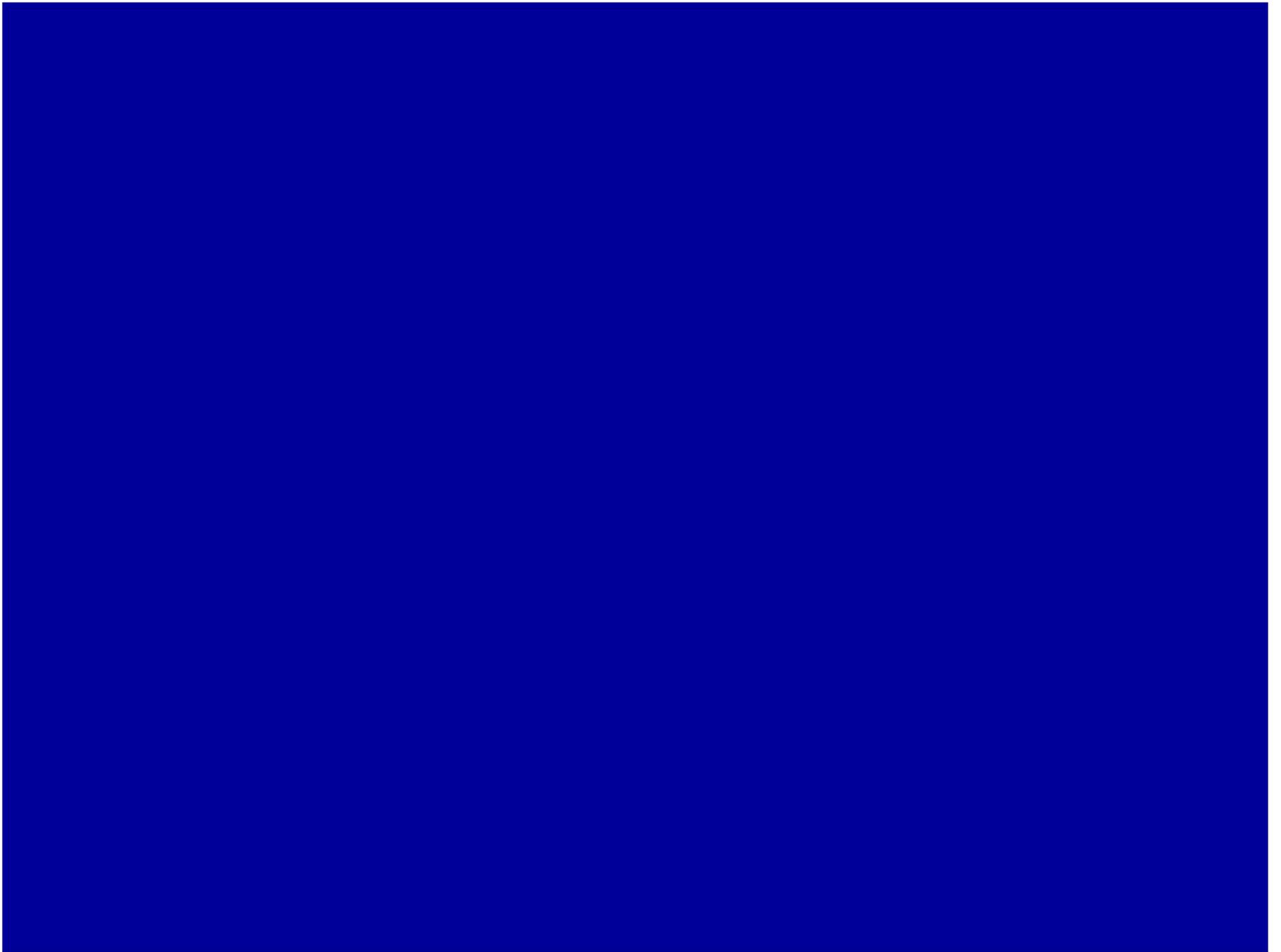
**About 60,000 PDEs, 48^3 spatial lattice (homogeneity assumed in 3rd direction),
Around 2,000,000 times steps, approximately 4-5 CPU-years for the time evolution**

Vortex generation and dynamics, see more movies at

http://www.phys.washington.edu/groups/gmbnt/vortices_movies.html

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 many 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



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

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**

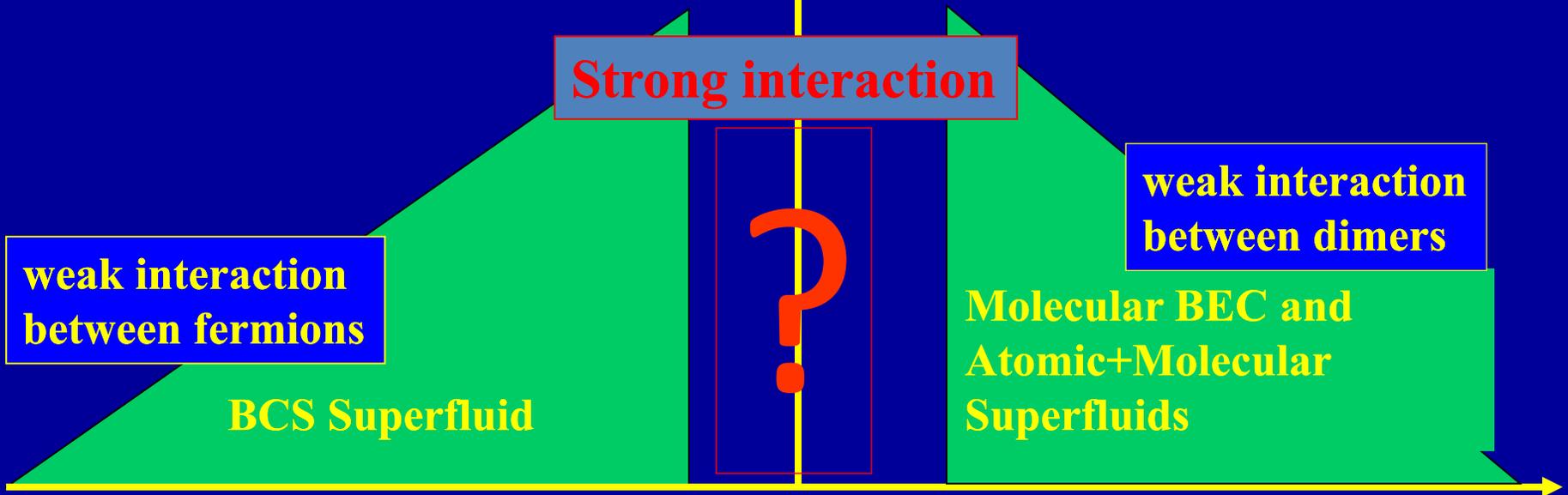
$a < 0$

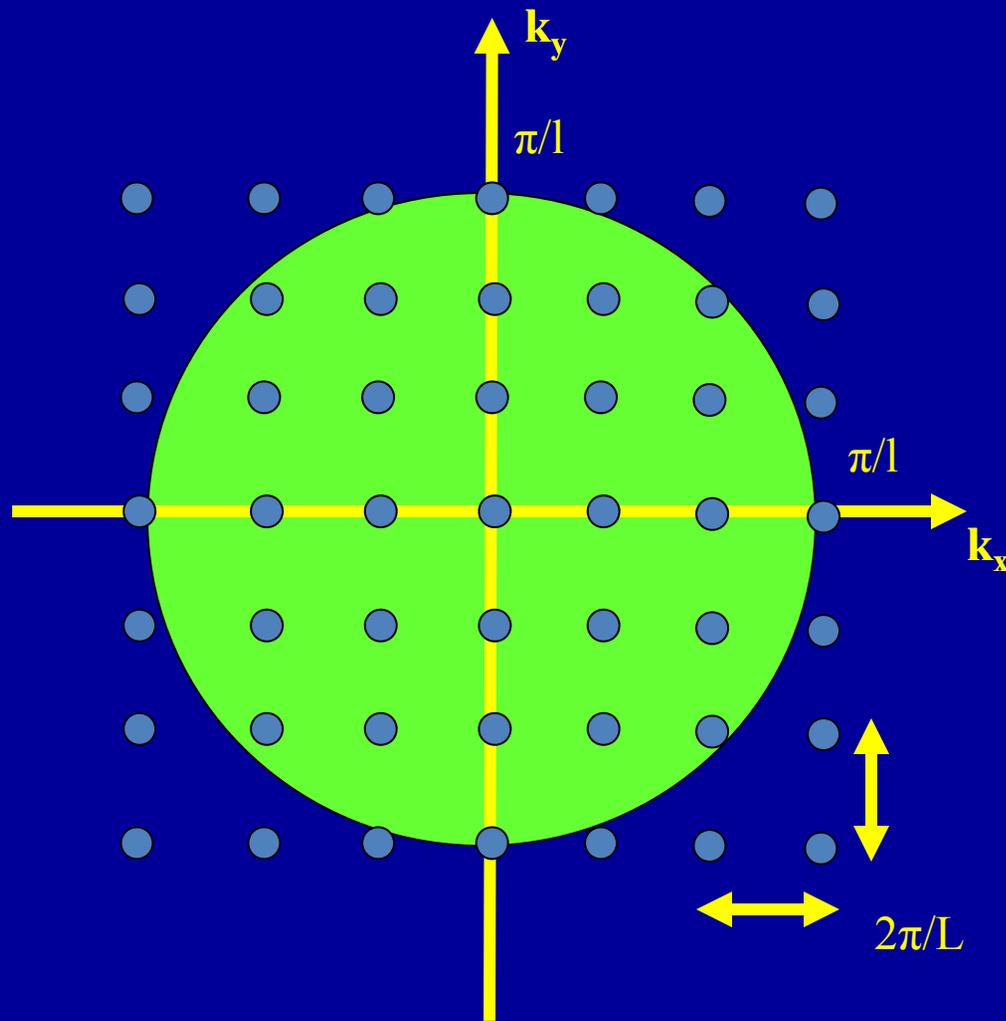
no 2-body bound state

$a > 0$

shallow 2-body bound state

$1/a$





Momentum space

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

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

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

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

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

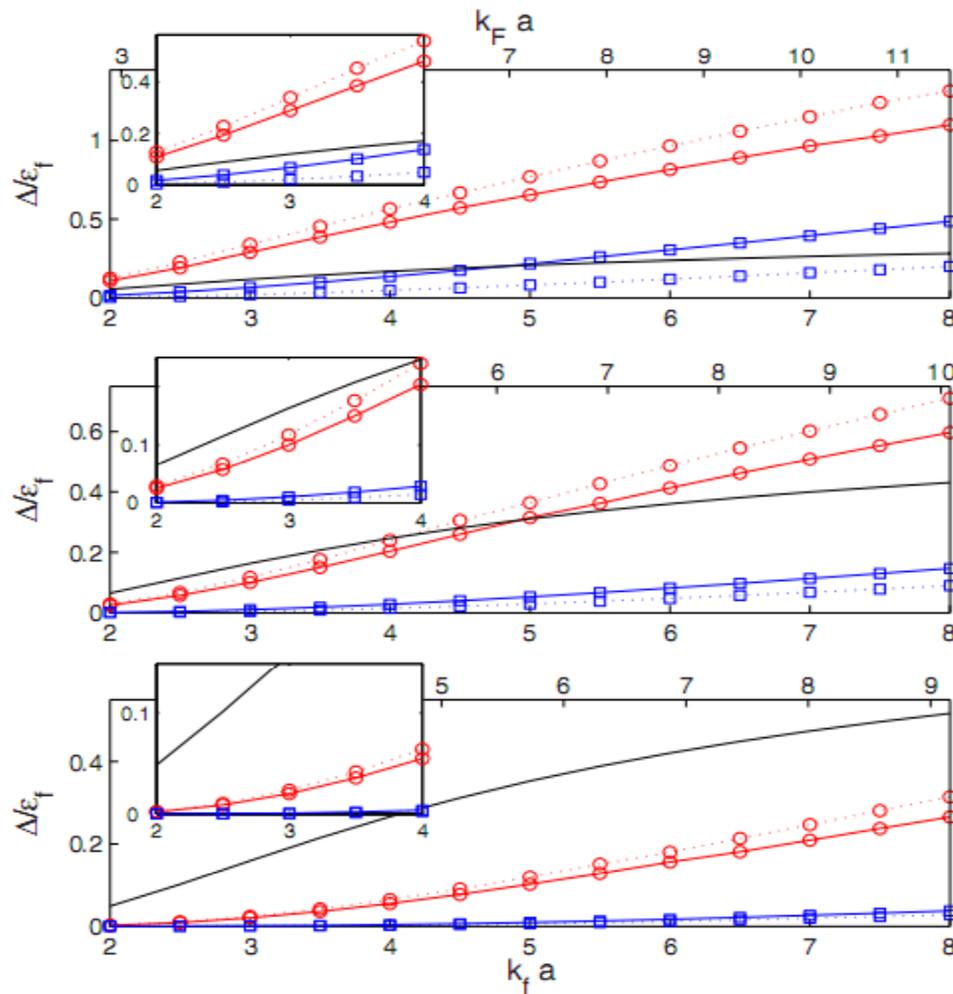
More details of the calculations:

- **Typical lattice sizes used from $8^3 \times 300$ (high Ts) to $8^3 \times 1800$ (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” $\approx 250 - 300$ time steps at $T \approx T_c$**

How to construct and validate an *ab initio* Energy Density Functional (EDF)?

- ❑ Given a many body Hamiltonian determine the properties of the infinite homogeneous system as a function of density
- ❑ Extract the EDF
- ❑ Add gradient corrections, if needed or known how (?)
- ❑ Determine in an *ab initio* calculation the properties of a select number of wisely selected finite systems
- ❑ Apply the energy density functional to inhomogeneous systems and compare with the *ab initio* calculation, and if lucky declare Victory!

Going beyond the naïve BCS approximation



Eliashberg approx. (red)

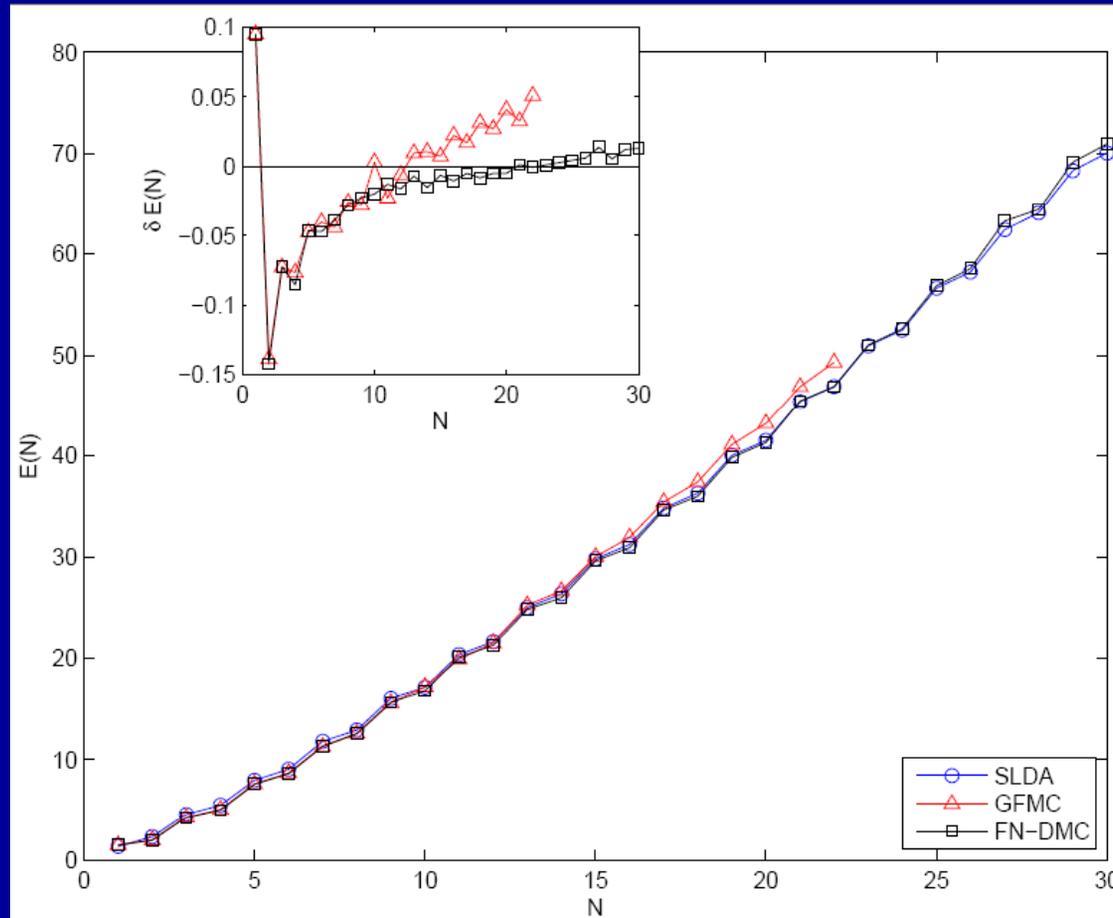
BCS approx. (black)

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

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

Fermions at unitarity in a harmonic trap

Total energies $E(N)$



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

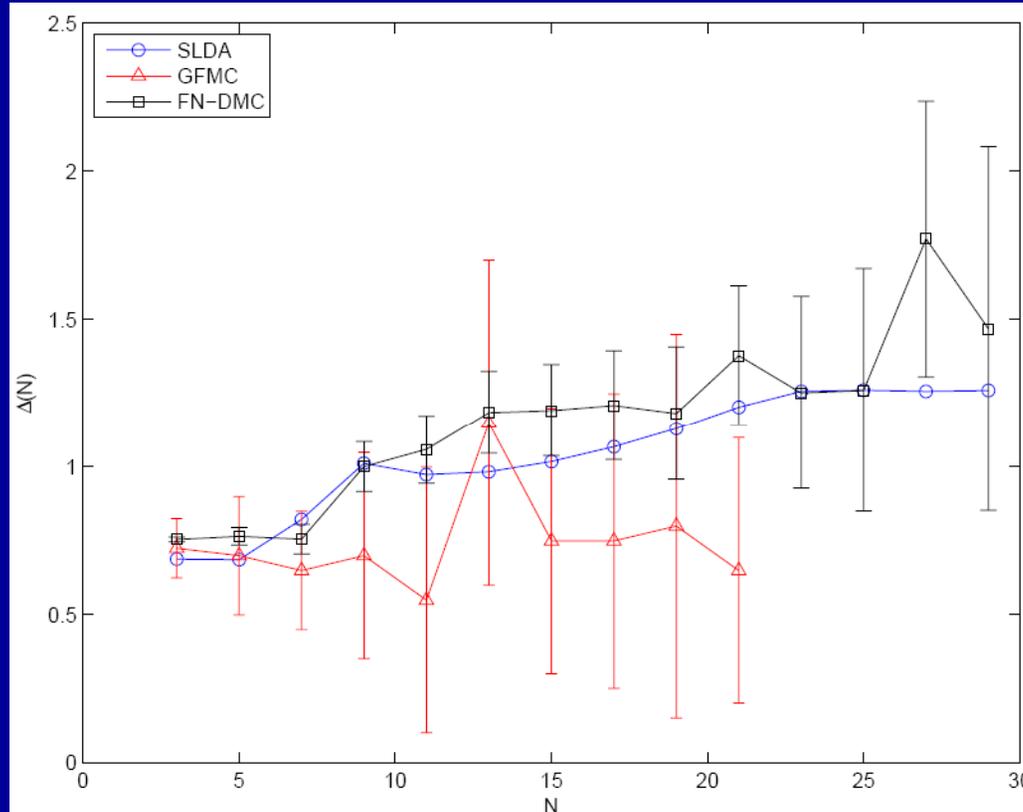
FN-DMC - von Stecher, Greene and Blume, PRL 99, 233201 (2007)

PRA 76, 053613 (2007)

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

Fermions at unitarity in a harmonic trap

Pairing gaps



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

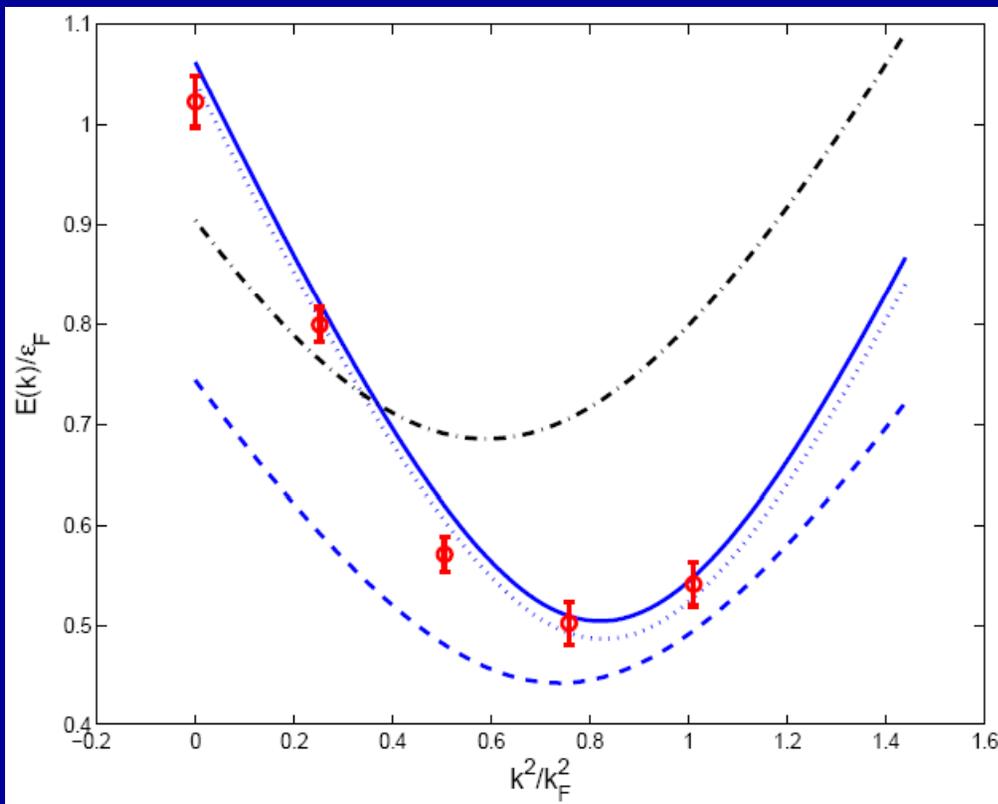
GFMC - Chang and Bertsch, Phys. Rev. A **76**, 021603(R) (2007)

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



- solid/dotted blue line - SLDA, homogeneous GFMC due to Carlson et al
- red circles - GFMC due to Carlson and Reddy
- dashed blue line - SLDA, homogeneous MC due to Juillet
- black dashed-dotted line - meanfield at unitarity

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

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

Asymmetric SLDA (ASLDA)

$$n_a(\vec{r}) = \sum_{E_n < 0} |\mathbf{u}_n(\vec{r})|^2, \quad n_b(\vec{r}) = \sum_{E_n > 0} |\mathbf{v}_n(\vec{r})|^2,$$

$$\tau_a(\vec{r}) = \sum_{E_n < 0} |\vec{\nabla} \mathbf{u}_n(\vec{r})|^2, \quad \tau_b(\vec{r}) = \sum_{E_n > 0} |\vec{\nabla} \mathbf{v}_n(\vec{r})|^2,$$

$$\nu(\vec{r}) = \frac{1}{2} \sum_{E_n} \text{sign}(E_n) \mathbf{u}_n(\vec{r}) \mathbf{v}_n^*(\vec{r}),$$

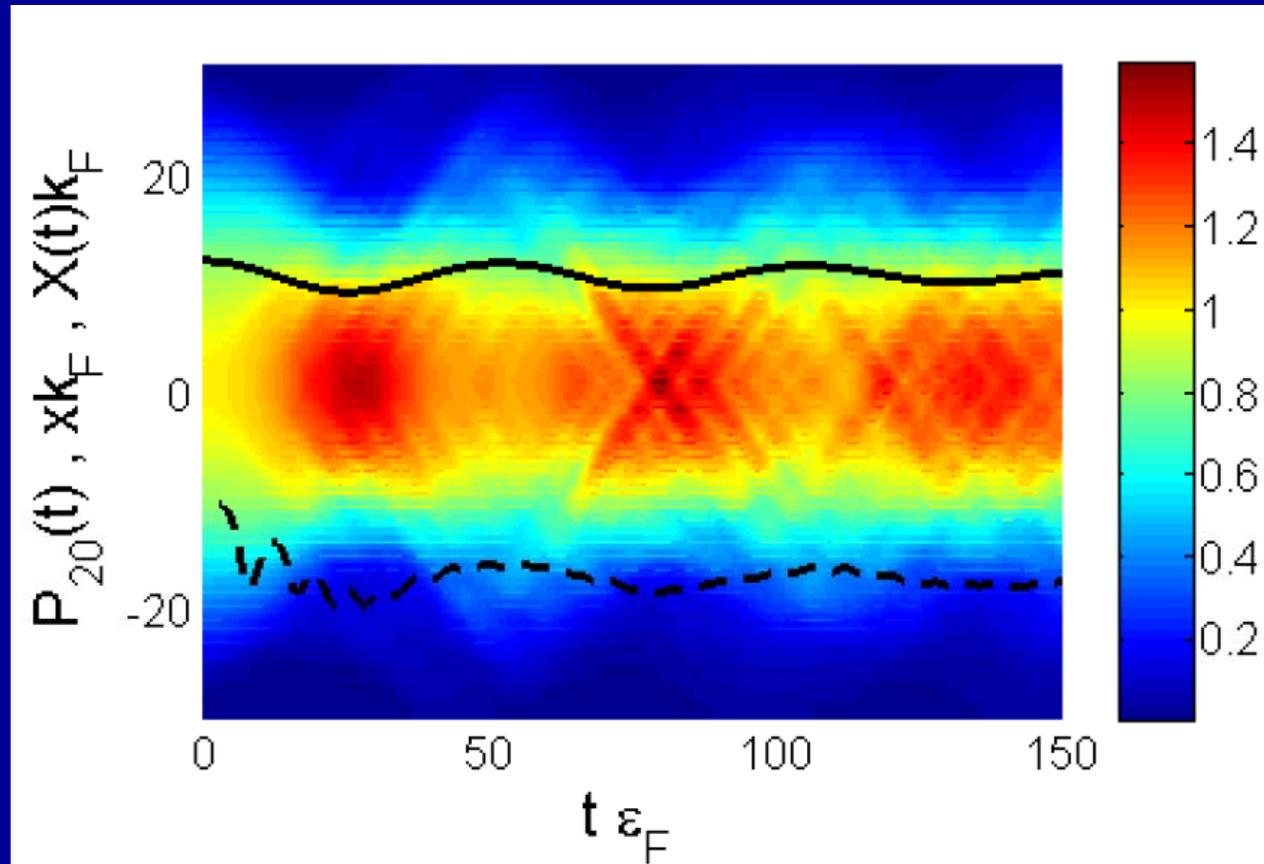
$$\begin{aligned} E(\vec{r}) = & \frac{\hbar^2}{2m} [\alpha_a(\vec{r}) \tau_a(\vec{r}) + \alpha_b(\vec{r}) \tau_b(\vec{r})] - \Delta(\vec{r}) \nu(\vec{r}) + \\ & + \frac{3(3\pi^2)^{2/3} \hbar^2}{10m} [n_a(\vec{r}) + n_b(\vec{r})]^{5/3} \beta[x(\vec{r})], \end{aligned}$$

$$\alpha_a(\vec{r}) = \alpha[x(\vec{r})], \quad \alpha_b(\vec{r}) = \alpha[1/x(\vec{r})], \quad x(\vec{r}) = n_b(\vec{r}) / n_a(\vec{r}),$$

$$\Omega = - \int d^3\vec{r} P(\vec{r}) = \int d^3\vec{r} [E(\vec{r}) - \mu_a n_a(\vec{r}) - \mu_b n_b(\vec{r})]$$

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)