# Fermionic atoms in the unitary regime

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Also in Warsaw

Now in Lund

# Outline

- Some general remarks
- T=0 equation of state and collective excitations
- Path integral Monte Carlo for many fermions on the lattice at finite temperatures, and some remarks about specific heat of clouds in traps
- Vortices, how to describe them and what has been observed recentlly
- Conclusions

# 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 $\approx 10^4$ K)*

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# A little bit of history

# Bertsch 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.***

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 (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.**

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

**Bertsch's regime is nowadays called *the unitary regime***

The system is very dilute, but strongly interacting!

$$n\, r_0^3 \ll 1$$

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

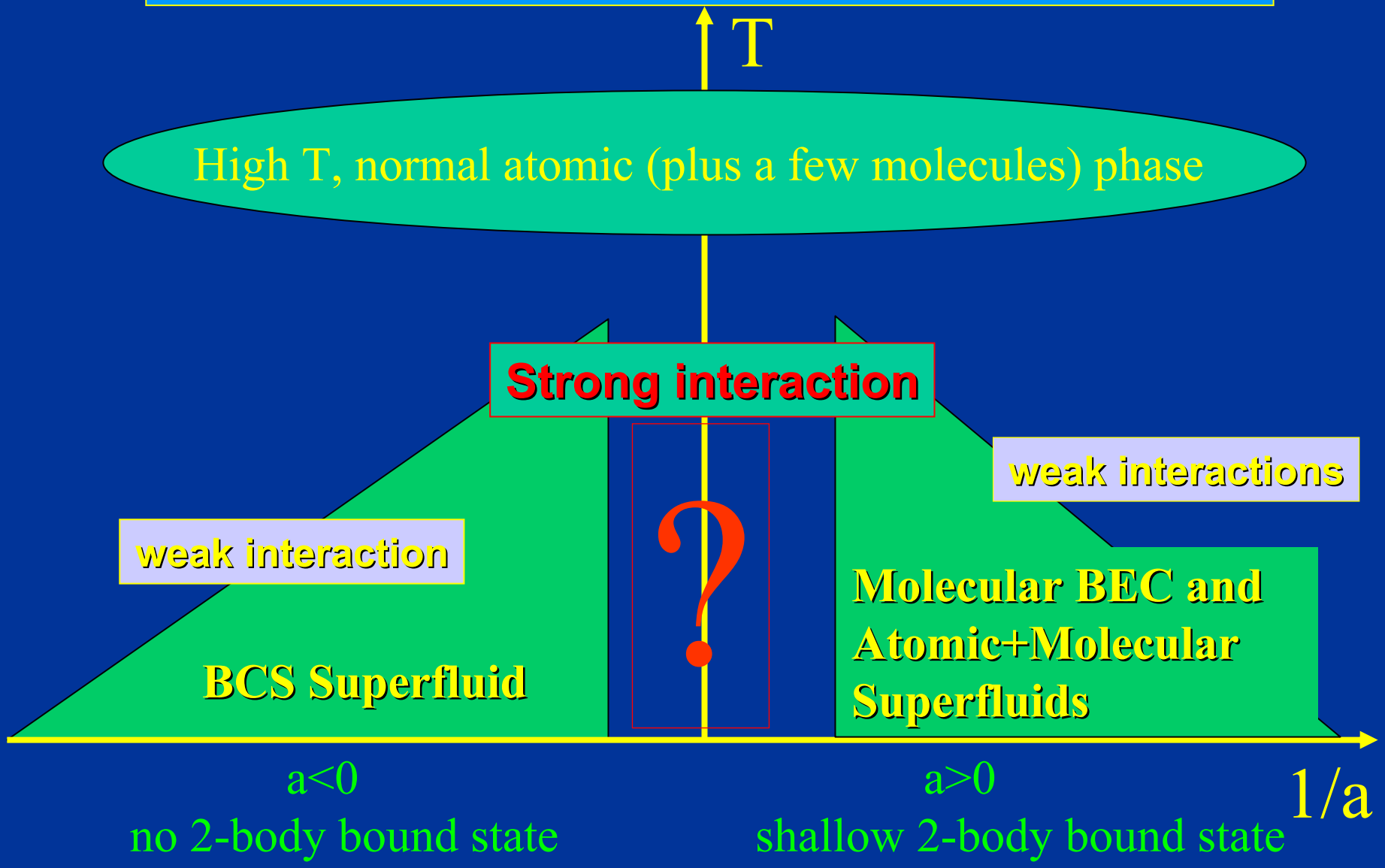
**n - number density**

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

$r_0$ - range of interaction

a - scattering length

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



# Early theoretical approach to BCS-BEC crossover

Dyson (?), Eagles (1969), Leggett (1980) …

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

$$\frac{m}{4\pi\hbar^2 a} = \sum_k \left(\frac{1}{2\varepsilon_k} - \frac{1}{2E_k}\right)$$ gap equation

$$n = 2\sum_k \left(1 - \frac{\varepsilon_k - \mu}{E_k}\right)$$ number density equation

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

$$E_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}$$ quasi-particle energy

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}, \quad u_k^2 + v_k^2 = 1, \quad v_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k - \mu}{E_k}\right)$$

$$\frac{E_{total}}{N} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} + \underline{\frac{\pi\hbar^2 a}{m}} n + \ldots - \frac{3\Delta^2}{8\mu}, \qquad n = \frac{k_F^3}{3\pi^2}$$

**Neglected/overlooked**

## Consequences:

- Usual BCS solution for small and negative scattering lengths, with exponentially small pairing gap

- For small and positive scattering lengths this equations describe a gas a weakly repelling (weakly bound/shallow) molecules, essentially all at rest (almost pure BEC state)

$$\Psi\left(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4,\ldots\right) \approx \mathcal{A}\left[\varphi(\vec{r}_{12})\varphi(\vec{r}_{34})\ldots\right]$$

In BCS limit the particle projected many-body wave function has the same structure (BEC of spatially overlapping Cooper pairs)

- For both large positive and negative values of the scattering length these equations predict a smooth crossover from BCS to BEC, from a gas of spatially large Cooper pairs to a gas of small molecules

# What is wrong with this approach:

- The BCS gap (a<0 and small) is overestimated, thus the critical temperature and the condensation energy are overestimated as well.

- In BEC limit (a>0 and small) the molecule repulsion is overestimated

- The approach neglects of the role of the "meanfield (HF) interaction," which is the bulk of the interaction energy in both BCS and unitary regime

- All pairs have zero center of mass momentum, which is reasonable in BCS and BEC limits, but incorrect <u>in the unitary regime</u>, where <u>the interaction between pairs is strong !!!</u> (this situation is similar to superfluid $^4$He)

**Fraction of non-condensed pairs (perturbative result)!?!**

$$\frac{n_{ex}}{n_0} = \frac{8}{3\sqrt{\pi}}\sqrt{n_m a_{mm}^3}, \qquad n_m = \frac{n}{2}, \qquad a_{mm} \approx 0.6a$$

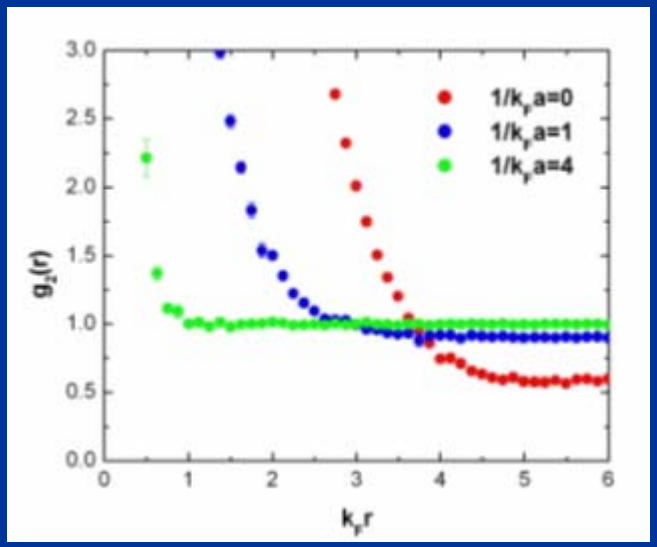
## Two-body density matrix and condensate fraction

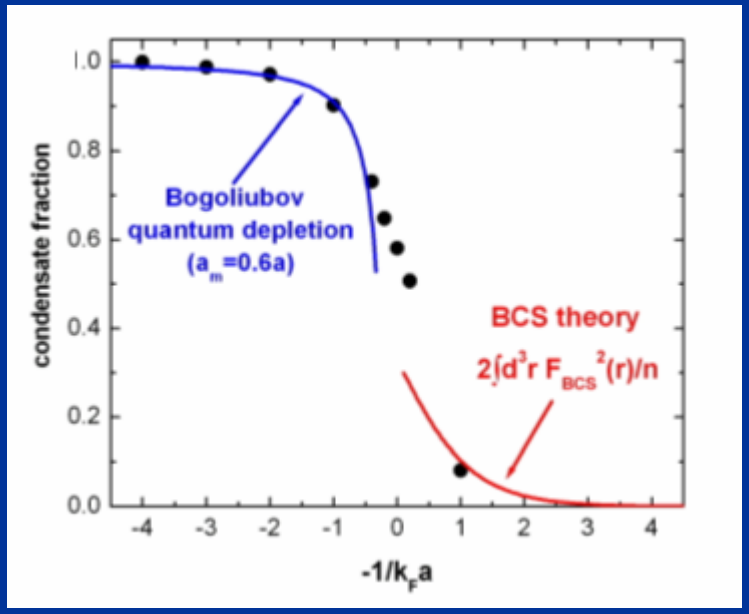
$$\left\langle \psi_\uparrow^+(\vec{r}_1+\vec{r})\psi_\downarrow^+(\vec{r}_2+\vec{r})\psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2)\right\rangle \xrightarrow[r\to\infty]{} F^2(|\vec{r}_1-\vec{r}_2|)$$

where

$$F(|\vec{r}_1-\vec{r}_2|)=\left\langle \psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2)\right\rangle$$ **order parameter**

$$g_2(r)=\frac{2}{N}\int d^3r_1 d^3r_2 \left\langle \psi_\uparrow^+(\vec{r}_1+\vec{r})\psi_\downarrow^+(\vec{r}_2+\vec{r})\psi_\uparrow(\vec{r}_1)\psi_\downarrow(\vec{r}_2)\right\rangle$$

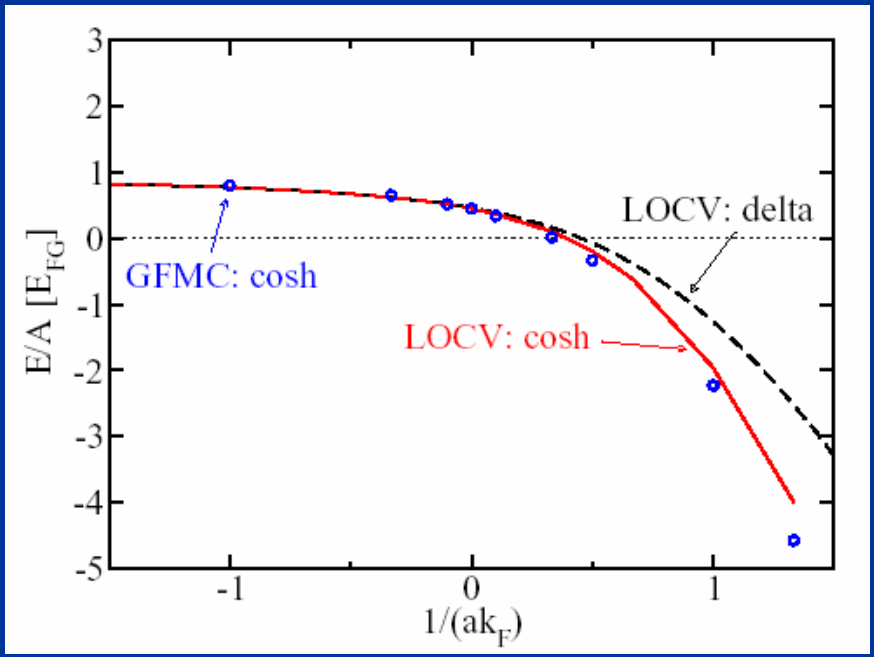


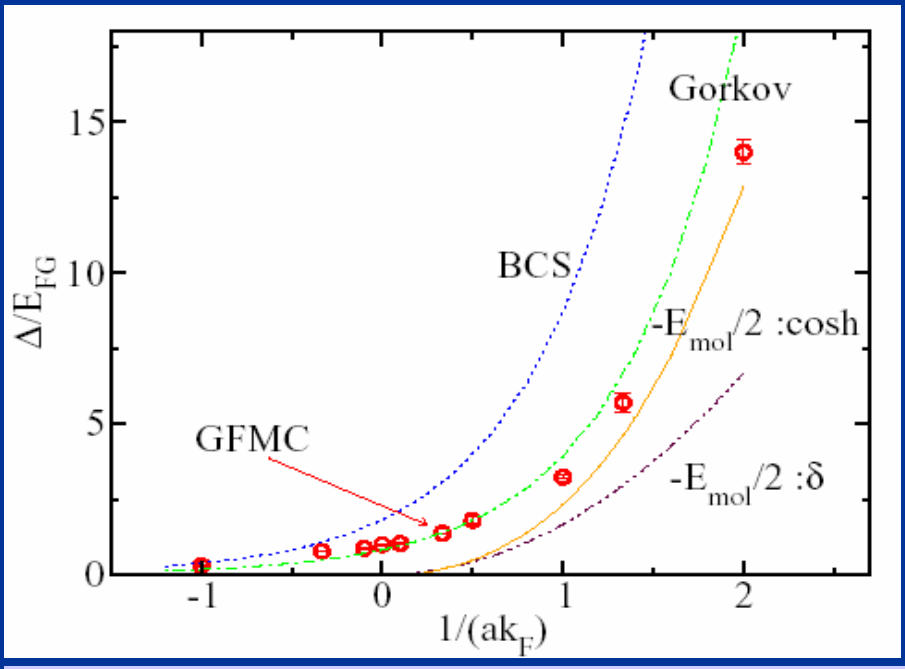



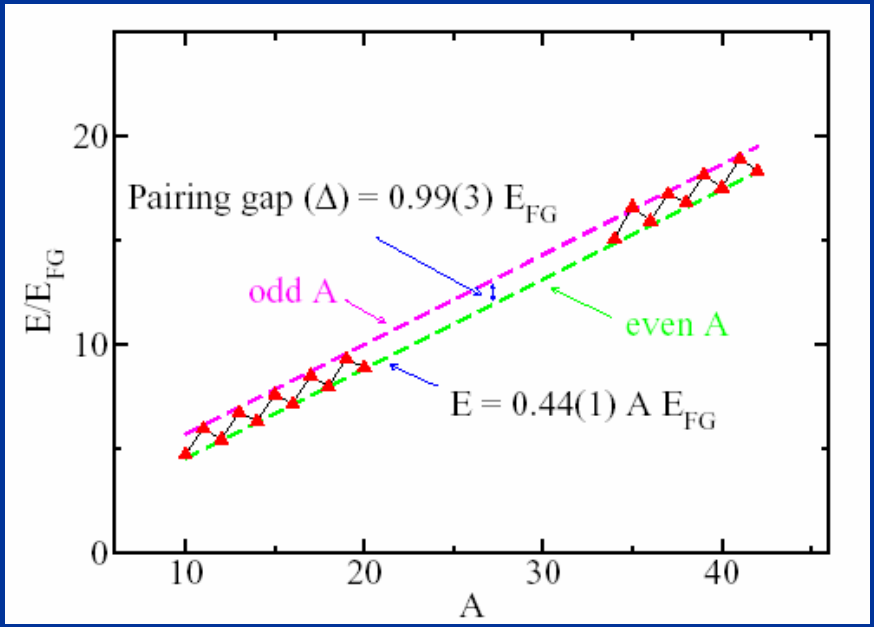

**From a talk of Stefano Giorgini (Trento)**

**What is the best theory for the T=0 case?**

# Fixed-Node Green Function Monte Carlo approach at T=0



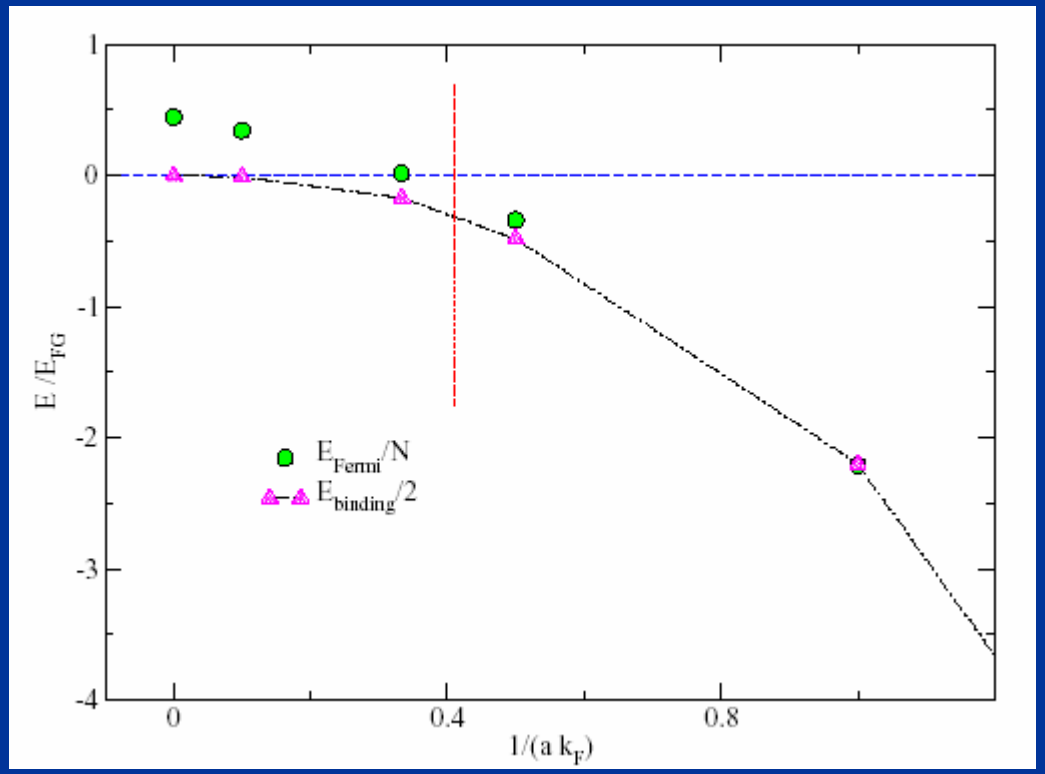




$$\Delta_{\mathrm{BCS}} \approx \frac{8}{\mathrm{e}^2}\varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

$$\Delta_{\mathrm{Gorkov}} \approx \left(\frac{2}{e}\right)^{7/3} \varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

Carlson *et al.* PRL 91, 050401 (2003)
Chang *et al.* PRA 70, 043602 (2004)
Astrakharchik *et al.* PRL 93, 200404(2004)




Even though two atoms can bind,
there is no binding among dimers!

Fixed node GFMC results, J. Carlson *et al.* (2003)

**One test of this theory:**

***Collective excitations***

$$\varepsilon(n) = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\left[\xi - \frac{\varsigma}{k_F a} - \frac{5\iota}{(k_F a)^2} + O\left(\frac{1}{(k_F a)^3}\right)\right]$$

$$\xi \approx 0.44, \qquad \varsigma \approx 1, \qquad \iota \approx 1$$

$$U = \frac{m\omega_0^2\left(x^2 + y^2 + \lambda^2 z^2\right)}{2}$$

$$\frac{\delta\omega^2}{\omega^2} = \frac{\varsigma}{\xi}\frac{1}{k_F(0)a}K$$

**Adiabatic regime, T=0**
**Spherical Fermi surface**

**Bogoliubov-Anderson modes in a trap**

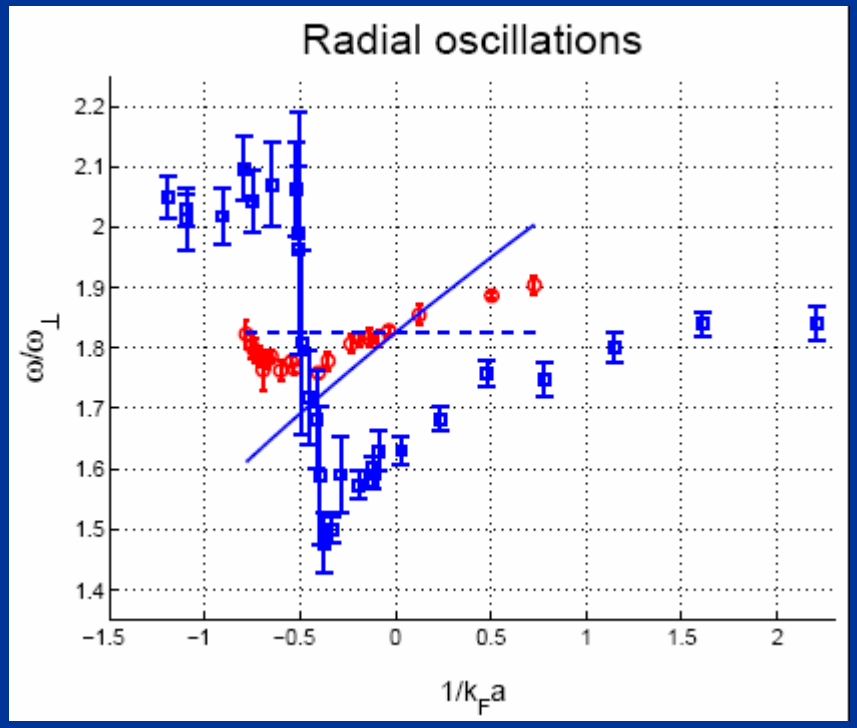
**Perturbation theory result using GFMC equation of state in a trap**

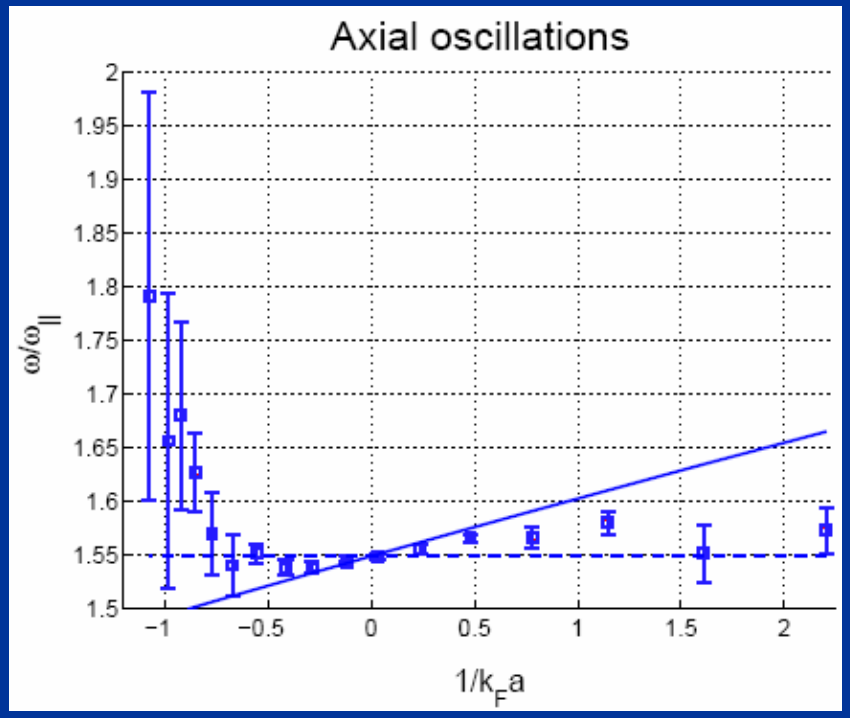
TABLE II: Results for $K$.

| trap type | mode | $f_1$ | $\omega$ | $K$ |
|---|---|---|---|---|
| spherical | dipole | $z$ | $\omega_0$ | 0 |
| $\lambda = 1$ | monopole | $1 - 2r^2$ | $2\omega_0$ | $\frac{256}{525\pi}$ |
| | quadrupole | $xy$ | $\sqrt{2}\omega_0$ | 0 |
| axial | $M = \pm 2$ | $xy,\ x^2 - y^2$ | $\sqrt{2}\omega_0$ | 0 |
| $\lambda \ll 1$ | $M = \pm 1$ | $xz,\ yz$ | $\omega_0$ | 0 |
| | radial | $x^2 + y^2 + \frac{2}{5}\lambda^2 z^2 - \frac{2}{5}$ | $\sqrt{\frac{10}{3}}\omega_0$ | $\frac{1024}{2625\pi}$ |
| | axial | $1 - 6\lambda^2 z^2$ | $\sqrt{\frac{12}{5}}\lambda\omega_0$ | $\frac{256}{2625\pi}$ |

**Only compressional modes are sensitive to the equation of state and experience a shift!**

Innsbruck's results - blue symbols
Duke's results - red symbols




First order perturbation theory prediction (blue solid line)

Unperturbed frequency in unitary limit (blue dashed line)
Identical to the case of non-interacting fermions

**If the matter at the Feshbach resonance would have a bosonic character then the collective modes will have significantly higher frequencies!**

# Theory for fermions at T >0 in the unitary regime

**Put the system on a spatio-temporal lattice and use a path integral formulation of the problem**

# 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

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

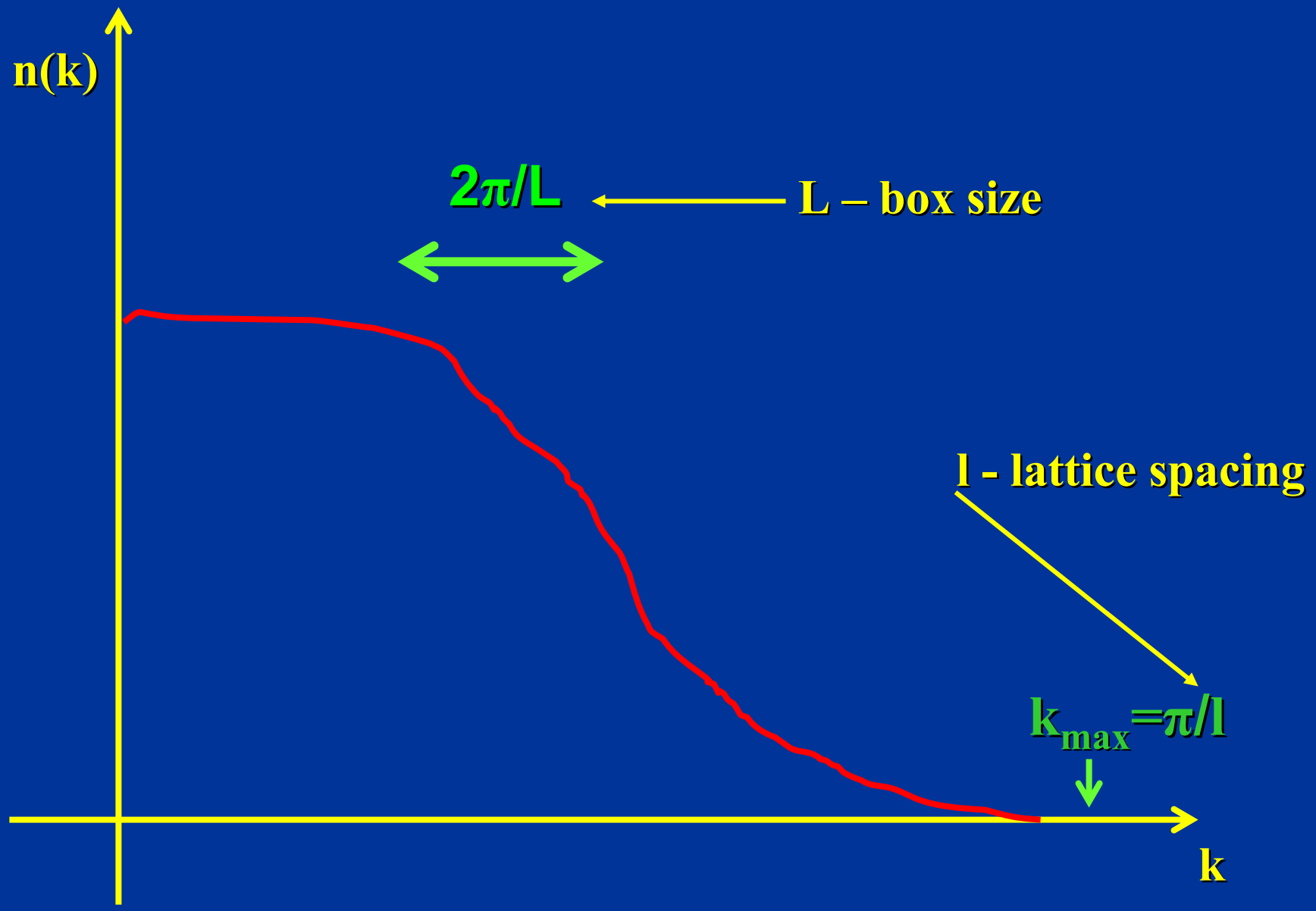
Discrete Hubbard-Stratonovich transformation

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

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




**How to choose the lattice spacing and the box size**

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

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

**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!**

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

**<u>All traces can be expressed through these single-particle density matrices</u>**

# More details of the calculations:

- Lattice sizes used from $\underline{6^3 \times 300}$ (high Ts) to $\underline{6^3 \times 1361}$ (low Ts)

$8^3$ running (incomplete, but so far no surprises) and larger sizes to come

- 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

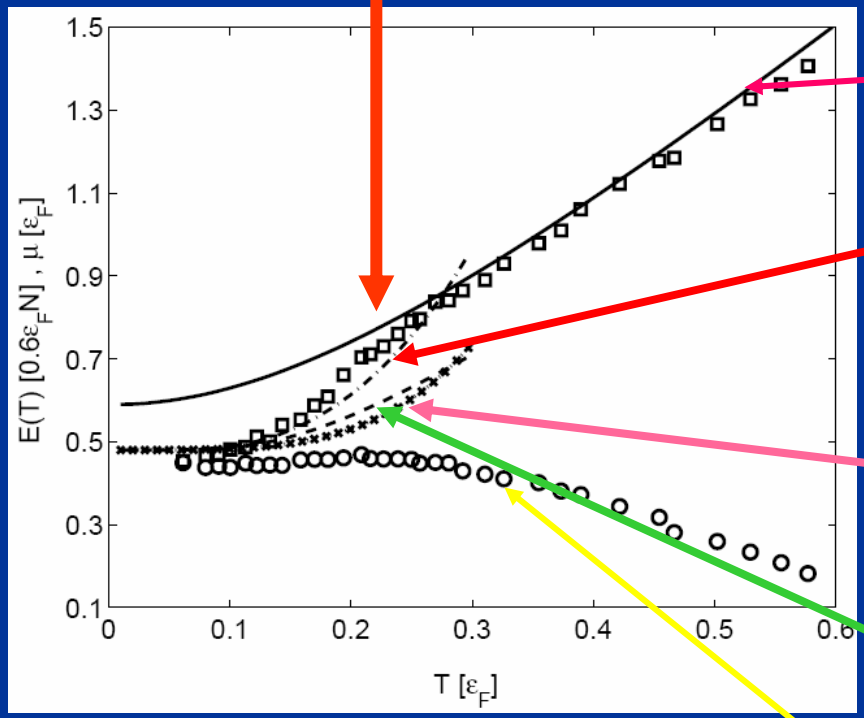
- At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics

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

- MC correlation "time" $\approx$ 250 – 300 time steps at $T \approx T_c$

# $a = \pm\infty$

# Superfluid to Normal Fermi Liquid Transition




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

Bogoliubov-Anderson phonons and quasiparticle contribution (dot-dashed lien )

Bogoliubov-Anderson phonons contribution only (little crosses)
People never consider this ???

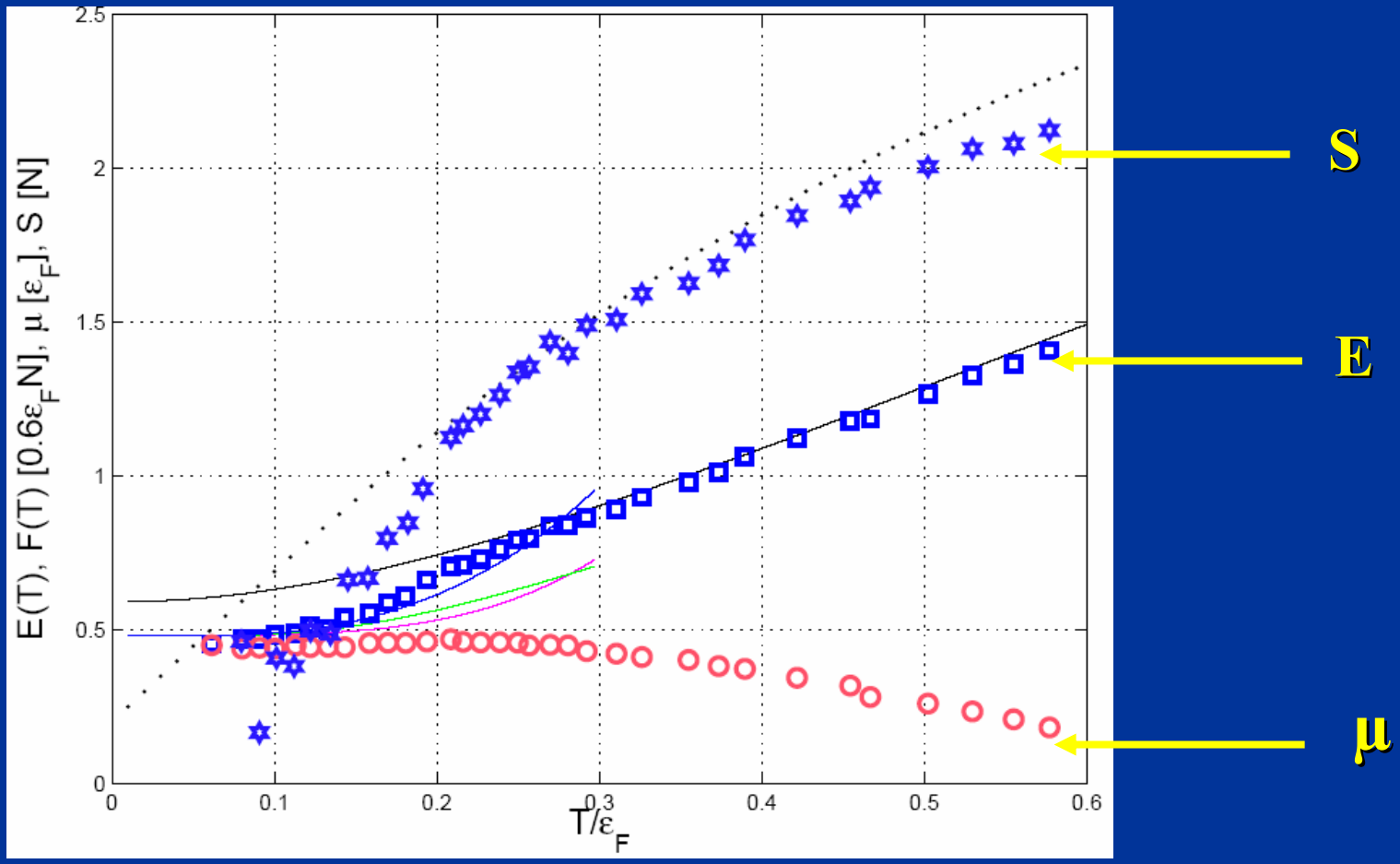
Quasi-particles contribution only (dashed line)

μ - chemical potential (circles)

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

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

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




$$E = \frac{3}{5}\varepsilon_F(n)N\ e\left(\frac{T}{\varepsilon_F(n)}\right) = \varepsilon(n)nV$$

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

$$S = N\sigma\left(\frac{T}{\varepsilon_F(n)}\right), \quad P = \frac{2}{3}\varepsilon(n)n$$

# Specific heat of a fermionic cloud in a trap

- Typical traps have a cigar/banana shape and one distinguish several regimes because of geometry only!
  - Specific heat exponentially damped if $T \ll \hbar\omega_{\parallel}$
  - If $\hbar\omega_{\parallel} \ll T \ll \hbar\omega_{\perp}$ then $E(T) \approx E_{gs} + \frac{\sqrt{3}\pi^2}{6}\frac{T^2}{\hbar\omega_{\parallel}}$
  - If $T \gg \hbar\omega_{\perp}$ then surface modes dominate

$$E(T) = E_{gs} + \sum_{nl} \frac{(2l+1)\hbar\Omega_{nl}}{\exp(\beta\hbar\Omega_{nl})-1} \approx E_{gs} + 142\frac{T^5}{\hbar^4\omega^4}$$

**Unexpected!**

$$\hbar\Omega_{nl} = \hbar\omega\sqrt{\frac{4}{3}n(n+l+2)+l} \approx \hbar\omega\sqrt{l}$$

$$E(T) = E_{gs} + \frac{3^{1/2}\pi^4}{10}\frac{T^4}{\hbar^3\omega^3}$$

**Expected bulk behavior (if no surface modes)**

# Experiments performed so far

Even though all these features are compatible with superfluidity, none of them really imply them. Their presence is merely a pretty good though circumstantial evidence.

- Existence of condensate
- Existence of an excitation gap
- Collective oscillations
- Expansion
- Caloric curve, specific heat

<u>Superfluidity means superflow</u> $\longrightarrow$ Vortices!

# Superfluid LDA (SLDA)

number and kinetic densities

anomalous density

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

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

Divergent!

$$\mathrm{E} = \int d^3r \left\{ \frac{\hbar^2}{2m}\tau(\vec{r}) + \frac{\hbar^2}{m}\beta\left[x(\vec{r})\right]n(\vec{r})^{5/3} - \Delta\left[x(\vec{r})\right]\nu^*(\vec{r}) \right\}$$

Cutoff and position running coupling constant!

$$\Delta\left[x(\vec{r})\right] = -\frac{\hbar^2}{m}\frac{\gamma_{eff}\left[x(\vec{r})\right]}{n(\vec{r})^{1/3}}\nu(\vec{r}), \qquad x(\vec{r}) = \frac{1}{k_F(\vec{r})a}$$

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

Bogoliubov-de Gennes like equations.
Correlations are however included by default!

# Vortex in fermion matter

$$\begin{pmatrix} \mathrm{u}_{\alpha\,\mathrm{kn}}(\vec{r}) \\ \mathrm{v}_{\alpha\,\mathrm{kn}}(\vec{r}) \end{pmatrix} = \begin{pmatrix} \mathrm{u}_{\alpha}(\rho)\exp[i(n+1/2)\phi - ikz] \\ \mathrm{v}_{\alpha}(\rho)\exp[i(n-1/2)\phi - ikz] \end{pmatrix}, \quad \mathrm{n} \text{ - half-integer}$$

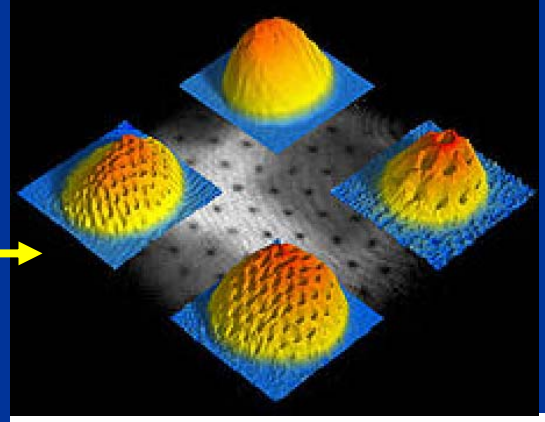
$$\Delta(\vec{r}) = \Delta(\rho)\exp(i\phi), \qquad \vec{r} = (\rho, \phi, z) \text{ [cyllindrical coordinates]}$$

Oz - vortex symmetry axis

Ideal vortex, Onsager's quantization (one $\hbar$ per Cooper pair)

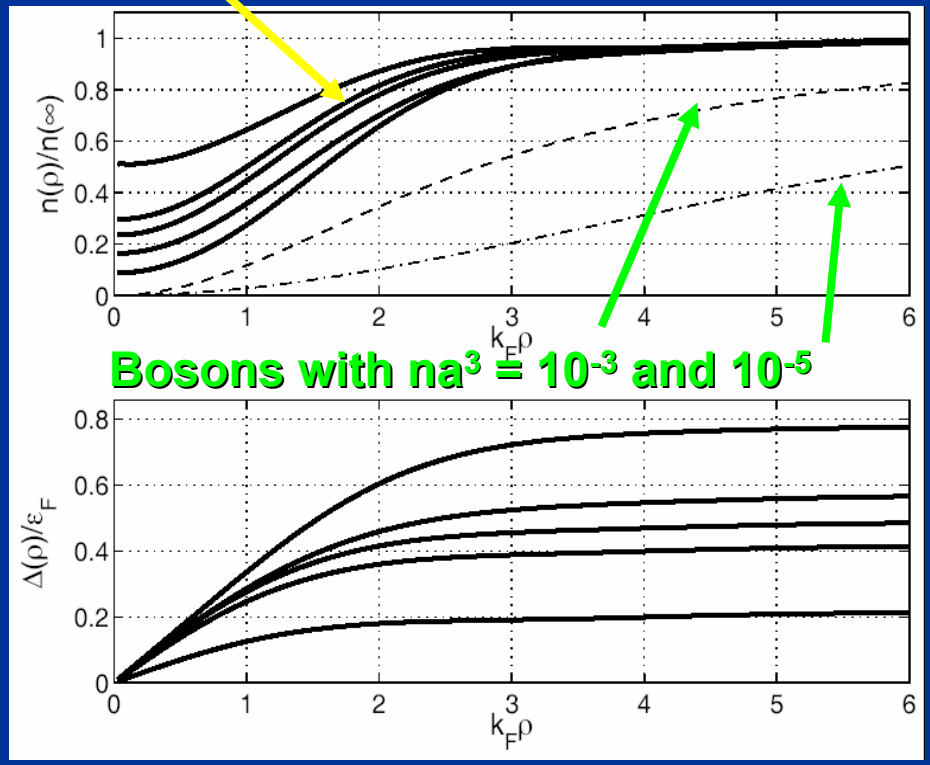
$$\vec{\mathrm{V}}_{\mathrm{v}}(\vec{r}) = \frac{\hbar}{2m\rho^2}(y, -x, 0) \quad \Leftarrow \quad \frac{1}{2\pi}\oint_C \vec{\mathrm{V}}_{\mathrm{v}}(\vec{r})\cdot d\vec{r} = \frac{\hbar}{2m}$$

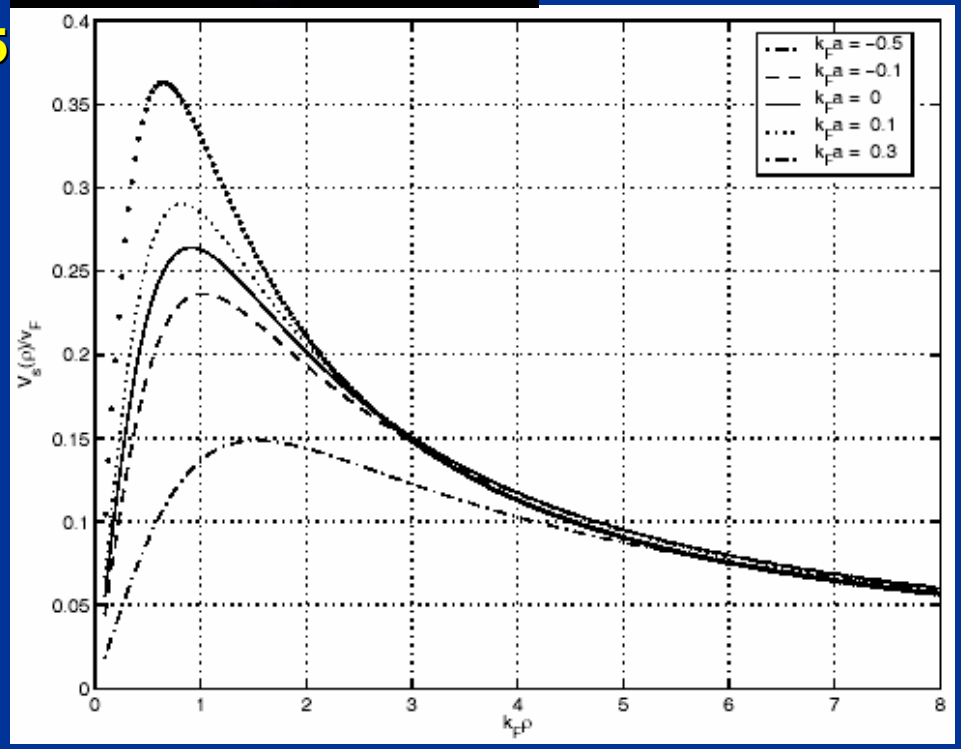
The depletion along the vortex core is reminiscent of the corresponding density depletion in the case of a vortex in a Bose superfluid, when the density vanishes exactly along the axis for 100% BEC.



From Ketterle's group

Fermions with $1/k_F a = 0.3, 0.1, 0, -0.1, -0.5$




Extremely fast quantum vortical motion!

Number density and pairing field profiles

Landau →

$$\frac{v_s}{v_F} < \frac{\Delta}{2\varepsilon_F} \propto \frac{T_c}{T_F}$$

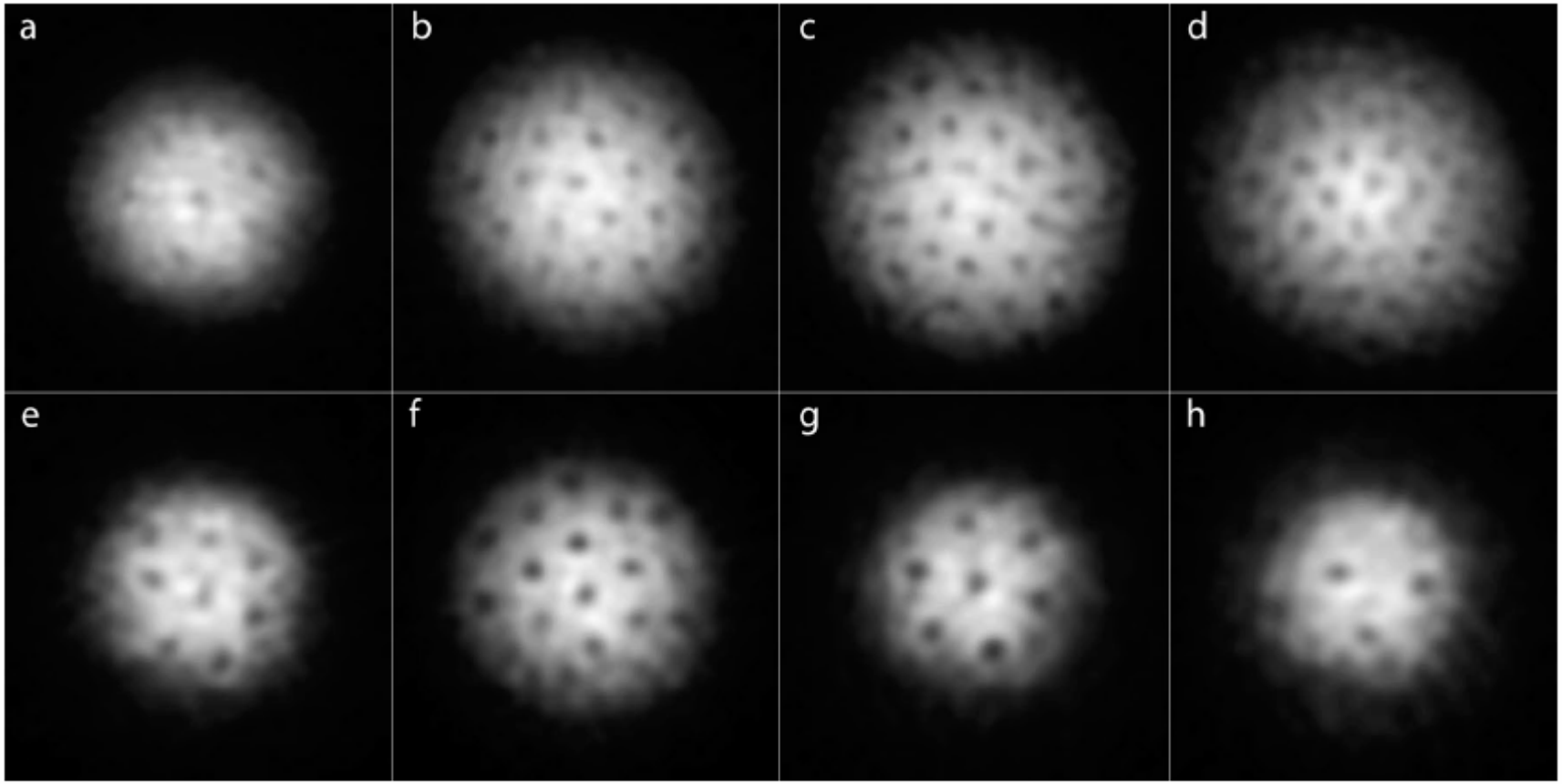



Fig. 2: Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) to 500 ms (b-h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the magnetic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

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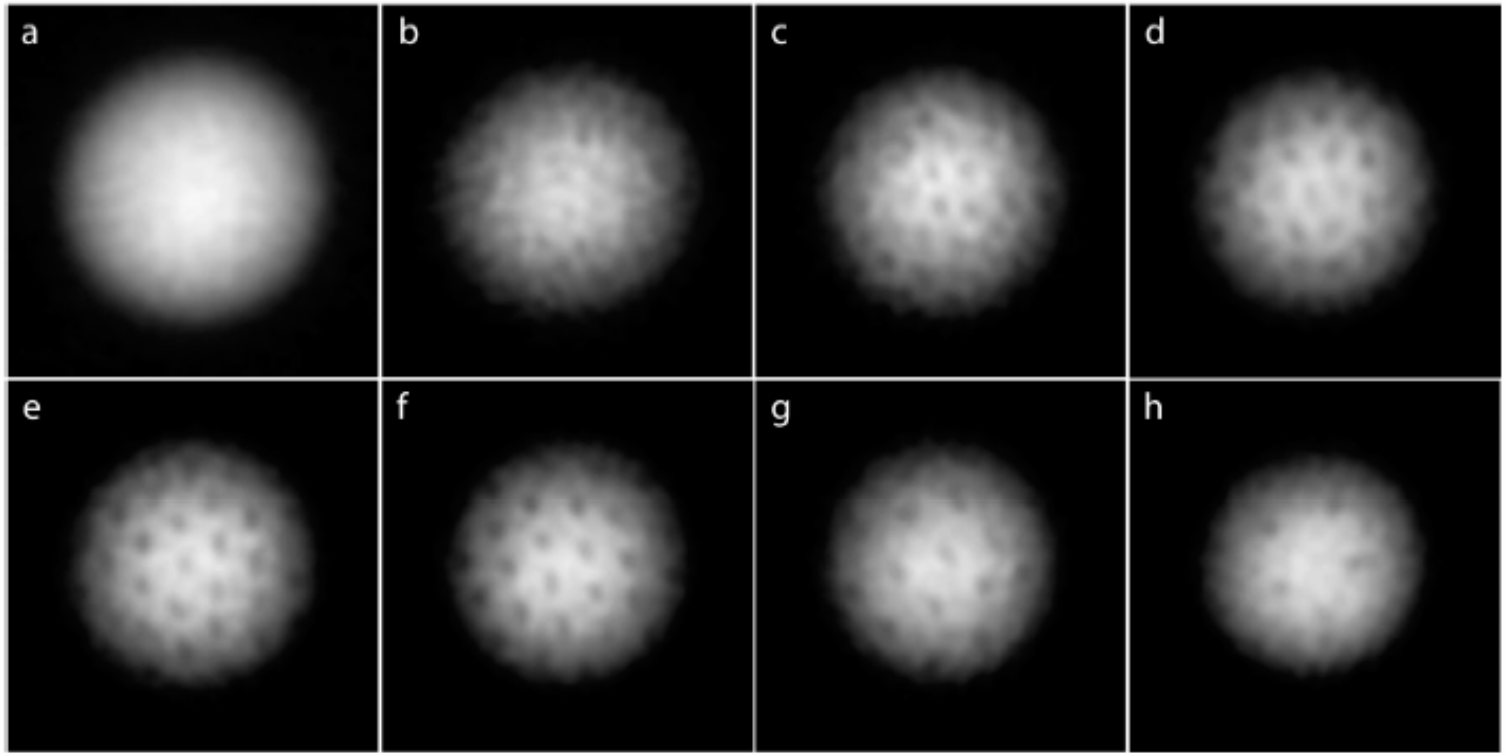


Fig. 6: Formation and decay of a vortex lattice in a fermion pair condensate on the BEC-side close to the Feshbach resonance. A molecular condensate, prepared at 766 G as shown in (a), was stirred for 800 ms. The field was then ramped to 812 G in 20 ms for equilibration. At this field, $1/k_F a = 0.35$, and the condensate was deep in the strongly interacting regime. To observe the vortex lattice, the field was ramped in 25 ms to 735 G ($1/k_F a = 2.3$), where the condensate was released from the trap and imaged after 12 ms time-of-flight. The equilibration times after the end of the stirring were (b) 40 ms, (c) 240 ms, (d) 390 ms, (e) 790 ms, (f) 1140 ms, (g) 1240 ms and (h) 2940 ms. Due to stirring, evaporation and vibrational relaxation, the number of fermion pairs decayed from $3\times10^6$ (a) to $1\times10^6$ (b-h). The field of view of each image is $830\ \mu\text{m}\times830\ \mu\text{m}$.

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

T

## "Before"- Life

Atoms form rather unstable couples, spread over large distances, with many other couples occupying the same space

## LIFE!

Atoms form strong couples, living as in an apartment building, in close proximity of one another, and obviously anoying each other quite a bit

## After – Life

Atoms form very strong couples, mostly inert and at rest, ***halo dimers***, widely separated from one another and weakly interacting

**weak interaction** | **Strong interaction** | **weak interactions**

$a<0$
no 2-body bound state

$a>0$
shallow 2-body bound state
**halo dimers**

1/a

# Conclusions

✓ **Fully non-perturbative calculations for a spin ½ many fermion system in the unitary regime at finite temperatures are feasible and apparently the system undergoes a phase transition in the bulk at Tc = 0.22 (3) εF**

(One variant of the fortran 90 program, version in matlab, has about 500 lines, and it can be shortened also. This is about as long as a PRL!)

✓ **Vortices and superfluidity became, <u>at last</u>, mainstream**