# BEC collisions

## Quantum dynamics simulation in a macroscopic system


Piotr Deuar

(LPTMS, Orsay)


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*Collaborations:*

Gora Shlyapnikov *(LPTMS)*

Chris Westbrook *(Institut d'Optique)*

Vanessa Leung

Aurelién Perrin

Denis Boiron

Karen Kheruntsyan *(Uni. Queensland)*

Marek Trippenbach *(Warsaw University)*

Paweł Ziń

Jan Chwedeńczuk

# To what degree is [ BEC = coherent matter wave ] ?

- Basic "canonical" description:
  $N \gg 1$ atoms all in one orbital ( $\implies$ needs low $T$).

- Mean-field description is the coherent boson field $\Psi(x,t)$.

- Dynamics "usually" has obeyed the mean field Gröss-Pitaevskii (GP) equation, with $g = 4\pi\hbar^2 a_s/m$

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \left\{-\frac{\hbar^2\nabla^2}{2m} + V(x) + g|\Psi(x,t)|^2\right\}\Psi(x,t)$$

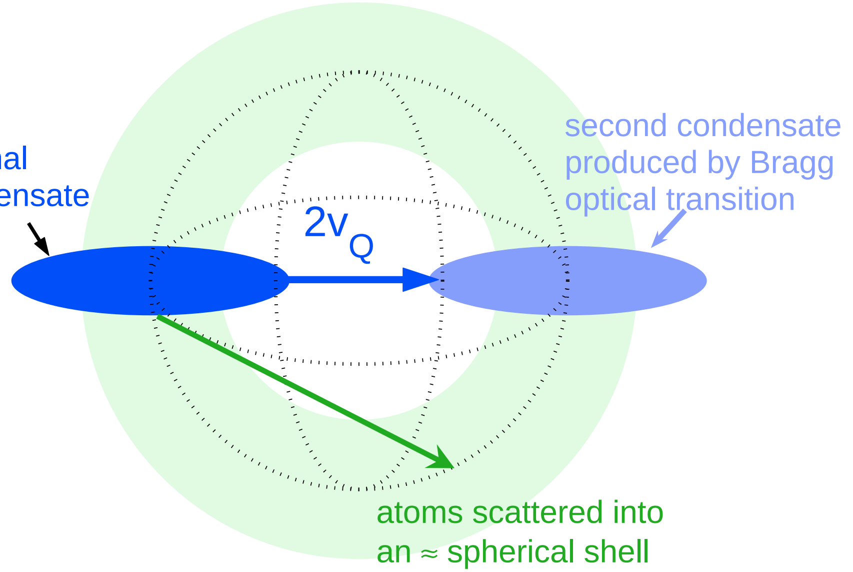
- similar to coherent laser field with Kerr $\chi^{(3)}$ nonlinearity.

- Well, it's been a good description, *UNLESS*:

1. Motion is supersonic — speed of sound $c(x) = \sqrt{gn(x)/m}$
2. OR, Details on scales smaller than the healing length $\xi(x) = \hbar/mc\sqrt{2}$ are important

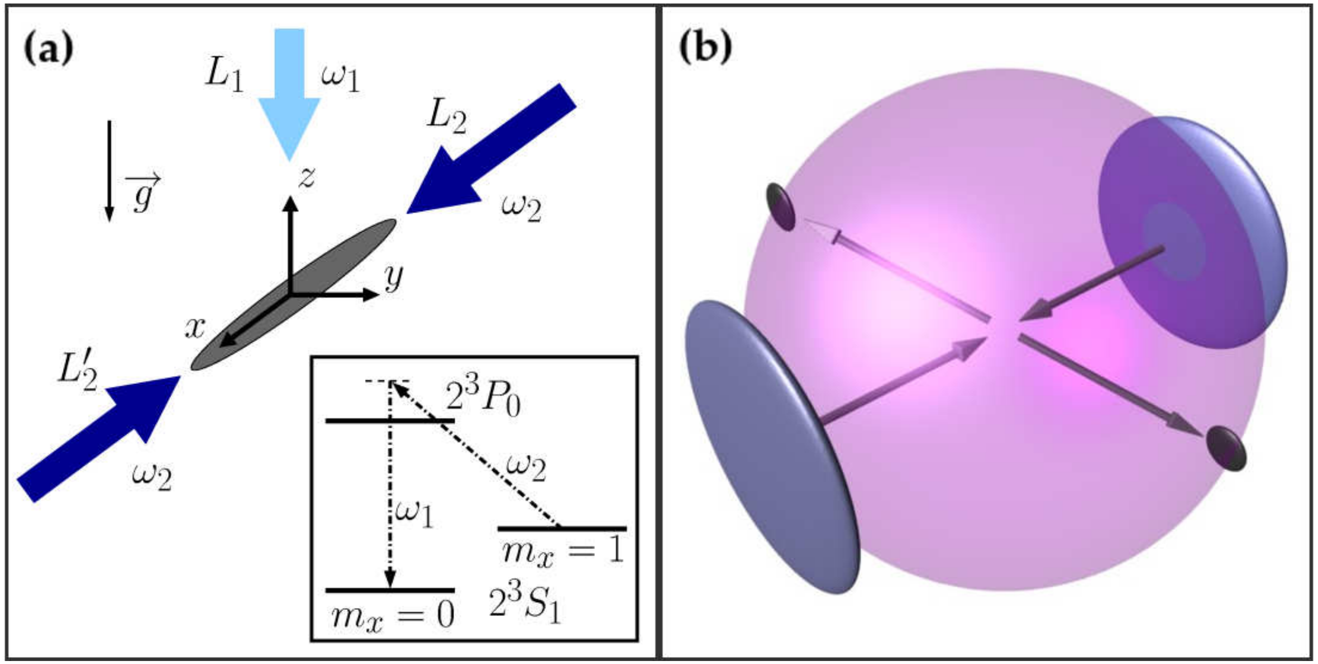
# Supersonic BEC collision

Schematic in x-space:



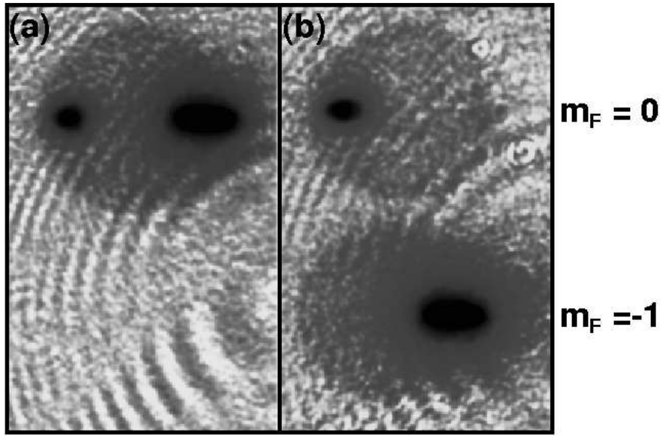

Lasers in x-space

View in k-space



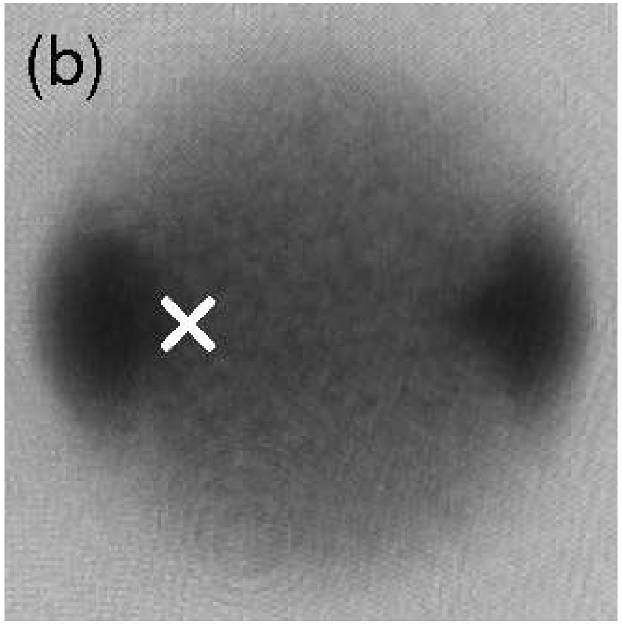

From A. Perrin *et al.*,
PRL **99** 150405 (2007)

# Experimental examples

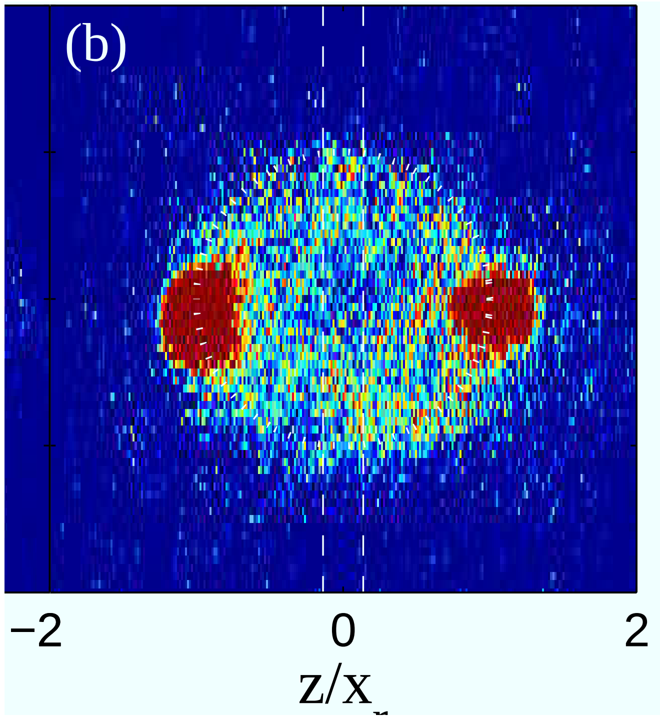



Integrated density

From A.P. Chikkatur *et al.*, PRL **85**, 483 (2000).



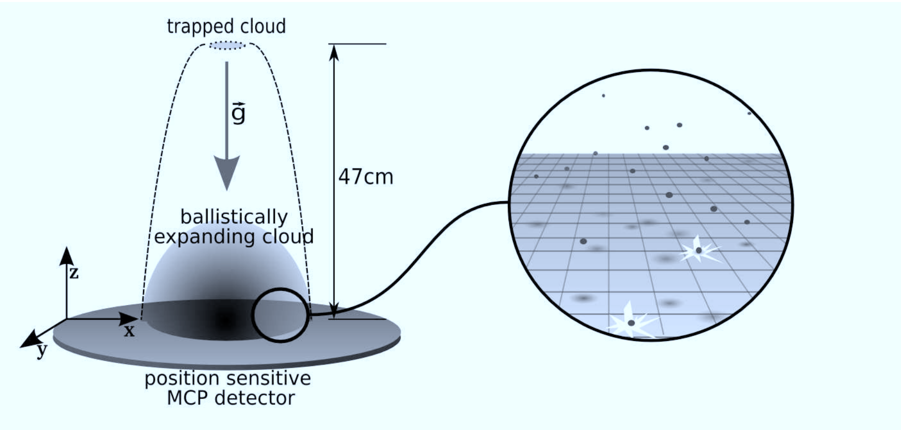

From J.M. Vogels *et al.*,
PRL **89**, 020401 (2002).




From N. Katz *et al.*, PRL **95**, 220403 (2005).

# Metastable He* experiment

Uses multi-channel plate – Allows mapping of 3D atom distribution

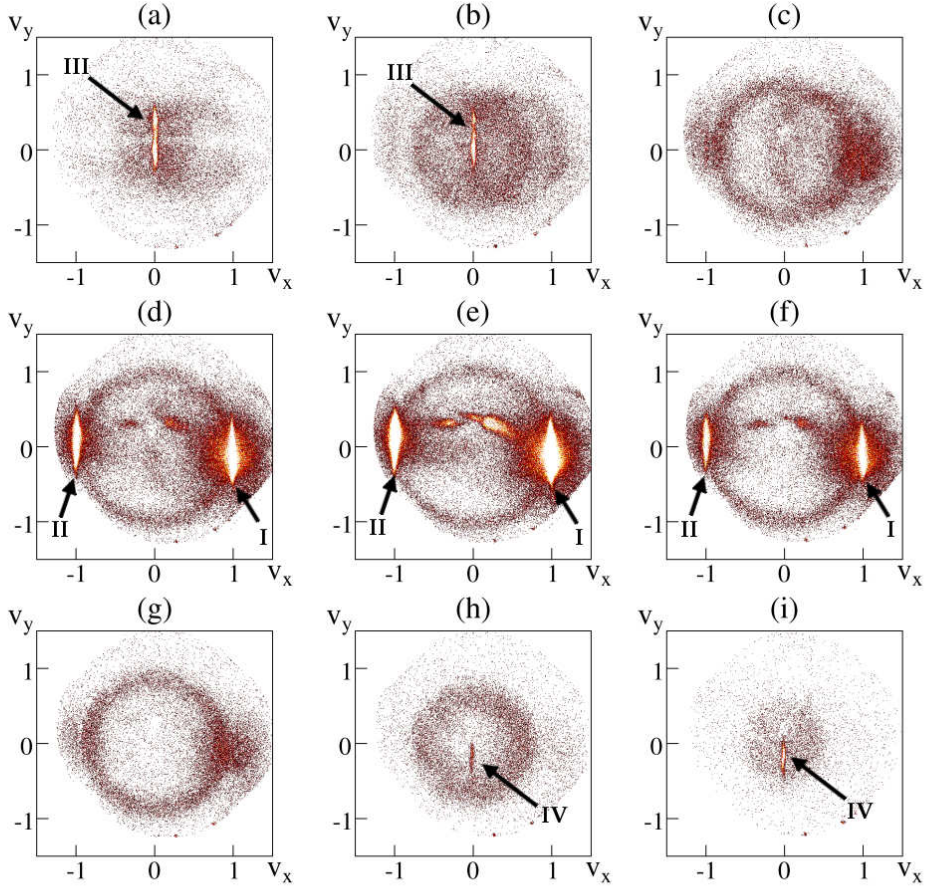



From M. Schellekens *et al.*,

Science **310**, 648 (2005).

After long time of flight,

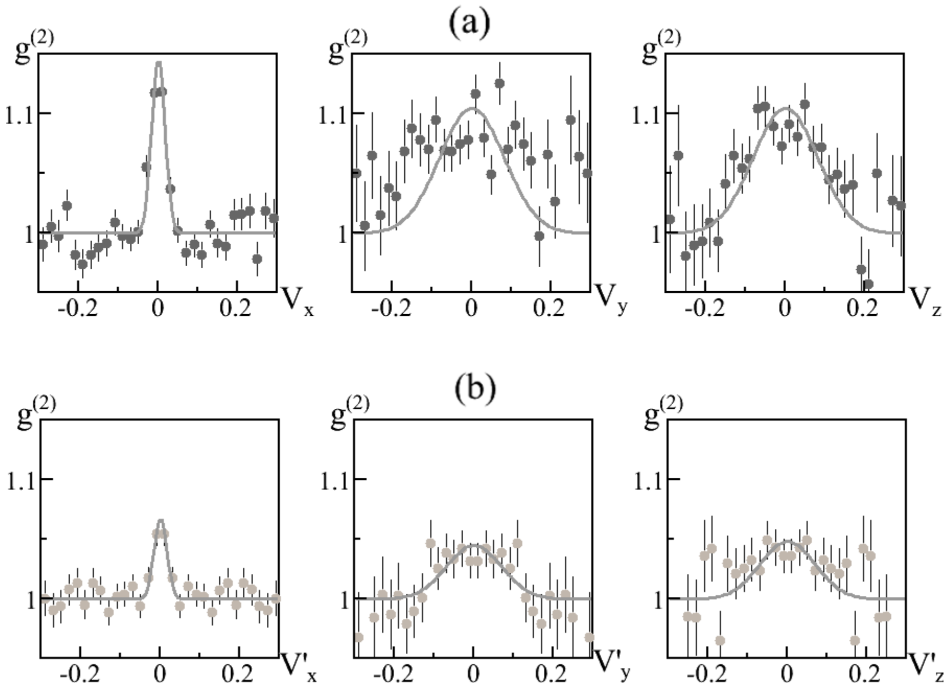
$n(x,t) \rightarrow n(k,0)$




From A. Perrin *et al.*, PRL **99** 150405 (2007)

# Allows measurement of correlations - density $g^{(2)}$

$$g^{(2)}(k,k') = \frac{\langle \hat{n}(k)\hat{n}(k')\rangle}{\langle \hat{n}(k)\rangle\langle \hat{n}(k)\rangle}$$




Back-to-Back $k' \sim -k$

Collinear $k' \sim k$

From A. Perrin *et al.*, PRL **99** 150405 (2007)

# Another interesting issue – Phase grains

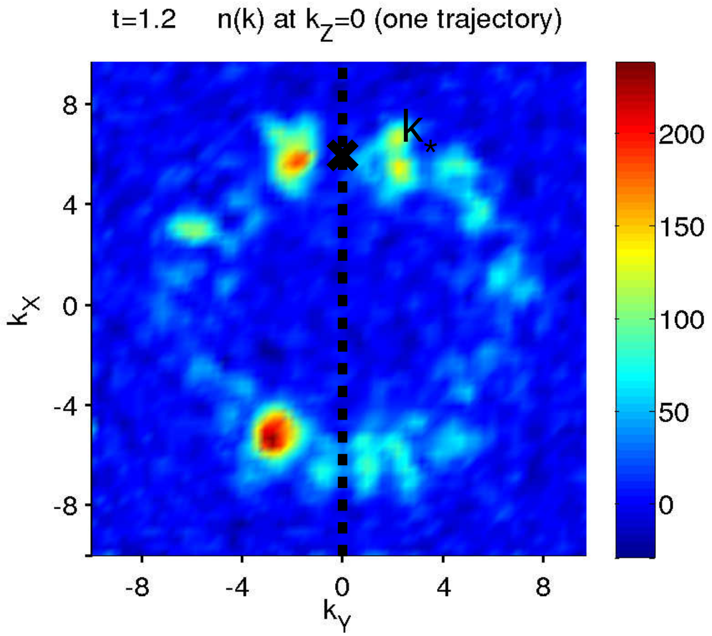
Coherence: $$g^{(1)}(k,k+\delta k) = \frac{\langle \widehat{\Psi}^\dagger(k)\widehat{\Psi}(k+\delta k)\rangle}{\sqrt{\langle \widehat{n}(k)\rangle\langle \widehat{n}(k+\delta k)\rangle}}$$

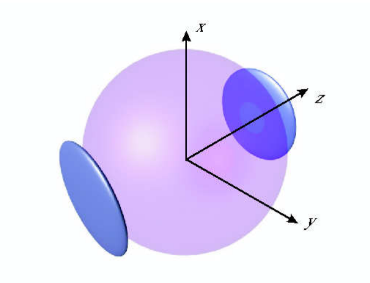
– Locally coherent regions. $|g^{(1)}| \gg 0$ Norrie *et al.*, PRL **94**, 040401 (2005)

– Scattering rate into such a coherent region with $n$ atoms is $\propto (1+n)$

$\longrightarrow$ Bose stimulation if $n \gtrsim 1$ leads to rapid coherent growth of occupation of the phase grain

$\longrightarrow$ Mini condensates formed.

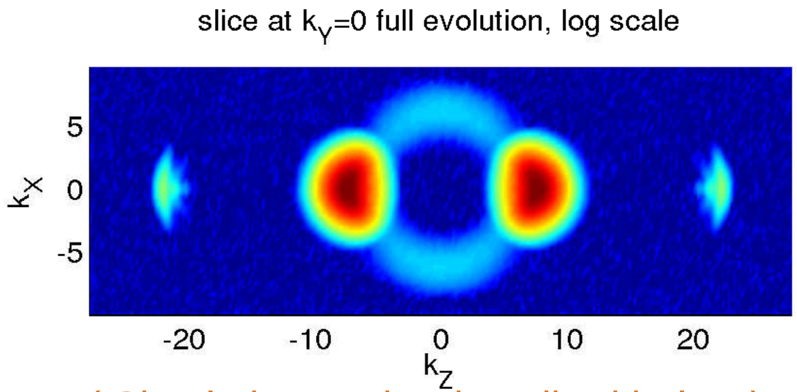


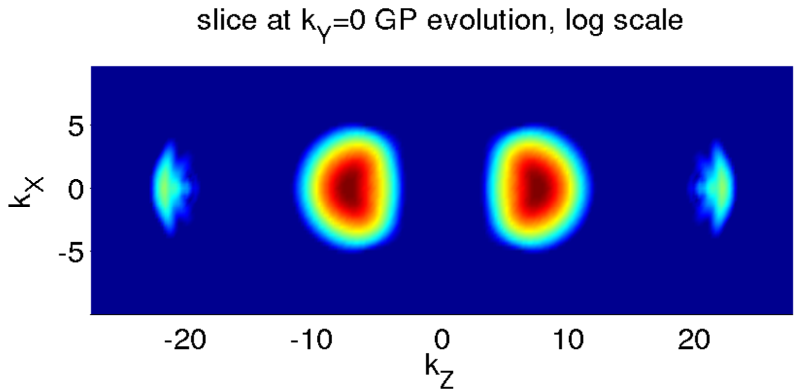
# Why is mean field no good here?

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t}=\left\{-\frac{\hbar^2\nabla^2}{2m}+V(x)+g|\Psi(x,t)|^2\right\}\Psi(x,t)$$

In the halo, initial condensate field $\Psi(x,0)$ is zero, and so stays that way.



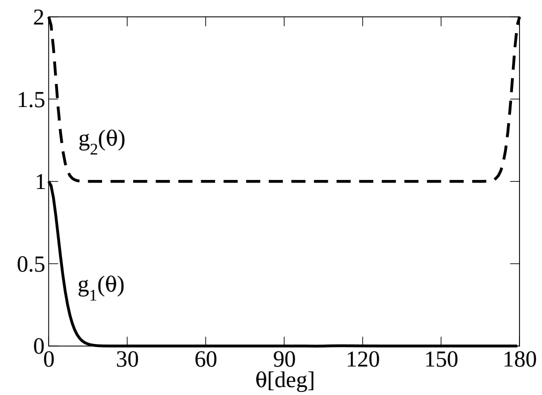

( Simulations to be described below )



# What about simple analytic models?

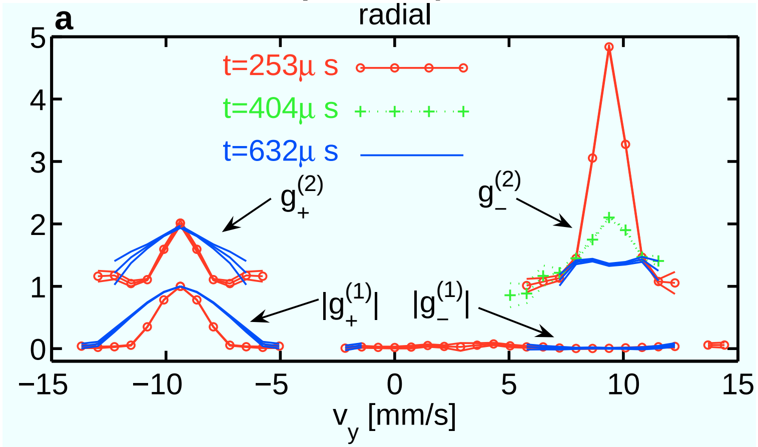
This has been done with Bogoliubov quasiparticles + extra simplifying assumptions. Works in special cases:

Limit of very fast collision



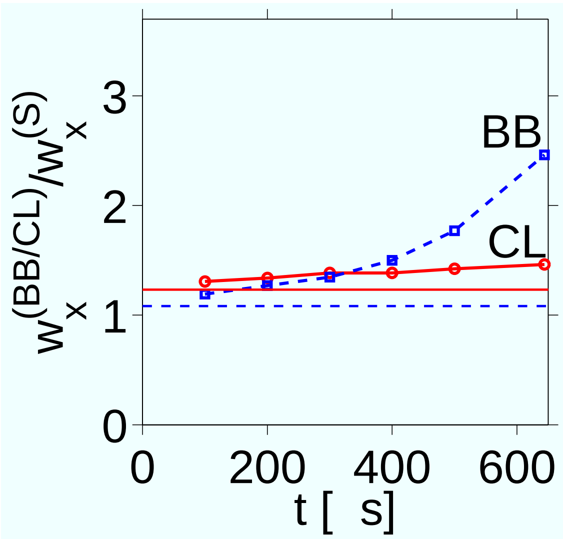

From P. Ziń *et al.*, PRL **94** 200401 (2005)

Moderate speed (ab initio simulation)




PD & P. Drummond, PRL **98** 120402 (2007)

Short-time evolution

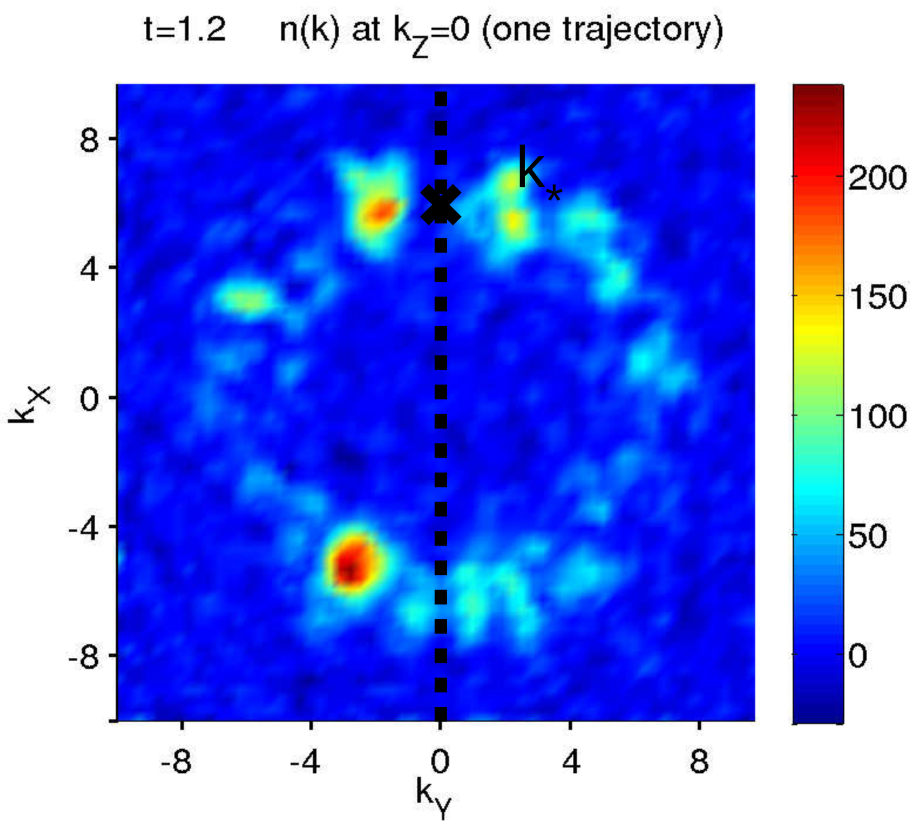


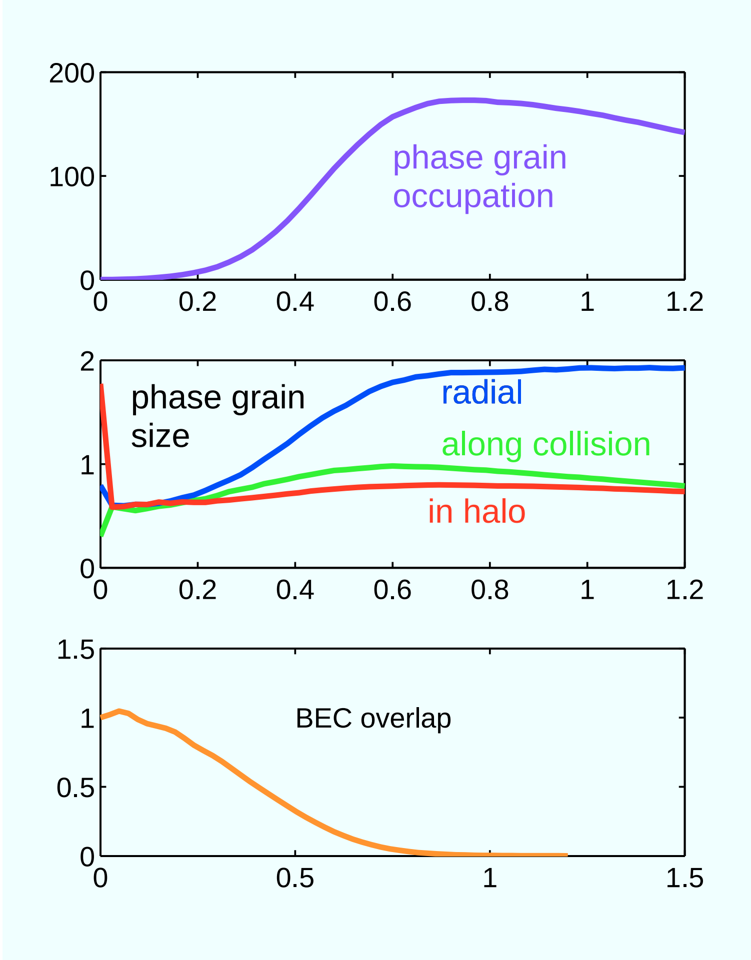

From:

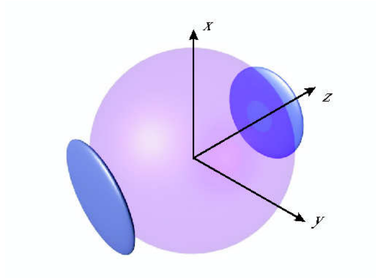
M. Ögren & K.V. Kheruntsyan,

PRA **79** 021606(R) (2009)

# Phase grain formation – a complicated business



# Understanding the dynamics – The plan

$$\widehat{H} = \int dx \widehat{\Psi}^{\dagger}(x) \left\{ -\frac{\hbar^2 \nabla^2}{2m} + \frac{g}{2} \widehat{\Psi}^{\dagger}(x) \widehat{\psi}(x) \right\} \widehat{\Psi}(x)$$

- Discretize the Hamiltonian onto a lattice : produces a Bose-Hubbard Hamiltonian

- Simulate the system numerically

- Pick a regime where the complicated business happens
  – Bose enhancement significant
  – Speed not *too* supersonic
  – Spherical condensates for simplicity

- Dissect the Hamiltonian term by term to see which process produces what.

# Bogoliubov Hamiltonian

1. Write $\widehat{\Psi}(x,t) = \phi(x,t) + \widehat{\psi}_B(x,t)$

2. Substitute into full $\widehat{H}$

3. <u>Assume</u> $\widehat{\psi}_B(x,t)$ is orthogonal to $\phi(x,t)$.

4. <u>Assume</u> $\delta N$ the number of particles contained in $\widehat{\psi}_B$ is $\ll N$, the total number.

5. Remove terms of high order in $\delta N/N$ (quantum depletion) from $\widehat{H}$ to obtain $\widehat{H}_B$

6. For later convenience, separate right- and left-moving condensates (velocities $\approx \pm k_C$) into $\phi(x,t) = \phi_L(x,t) + \phi_R(x,t)$.

# time-dependent Bogoliubov Hamiltonian

$$\widehat{H}_B = \int dx \left\{ \widehat{\psi}_B^\dagger \left( -\frac{\hbar^2 \nabla^2}{2m} \right) \widehat{\psi}_B \right.$$ K.E.

$$+2g|\phi(t)|^2 \widehat{\psi}_B^\dagger \widehat{\psi}_B$$ collective potential

$$+2g\phi_L(t)\phi_R(t)(\widehat{\psi}_B^\dagger)^2 + \text{h.c.}$$ pair production

$$\left. +g\left[\phi_L(t)^2 + \phi_R(t)^2\right](\widehat{\psi}_B^\dagger)^2 + \text{h.c.} \right\}$$ off-resonant

$$\phi(x,t) = \phi_L(x,t) + \phi_R(x,t)$$

$$i\hbar \frac{d\phi_R(x,t)}{dt} = \left\{ -\frac{\hbar^2}{2m}\nabla^2 + g\left[|\phi_R(x,t)|^2 + 2|\phi_L(x,t)|^2 + \phi_L^*(x,t)\phi_R(x,t)\right] \right\} \phi_R(x,t)$$

$$i\hbar \frac{d\phi_L(x,t)}{dt} = \left\{ -\frac{\hbar^2}{2m}\nabla^2 + g\left[|\phi_L(x,t)|^2 + 2|\phi_R(x,t)|^2 + \phi_R^*(x,t)\phi_L(x,t)\right] \right\} \phi_L(x,t)$$

# A “technical” difficulty

- Experimentally realistic situations require $10^5 - 10^7$ lattice points.

- Standard Bogoliubov quasiparticle evolution procedure requires diagonalization, finding of eigenstates, etc.

- For a strongly evolving condensate as here — need to diagonalize at each time step, and project old $\widehat{\psi}_B(x,t)$ onto new $\widehat{\psi}_B(x,t+\Delta t)$.

SOLUTION:

Instead, the dynamics of $\widehat{\psi}_B$ can be treated stochastically using the positive-P representation…

# Positive-P method

One writes the density matrix of the system on $M$ lattice points in coherent states $|\psi_j(x)\rangle = e^{\psi_j(x)\widehat{\Psi}_B^\dagger(x)}|0\rangle$ as

$$\widehat{\rho} = |\Psi\rangle\langle\Psi| = \int \mathcal{D}^{2M}\psi_1(x)\mathcal{D}^{2M}\psi_2(x)\, P(\psi_1(x),\psi_2(x),t)\, |\psi_1(x)\rangle\langle\psi_2(x)|$$

– The distribution $P(\ldots)$ can be guaranteed non-negative real

– The complete quantum evolution of the state

$$i\hbar\frac{\partial\widehat{\rho}}{\partial t} = \left[\widehat{H}_B,\widehat{\rho}\right]$$

is equivalent to the random walk of an ensemble of $2M$ random variables $\psi_j(x,t)$.

– Expectation values of observables are equivalent to ensemble averages of the variables.

– Most complexity gets shoved into the ensemble, and hopefully averages out for most quantities of interest.

# Positive-P : evolution equations

GP + appropriate noise

$$
\begin{aligned}
i\hbar\frac{d\psi_1(x,t)}{dt} &= \left[-\frac{\hbar^2}{2m}\nabla^2 + 2g|\phi(x,t)|^2\right]\psi_1(x,t) \\
&= +g\phi(x,t)^2\psi_2(x,t)^* + i\sqrt{ig}\psi_1(x,t)\ \xi_1(x,t) \\
i\hbar\frac{d\psi_2(x,t)}{dt} &= \left[-\frac{\hbar^2}{2m}\nabla^2 + 2g|\phi(x,t)|^2\right]\psi_2(x,t) \\
&= +g\phi(x,t)^2\psi_1(x,t)^* + i\sqrt{ig}\psi_2(x,t)\ \xi_2(x,t)
\end{aligned}
$$

Here, $\xi_j(x,t)$ are independent Gaussian random variable fields with mean zero and variances $\langle\xi_i(x,t)\xi_j(x',t')\rangle = \delta_{ij}\delta(x-x')\delta(t-t')$.

The condensate field $\phi(x,t) = \phi_L(x,t) + \phi_R(x,t)$ itself evolves according to the unchanged GP evolution from before

# Positive-P : caveats

- Noisy and limited precision $\propto \sqrt{\text{number of trajectories}}$
- Amplification of noise can produce a signal-to-noise catastrophe after some evolution time.

# Positive-P : benefits

- Contains all two-body processes in the Hamiltonian

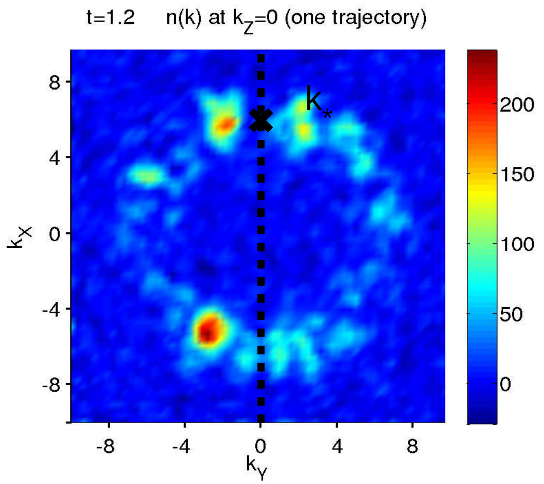
  With some small print

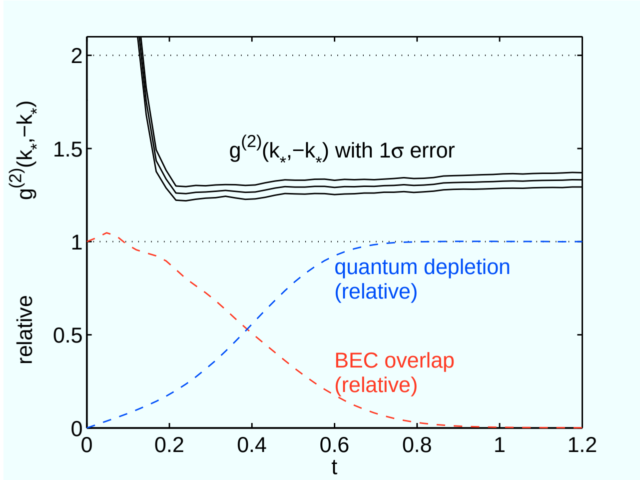
- Complexity of the description grows very slowly — linear in lattice size/atom number! $10^7$ atoms or lattice points is fine to simulate on a PC.

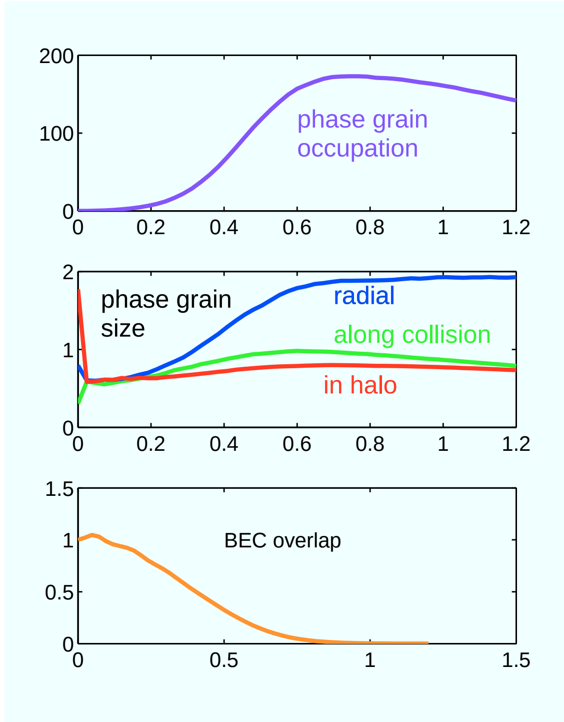
  With some small print

- Uncertainty in results can be reliably computed from the ensemble
- Equations and their integration in $t$ are only of similar complexity to the usual mean field GP equations.
- Lucky bonus: for our Bogoliubov Hamiltonian $\widehat{H}_B$, there is no noise catastrophe.

# What does one see?




QUESTIONS

– The dominant, resonant process is pair production. $k_C \& -k_C \implies k \& -k$

Such models give $g^{(2)}(k,-k) \to \geq 2$ (perfect pairs) at long times.

– How can the other "weak" processes destroy the pairing – and by so much?

– Why do the phase grains become elongated radially?

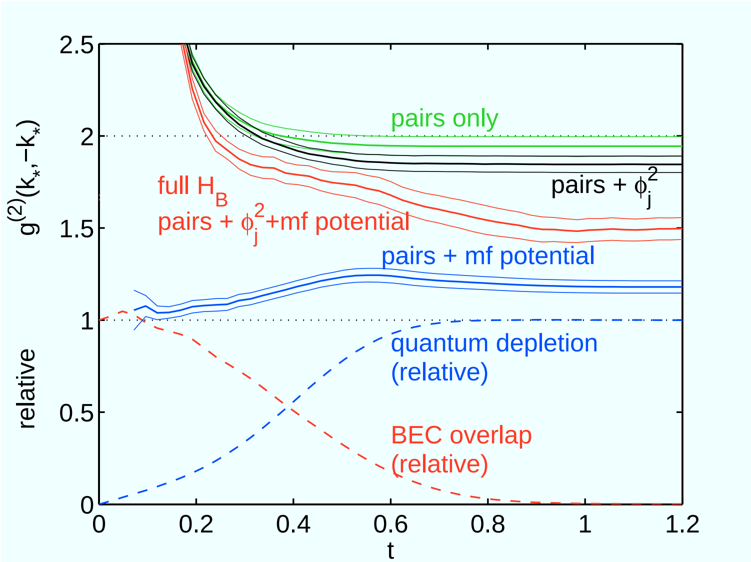
– Why do they degrade after the collision is finished?

– Other fun issues: halo mean radius $< k_C$, anisotropy in radius and width, evolution after apparent end of collision,. . .

# Pairing loss mechanism 1

Consider only rudimentary condensate evolution (stiff wavepackets)

$i\frac{d\phi_{L,R}}{dt} = -\frac{\hbar^2}{2m}\nabla^2\phi_{L,R}$, but various $\widehat{H}_B$

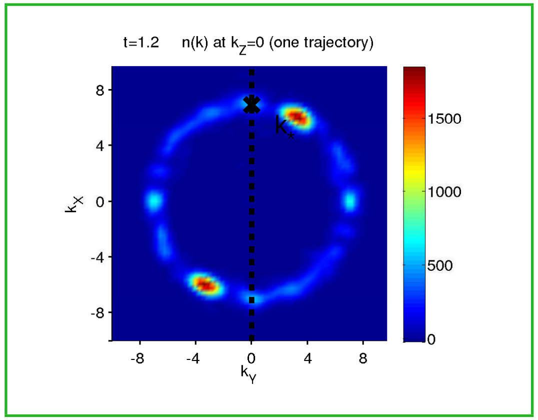


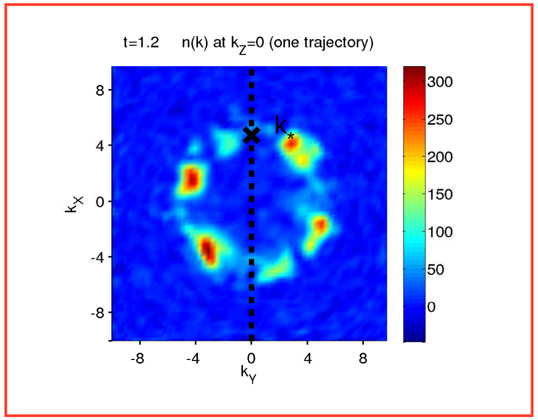

$$\widehat{\mathcal{H}}_B = \widehat{\Psi}_B^\dagger\left(-\frac{\hbar^2\nabla^2}{2m}\right)\widehat{\Psi}_B + 2g\phi_L\phi_R(\widehat{\Psi}_B^\dagger)^2 + \text{h.c.}$$

$$\widehat{\mathcal{H}}_B = \widehat{\Psi}_B^\dagger\left(-\frac{\hbar^2\nabla^2}{2m}\right)\widehat{\Psi}_B + g\phi^2(\widehat{\Psi}_B^\dagger)^2 + \text{h.c.}$$

$$\widehat{\mathcal{H}}_B = \widehat{\Psi}_B^\dagger\left(-\frac{\hbar^2\nabla^2}{2m}\right)\widehat{\Psi}_B + 2g|\phi|^2\widehat{\Psi}_B^\dagger\widehat{\Psi}_B + 2g\phi_L\phi_R(\widehat{\Psi}_B^\dagger)^2 + \text{h.c.}$$

$$\widehat{\mathcal{H}}_B = \widehat{\Psi}_B^\dagger\left(-\frac{\hbar^2\nabla^2}{2m}\right)\widehat{\Psi}_B + 2g|\phi|^2\widehat{\Psi}_B^\dagger\widehat{\Psi}_B + g\phi^2(\widehat{\Psi}_B^\dagger)^2 + \text{h.c.}$$



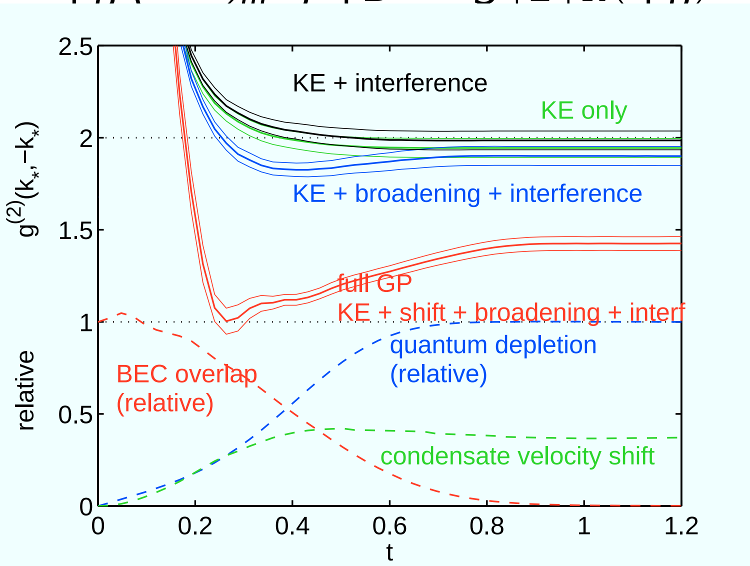




$\Longrightarrow$ After production, pairs can veer away from back-to-back alignment by rolling around on the anisotropic collective mean field of the condensates

# Pairing loss mechanism 2

Consider only rudimentary Bogoliubov process (pairs+K.E.)

$$\widehat{\mathcal{H}}_B = \widehat{\Psi}_B^\dagger \left(-\frac{\hbar^2\nabla^2}{2m}\right)\widehat{\Psi}_B + 2g\phi_L\phi_R(\widehat{\Psi}_B^\dagger)^2 + \text{h.c.},$$ but various GP evolutions

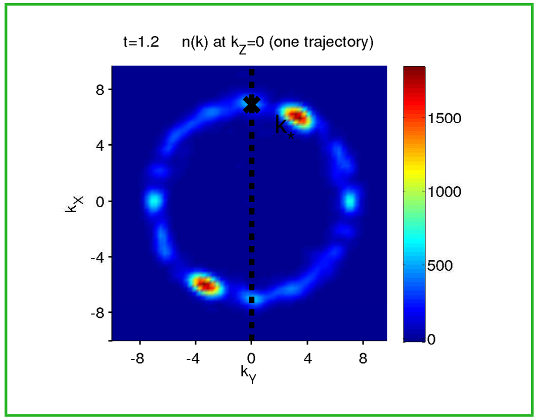


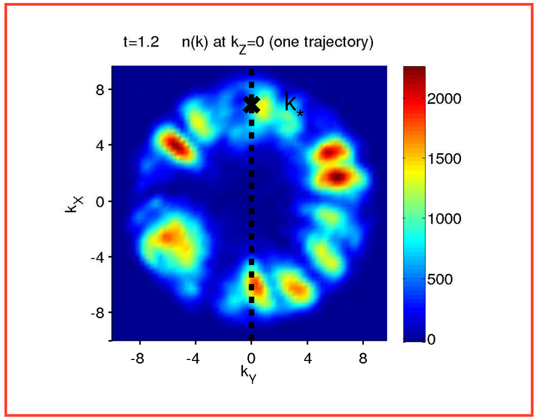

$$i\hbar\frac{d\phi_R}{dt} = -\frac{\hbar}{2m}\nabla^2\phi_R$$

$$i\hbar\frac{d\phi_R}{dt} = \left[-\frac{\hbar}{2m}\nabla^2 + g\phi_L^*\phi_R\right]\phi_R$$

$$i\hbar\frac{d\phi_R}{dt} = \left[-\frac{\hbar}{2m}\nabla^2 + g\left(|\phi_R|^2 + \phi_L^*\phi_R\right)\right]\phi_R$$

$$i\hbar\frac{d\phi_R}{dt} = \left[-\frac{\hbar}{2m}\nabla^2 + g\left(2|\phi_L|^2 + |\phi_R|^2 + \phi_L^*\phi_R\right)\right]\phi_R$$

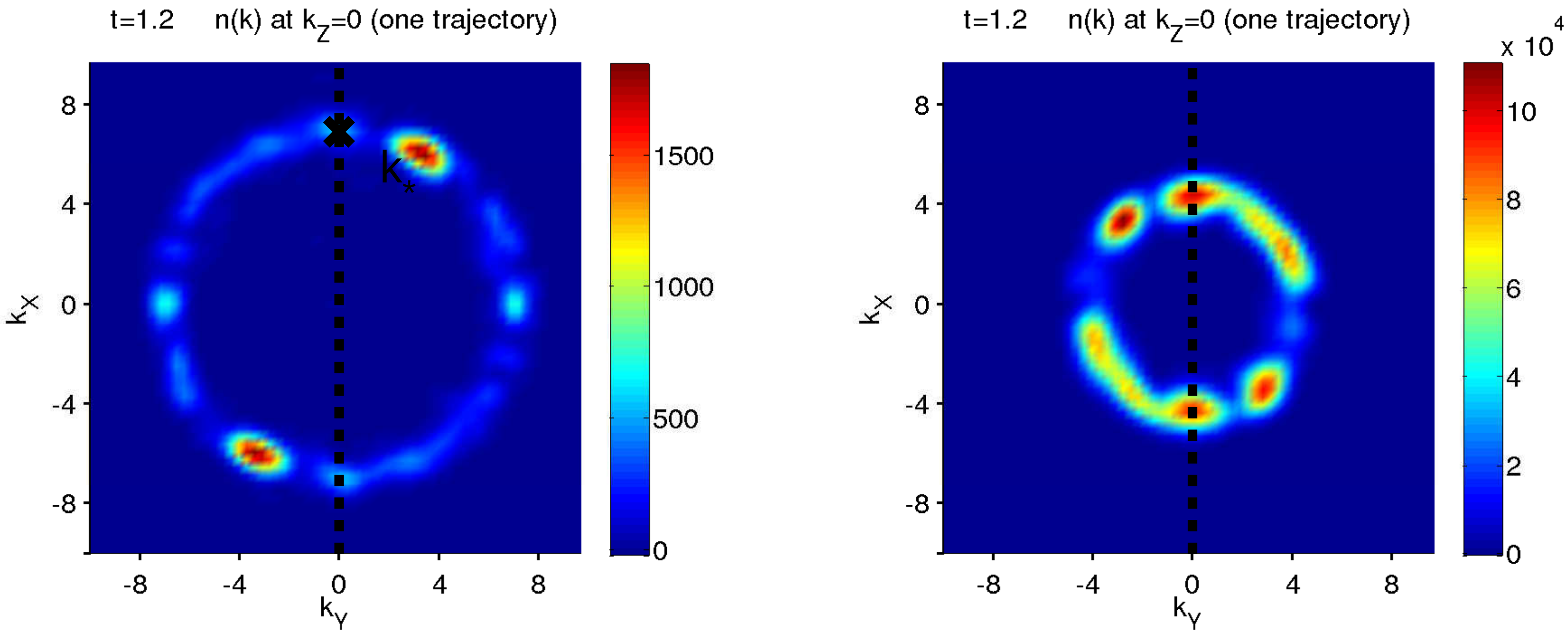



Not fully understood – clearly due to nonlinear evolution of BECs during the collision, and primarily due to mutual repulsion between wavepackets (Is the resulting anisotropy or the extra velocity kick more important?) Why is $g^{(2)}$ non-monotonic?

# Pairing loss mechanism 3

There is some degradation of pairing even in the simplest pairing Hamiltonian with stiff wavepackets:




Probable cause: finite wavepacket size $\longrightarrow$ variable mean-field energy cost to produce a pair depending on position

$\longrightarrow$relaxation of requirements for pair to have zero total momentum $\longrightarrow$ some atoms with $k$ not necessarily paired with exactly $-k$.

# Finally

- BECs display rich non-mean-field dynamics when beyond superfluidity
- Numerics *can* be used to gain physical understanding via a term-by-term dissection of the dynamics.
- Bogoliubov dynamics can be simulated without the need to find any eigenstates (or eigenvalues).
- Related topics that are amenable to this approach:
  - Scattering around an impurity or sharp potential
  - Fast flow over disordered potential
  - Shocks introduced by rapidly varying potentials.