Simulating quantum dynamics in colliding Bose-Einstein Condensates "directly" from the microscopic Hamiltonian

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Plan

- Condensed and uncondensed fractions in a BEC “Matter wave”
- Studying the uncondensed with collisions of BECs
- Describing the BEC using the so-called positive-P representation
- The noisy evolution that results
- some movies
- Interesting features of the stochastic equations
- How quantum many-body dynamics defends itself against this attempt
- Comparison to precision experiments

Condensed and uncondensed fractions in a BEC

Consider the wavelength of a particle of mass m

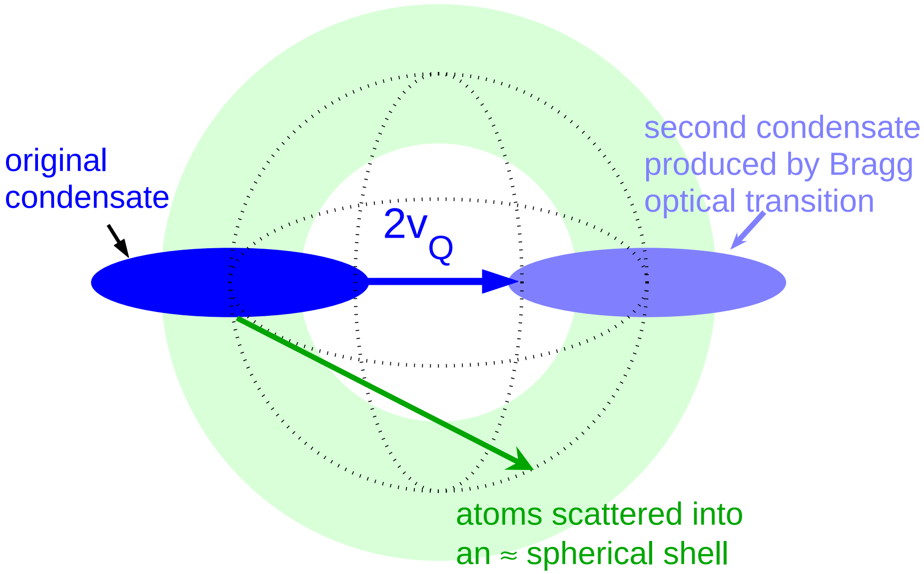
$$\lambda = \frac{h}{p} \sim \frac{h}{\sqrt{2mE}} \sim \frac{h}{\sqrt{2mk_B T}} \propto \frac{1}{\sqrt{T}}.$$

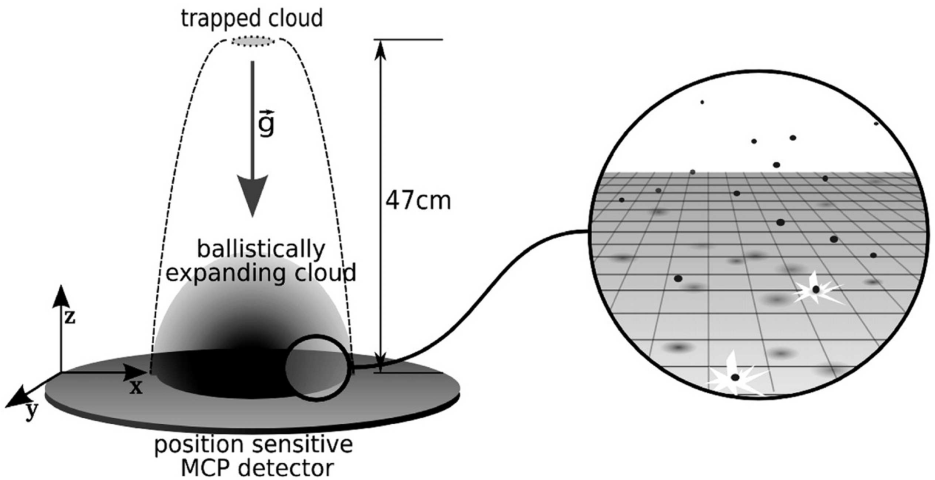
A rough picture: *When single wavelengths of different particles overlap, they become better described by a matter wave, and the BEC forms*

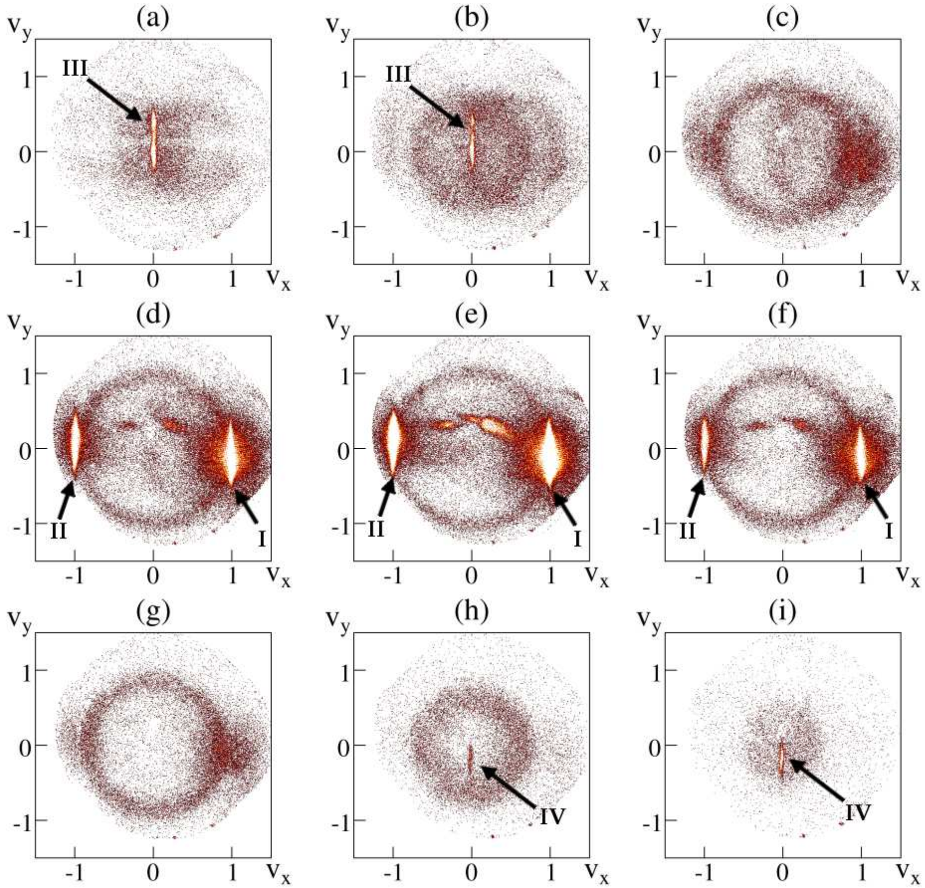
Types of uncondensed atoms

- **Thermal** (*Very* nicely treated by the SGPE methods of Stoof, Proukakis, et al.)
- **Quantum depletion** (equlibrium effect, T=0, due to interaction between individual atoms)
- **Supersonic** (non-equilibrium) These can physically separate from the main condensate.

Colliding BECs – experiment

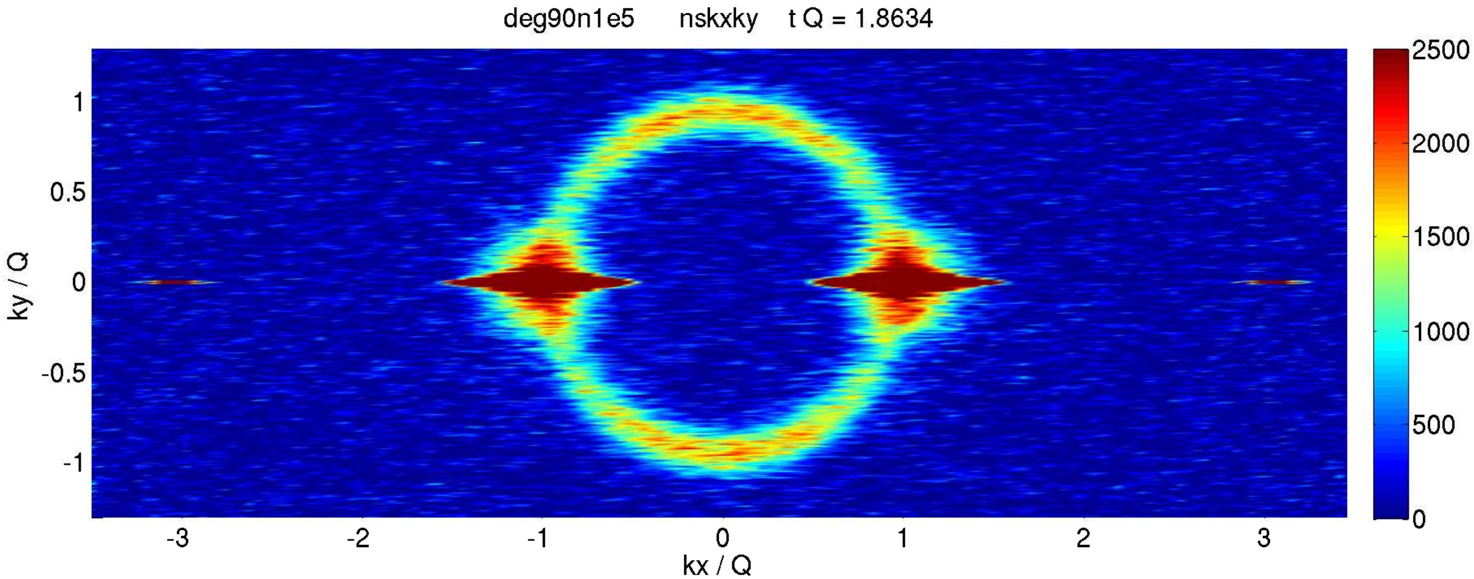


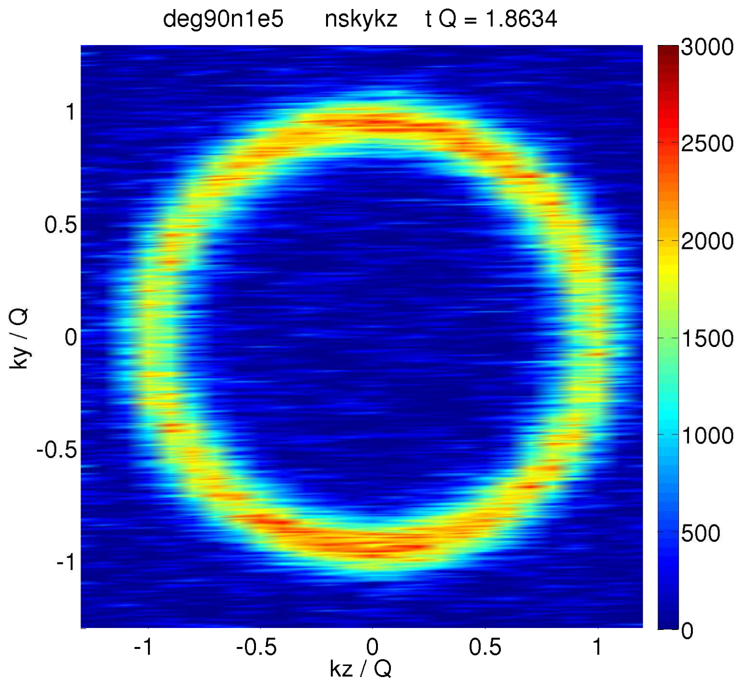




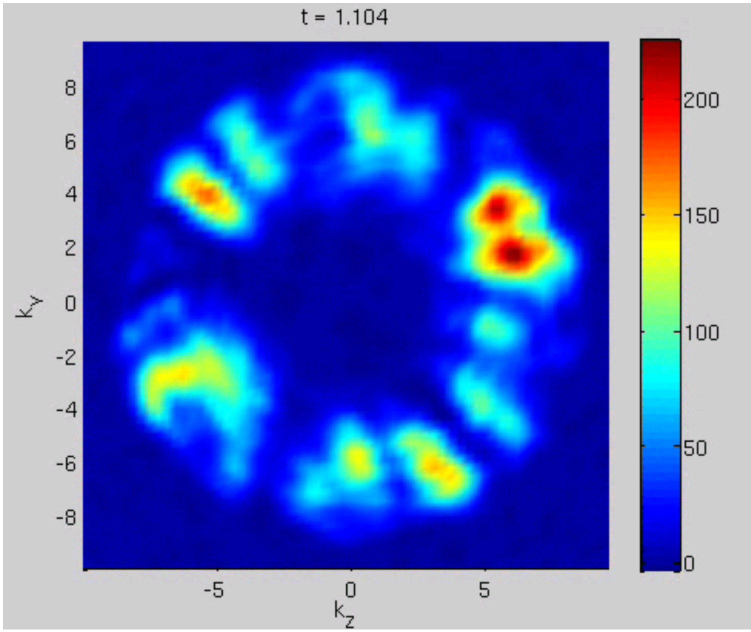
A. Perrin *et al.*, Phys. Rev. Lett. **99**, 15 (2007)

The uncondensed ones – in velocity-space





mean



single shot

Microscopic quantum mechanical description

First-quantized: Wave function $\psi(x_1, x_2, \ldots, x_N)$

$$H = -\frac{\hbar^2}{2m} \sum_j \frac{d^2}{dx_j^2} + \sum_j V(x_j) + \frac{g}{2} \sum_{\langle i,j \rangle} \delta(x_i - x_j)$$

Second-quantized: Boson field operators $\widehat{\Psi}(x)$.

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

Difficulty of microscopic description

The Hilbert space of the relevant quantum states grows exponentially with N and/or the number of single-particle orbitals to consider.

For example M orbitals with up to n particles in each, have a Hilbert space dimension of

$$D = (n+1)^M$$

To get eigenstates, eigenvalues, etc, in practice, one needs to diagonalise (or just even *STORE*!) matrices of size D^2

Gröss-Pitaevskii Equation – GPE

The standard description of a pure condensate.

The assumption – All the N particles are in the same orbital $\Phi(x,t)$.

$$\widehat{\Psi}(x,t) \rightarrow \psi(x,t) = \sqrt{N}\Phi(x,t)$$

The order parameter $\Psi(x)$ obeys the (superfluid, mean-field) Gröss-Pitaevskii (GP) equation:

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

Stochastic descriptions of departures from GPE

Thermal - SGPE

$$\frac{d\psi(x,t)}{dt} = \frac{-i}{\hbar}\left[-\frac{\hbar^2}{2m}\nabla^2 + g|\psi(x,t)|^2 - iR(x,t,T)\right]\psi(x,t) + \sqrt{\Sigma(x,t,T)}\eta(x,t)$$

White complex noise $\eta : \langle\eta^*(x,t)\eta(x',t')\rangle = \delta(t-t')\delta(x-x'), \quad \langle\eta(x,t)^2\rangle = 0$.

Positive-P

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

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

White real multiplicative independent noises $\xi_j : \langle\xi_i(x,t)\xi_j(x',t')\rangle = \delta(t-t')\delta(x-x')\delta_{ij}$.

positive-P representation

Write the density matrix of the system

$$\rho = |\psi\rangle\langle\psi|$$

as a probability distribution over coherent state operators

$$\rho = \int D[\psi_1(x)]D[\psi_2(x)] \quad |\psi_1(x)\rangle\langle\psi_2(x)^*| \quad P(\psi_1(x), \psi_2(x))$$

This leads to a Fokker-Planck equation for the probability P

And to random walk equations for samples $\psi_1(x), \psi_2(x)$ of P.

Averages of the samples correspond to quantum mechanical expectation values. E.g. density:

$$n(x) = \langle\psi_2(x)^*\psi_1(x)\rangle.$$

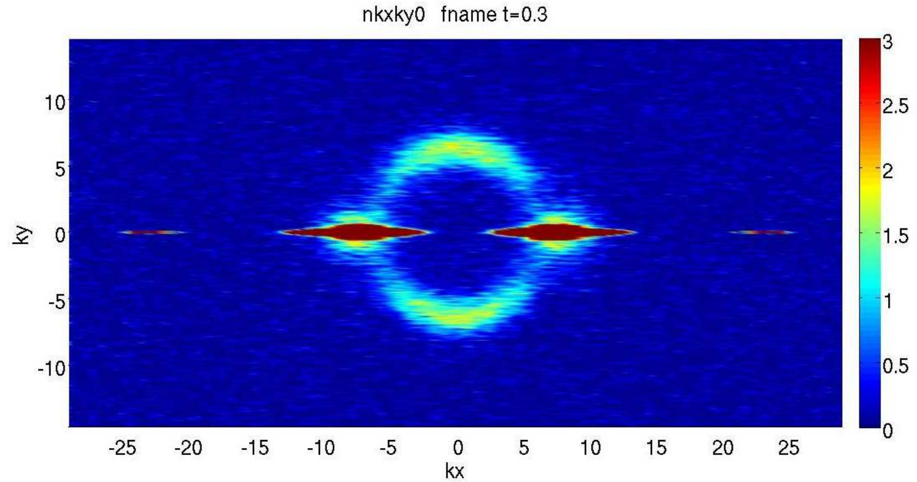
Simulations

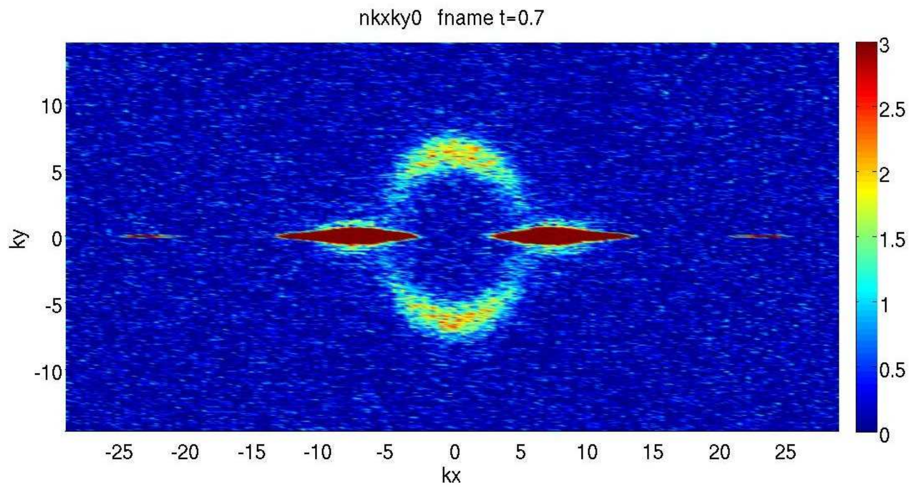
insert movie here

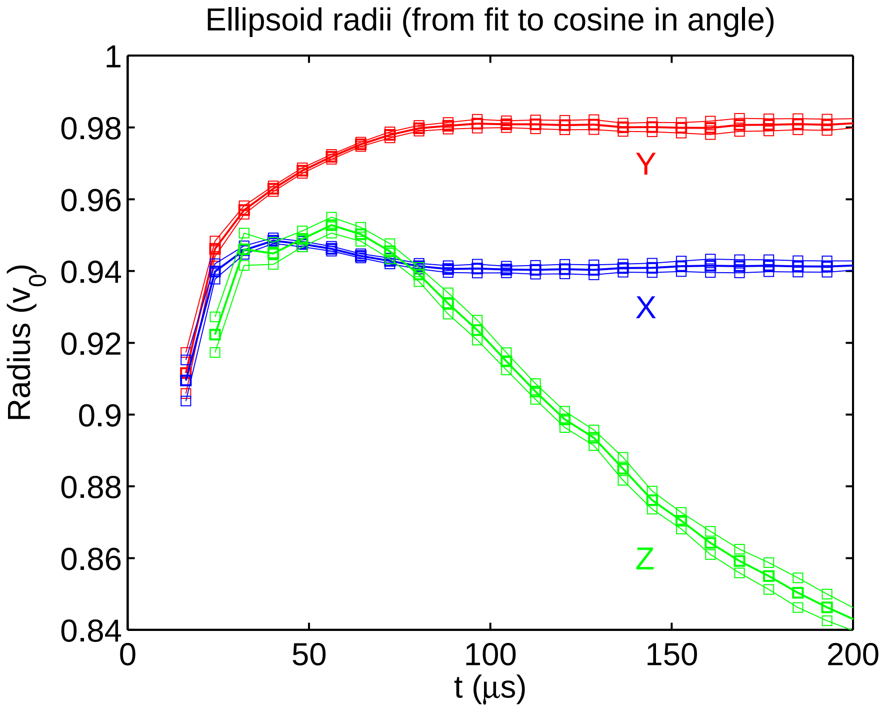
insert movie here

Advantages of simulations

Can “observe” what happens during the collision, rather than just the final debris.







Stochastic subtleties

- Multiplicative noise requires care when numerically integrating

- Since $\psi(t) \sim \psi(0)e^{(1+i)\sqrt{g}\zeta(t)}$, where $\zeta(t) \approx \int_0^t \xi(s)ds$ is a noise, one must watch that the phase variance is not too large.
  $\rightarrow$ if phase variance $\gtrsim O(10)$, systematic sampling errors can result.

- Two fields ψ_1 and ψ_2 allow one to add noise without adding new particles:
  This is because $\langle \psi_2^* \psi_1 \rangle$ does not necessarily grow even though $\langle |\psi_j|^2 \rangle$ do.

Noise amplification

The Hilbert Space Strikes Back

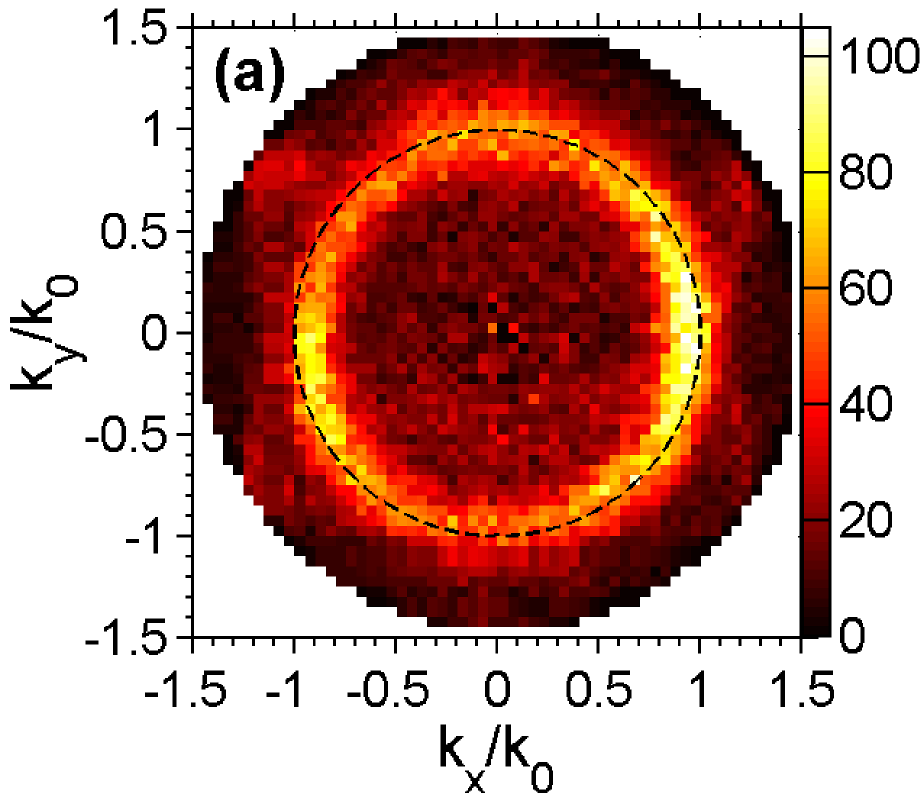
$$\frac{d\,\psi_1(x,t)}{dt} = \frac{-i}{\hbar}\left[-\frac{\hbar^2}{2m}\nabla^2 + g\,\psi_2(x,t)^*\psi_1(x,t) + i\sqrt{ig}\,\xi_1(x,t)\right]\psi_1(x,t)$$

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

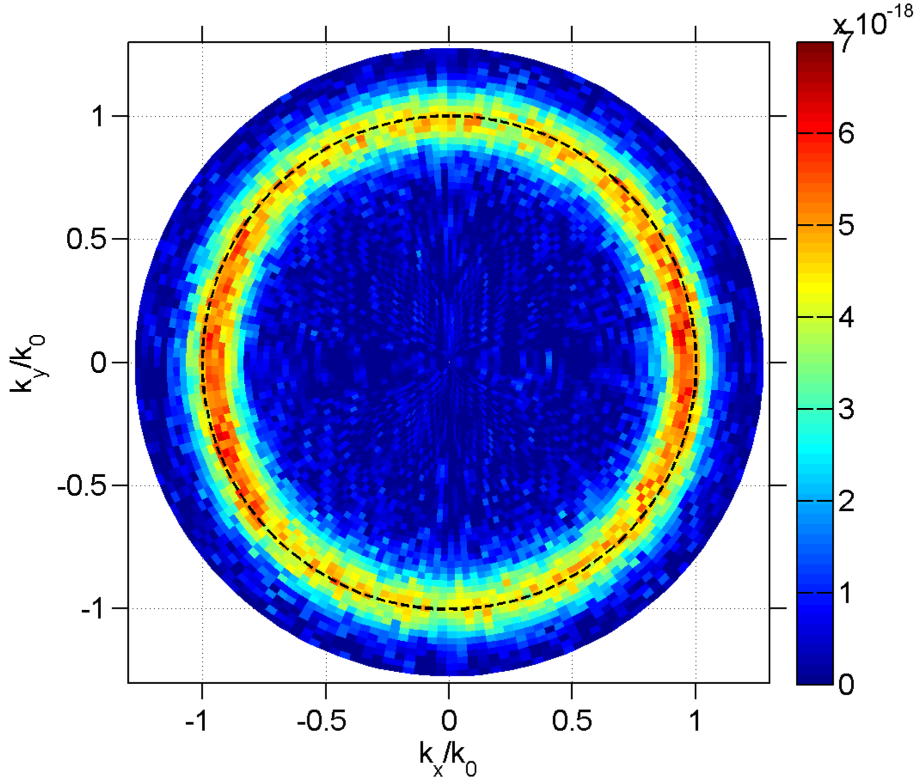
- The “density”, $\psi_2^*\psi_1$ was initially real since $\psi_2(0) = \psi_1(0)$ at $t = 0$
- Different noises xi_1 and ξ_2 make it acquire an imaginary part.
- Then ψ_1 (say) starts to grow exponentially, while ψ_2 decays, keeping
  $\longrightarrow$ noise takes off and becomes unmanageable after an “effective simulation time”

$$t_{\rm sim} \sim \left(\frac{\hbar}{g}\right)\frac{(\Delta V)^{(1/3)}}{(\max_x\{n(x)\})^(2/3)}$$

Comparison to experiment – halo position & shape



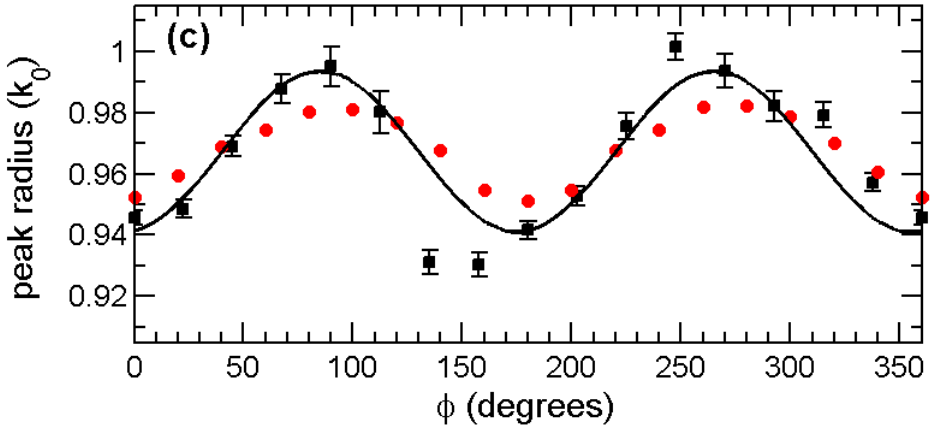
Experiment



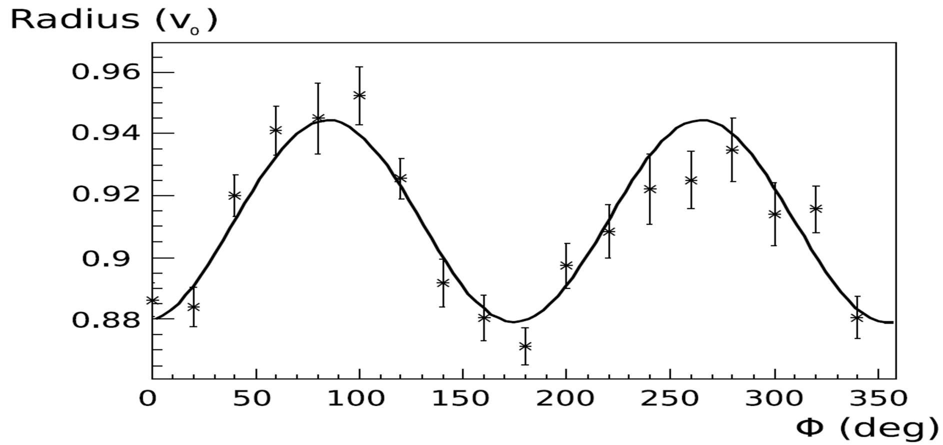
Simulation

Precision comparisons to experiment

- The scattering halo is not a sphere;
- The experiment can make precision measurements of the shifts;
- Is the current theory complete enough to explain them?



Experiment (□) + theory (○)



Old calibration

The future – treating both kinds of incoherence

SGPE / positive-P hybrid shoudl be able to treat both the thermal atoms and the quantum depletion in a “quasi-complete” manner.

Positive-P

$$\frac{d\psi_1(x,t)}{dt} = \frac{-i}{\hbar}\left[-\frac{\hbar^2}{2m}\nabla^2 + g\psi_2(x,t)^*\psi_1(x,t) + i\sqrt{ig}\,\xi_1(x,t) - iR(x,t,T)\right]\psi_1(x,t) + \sqrt{\Sigma(x,t,T)}\,\eta(x,t)$$

$$\frac{d\psi_2(x,t)}{dt} = \frac{-i}{\hbar}\left[-\frac{\hbar^2}{2m}\nabla^2 + g\psi_1(x,t)^*\psi_2(x,t) + i\sqrt{ig}\,\xi_2(x,t) - iR(x,t,T)\right]\psi_1(x,t) + \sqrt{\Sigma(x,t,T)}\,\eta(x,t)$$

White real multiplicative independent noises $\xi_j : \langle \xi_i(x,t)\xi_j(x',t')\rangle = \delta(t-t')\delta(x-x')\delta_{ij}$.

Thank you :)