AB INITIO SIMULATIONS OF COLLISIONS OF HELIUM CONDENSATES

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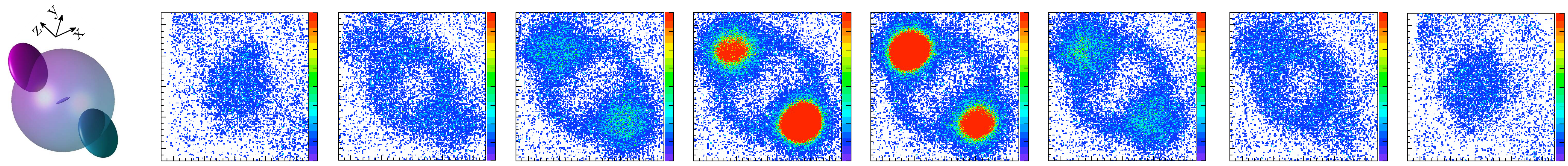

1. Motivation

- Interested in mechanisms of pair production of particles for ***quantum-atom optics*** (pair correlated photons have been pivotal to quantum optics; e.g., demonstrations of EPR paradox and violations of Bell's inequalities)
- Pair-correlated atoms in BEC collisions have been detected in [1]
- Modified experiments are underway; the new geometry gives better detection access
- First-principles simulations are now possible for the entire collision duration (in contrast to [2])

2. Hamiltonian and positive-P equations

$$\hat{H} = \int d^3\mathbf{x}\left(\tfrac{\hbar^2}{2m}\left|\nabla\hat{\Psi}\right|^2 + \tfrac{U_0}{2}\hat{\Psi}^+\hat{\Psi}^+\hat{\Psi}\hat{\Psi}\right) \qquad (1)$$

Positive-P (phase-space) method: the quantum many-body dynamics, governed by the Hamiltonian (1), is simulated exactly via stochastic differential equations for c-fields [2]:

$$\frac{\partial\psi(\mathbf{x},t)}{\partial t} = \frac{i\hbar}{2m}\nabla^2\psi - i(U_0/\hbar)\tilde{\psi}\psi\psi + \sqrt{-i(U_0/\hbar)\psi^2}\,\xi_1(\mathbf{x},t)$$

$$\frac{\partial\tilde{\psi}(\mathbf{x},t)}{\partial t} = \frac{-i\hbar}{2m}\nabla^2\tilde{\psi} + i(U_0/\hbar)\tilde{\psi}\psi\psi + \sqrt{i(U_0/\hbar)\tilde{\psi}^2}\,\xi_2(\mathbf{x},t)$$

- $\xi_i(\mathbf{x},t)$ – noise terms, with $\langle\xi_i(\mathbf{x},t)\xi_j(\mathbf{x}',t')\rangle = \delta_{ij}\delta^{(3)}(\mathbf{x}-\mathbf{x}')\delta(t-t')$
- $U_0 = 4\pi\hbar^2 a/m$ – s-wave scattering interaction

3. Simulation parameters

- Total No. of ^{4}He* atoms in the initial BEC: 10^5
- Initial condition: pure BEC in a coherent state, split into two counter-propagating halves
  $$\psi(\mathbf{x},0) = \sqrt{n(\mathbf{x})/2}\,[\exp(ik_0 z) + \exp(-ik_0 z)]$$
- Harmonic trap: 47/1150/1150 Hz
- Relative collision velocity: $2v_0$=2 x 7.36 cm/s
- Numerical lattice: 1024 x 48 x 112 lattice points
- Number of modes simulated: 5505024
- Positive-P simulations run for 70 μs
- Number of stochastic trajectory averages: 2000
- Computing time: 6-7 days on 10 CPUS

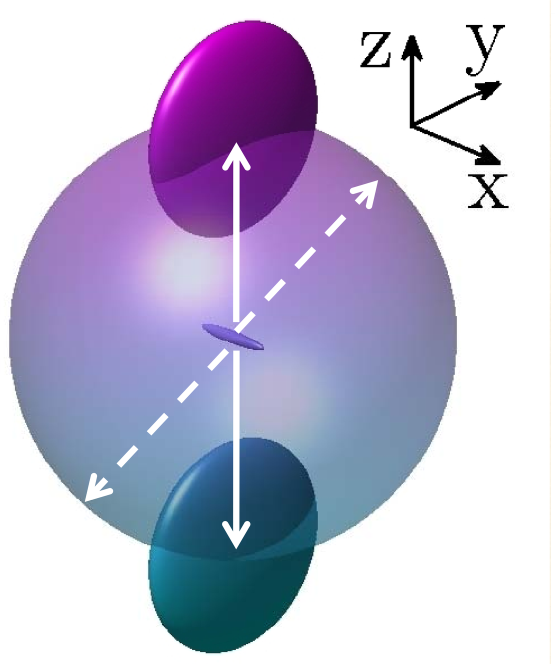

Figure 1. Schematic diagram of the collision geometry: The two disks represent the colliding condensates; the sphere represents the scattered atoms. The cigar shaped initial condensate is shown in the middle.

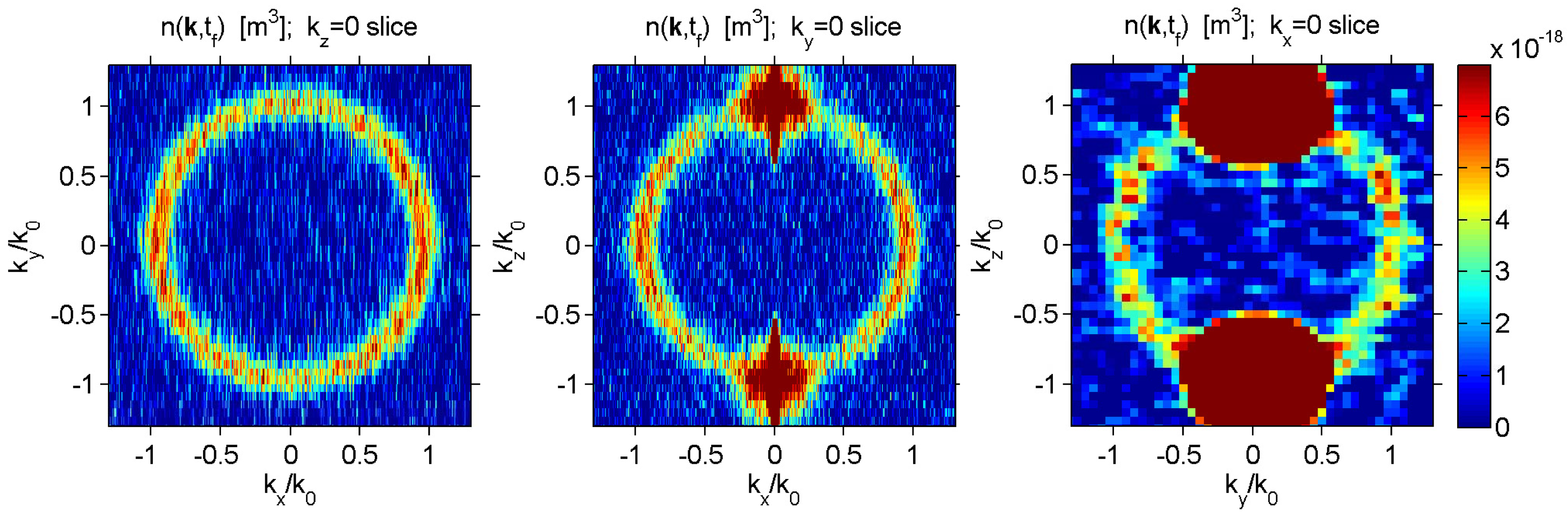

Figure 2. Atomic momentum distribution (positive-P simulation, average of 2000 stochastic trajectories): Three orthogonal cuts through the origin after 70 μs collision duration, by which time the collision has essentially ceased. The (nearly) spherical shell of scattered atoms is clearly seen, with the darker regions corresponding to the colliding condensates. ***A more careful quantitative analysis reveals a surprise***: *the scattering shell renders itself as an ellipsoid (see Fig. 4); the experiment also shows this!*

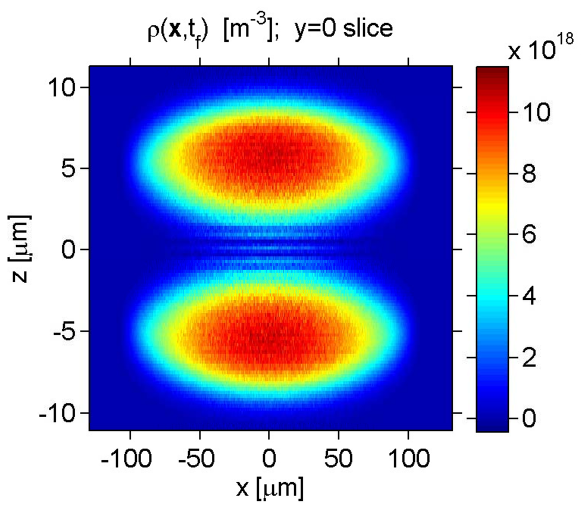

Figure 3. Real-space density of the atomic cloud after 70 μs, showing the spatial separation of the two colliding condensates.

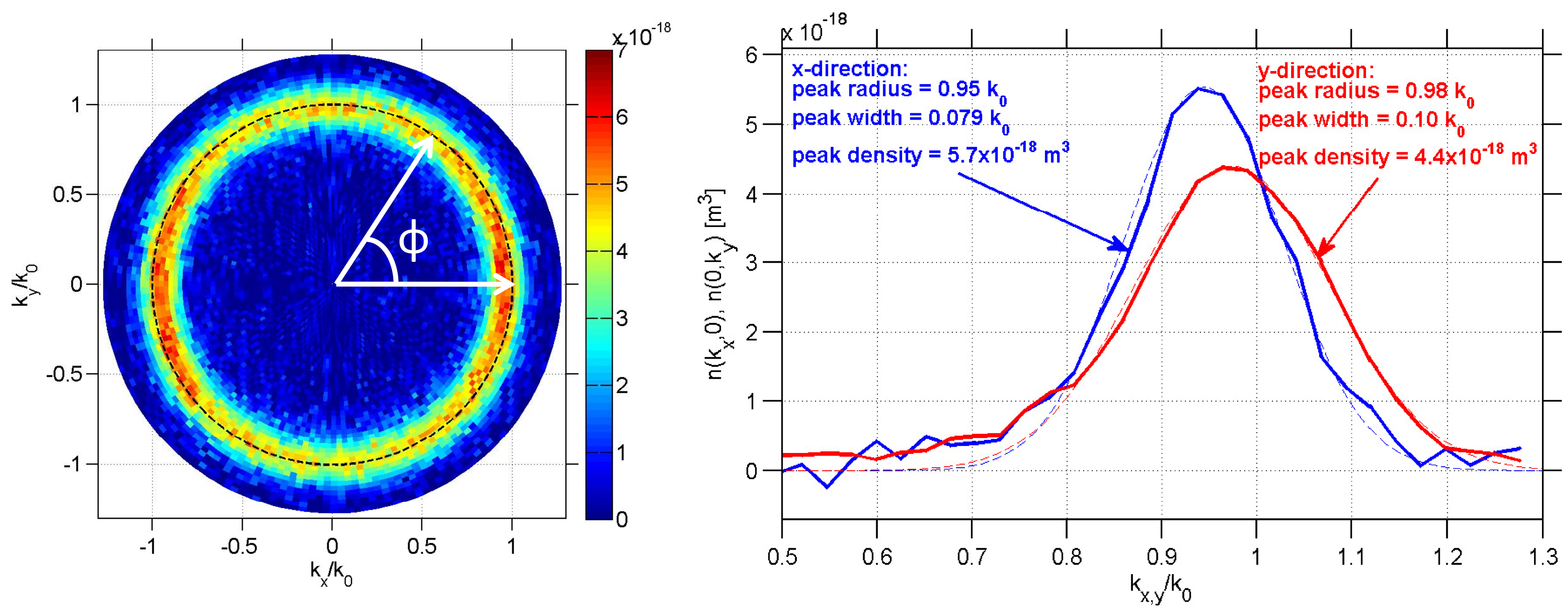

Figure 4. Slice of the atomic momentum distribution through the origin in the k_x-k_y plane in ***polar coordinates*** (left panel); the respective radial densities along k_x and k_y axis (right panel) show the anisotropy of the distribution and its ellipticity (ε=1.03). The axis are in units of $k_0 = mv_0/\hbar$.

Comparison table:	Peak position (units of k_0)		Peak width (units of k_0)		Peak density (arb. units)		$N_{scattered}$
	along k_x	k_y	k_x	k_y	k_x	k_y	
Theory	0.95±0.01	0.98±0.01	0.08±0.005	0.10±0.005	1.40±0.1	1	1400±50
Experiment	0.88±0.02	0.94±0.02	0.09±0.01	0.11±0.01	1.48±0.16	1	1600±200

Stochastic Hartree-Fock-Bogoliubov approach

- Apply the HFB scheme: $\hat{\Psi}(\mathbf{x},t) = \psi_0(\mathbf{x},t) + \hat{\delta}(\mathbf{x},t)$
- Re-formulate the Heisenberg equations of motion for $\hat{\delta}(\mathbf{x},t)$
  $$i\hbar\frac{\partial\hat{\delta}(\mathbf{x},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + 2U_0|\psi_0(\mathbf{x},t)|^2\right]\hat{\delta}(\mathbf{x},t) + 2U_0\psi_0(\mathbf{x},t)^2\hat{\delta}^+(\mathbf{x},t)$$
  according to the positive-P method
  - easier to solve than the standard Bogoliubov method in 3D
  - can incorporate the mean field dynamics of the colliding condensates [$\psi_0(\mathbf{x},t)$] as the solution to the GP equation
  - ***agreement with the full positive-P simulation!***
- Scattered atoms move in a complicated mean-field potential landscape of the separating and expanding condensates
- Shift $\delta k = k_0 - k_s$ in the radius of the sphere can be estimated as
  $$\frac{\hbar^2 k_0^2}{2m} + U_0 n_0 = \frac{\hbar^2 k_s^2}{2m} + 2U_0 n_0 \;\Rightarrow\; \frac{\hbar^2 k_s^2}{2m} = \frac{\hbar^2 k_0^2}{2m} - U_0 n_0 \;\Rightarrow\; \frac{\delta k}{k_0} \approx \frac{mU_0 n_0}{\hbar^2 k_0^2}$$
- Ellipticity: atoms moving along y slide down a steeper hill of the mean-field potential and regain the energy shift $U_0 n_0$ as kinetic energy (radius is back to k_0), unlike the atoms along x

REFERENCES

[1] *Observation of Atom Pairs in Spontaneous Four-Wave Mixing of Two Colliding Bose-Einstein Condensates*. A. Perrin, H. Chang, V. Krachmalnicoff, M. Schellekens, D. Boiron, A. Aspect, and C. I. Westbrook , Phys. Rev. Lett. **99**, 150405 (2007).

[2] *Atomic four-wave mixing via condensate collisions.* A. Perrin, C. M. Savage, D. Boiron, V. Krachmalnicoff, C. I. Westbrook, K. V. Kheruntsyan, New J. Physics **10**, 045021 (2008).

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