Simulating the quantum dynamics of many interacting bosons beyond the GP equation

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Main points

1. Quantum dynamics of a Bose gas

$$\widehat{H} = \int d^dx \left\{ \widehat{\Psi}^\dagger(x) \left[V_{\text{ext}}(x) - \frac{\hbar^2}{2m}\nabla^2 \right] \widehat{\Psi}(x) + \frac{g}{2}\, \widehat{\Psi}^\dagger(x)^2 \widehat{\Psi}(x)^2 \right\}$$

interacting via a 2-particle contact potential
is described “fully” by these simple, though noisy, field equations:

$$i\hbar \frac{d}{dt}\psi(x) = \left[V_{\text{ext}}(x) - \frac{\hbar^2}{2m}\nabla^2 + g\,\psi(x)\phi(x)^* + \sqrt{i\hbar g}\;\xi(x) \right] \psi(x)$$

$$i\hbar \frac{d}{dt}\phi(x) = \left[V_{\text{ext}}(x) - \frac{\hbar^2}{2m}\nabla^2 + g\,\phi(x)\psi(x)^* + \sqrt{i\hbar g}\;\zeta(x) \right] \phi(x)$$

2. Example with N=150 000 atoms: the fate of the scattered atoms in a BEC collision.

[PD & Drummond, PRL **98**, 120402 (2007)]

Discretization

- Divide space up into small bins of volume ΔV, label them by "x"
  $\widehat{a}_x$ is the bosonic anihilation operator for particles in box x

$$\widehat{H} \quad \Longrightarrow \quad \sum_{x,y} \hbar\omega_{xy}\, \widehat{a}_x^\dagger \widehat{a}_y + \frac{g}{2\Delta V} \sum_x \widehat{a}_x^{\dagger 2} \widehat{a}_x{}^2$$

where

$$\hbar\omega_{xy} = \delta_{xy}\, V_{\mathrm{ext}}(x) \quad + \quad \mathrm{kinetics}$$

- Provided bins are $\ll$ smallest relevant length scale, processes in continuum will be modeled accurately.

- Bose-Hubbard model is a special case with one bin per lattice site, and a particular choice of ω_{xy} to obtain $-J\sum_{\langle i,j\rangle} \widehat{a}_i^\dagger \widehat{a}_j$ etc.

Positive P representation

- From quantum optics: Density matrix $\widehat{\rho} = \sum_i C_i \left|\Phi_j\right\rangle \left\langle\Phi_j\right|$ is equivalent to

  [Drummond & Gardiner, J. Phys. A **13**, 2353 (1980)]

$$\widehat{\rho} = \int \mathcal{D}\psi(x)\ \mathcal{D}\phi(x)\quad P(\ \{\psi(x)\},\{\phi(x)\}\ )\quad \bigotimes_x \frac{\|\psi(x)\rangle\,\langle\phi(x)\|}{\mathcal{N}(x)}$$

with coherent states of mean particle density $|\psi(x)|^2$ in each bin "x"

$$\|\psi(x)\rangle = \exp\left[\left(\sqrt{\Delta V}\ \psi(x)\right)\widehat{a}_x^\dagger\right]\ |0\rangle$$

- The distribution P is positive and real — it's a probability distribution.

$$\hookrightarrow\qquad \widehat{\rho}\quad\equiv\quad \lim_{\mathcal{S}\to\infty}\left\{\quad \mathcal{S}\ \text{random samples of fields}\ \psi(x)\ \text{and}\ \phi(x)\quad\right\}$$

Dynamics

- Schrodinger equation is:

$$i\hbar\,\dot{\widehat{\rho}} = \widehat{H}\widehat{\rho} - \widehat{\rho}\widehat{H}.$$

- Without going into gory details, this is equivalent to a Fokker-Planck equation for the distribution $P(\psi,\phi)$:

$$i\hbar\frac{\partial P}{\partial t} = \sum_x \left[-\frac{\partial}{\partial\psi(x)}A_x + \frac{\partial^2}{\partial\psi(x)^2}D_x + \text{ etc. with } \frac{\partial}{\partial\phi(x)} \right] P$$

with diffusion coefficients D_x and drift rates A_x, etc.

- This in turn is is equivalent to Langevin equations for the random samples $\psi(x)$ and $\phi(x)$ such as:

$$\frac{d}{dt}\psi(x) = A_x(\psi,\phi) + \sqrt{D_x(\phi,\psi)}\,\xi(x,t)$$

with $\xi(x,t)$ being a real white noise field, delta-correlated in both x and t.

Gross-Pitaevskii + Noise

For our case of the contact–s wave–interacting Bose gas, one has:

[Drummond & Corney PRA **60**, R2661 (1999)], [PD & Drummond J. Phys. A **39**, 1163 (2006)]

$$\begin{aligned} i\hbar\frac{d}{dt}\psi(x) &= \left[V_{\text{ext}}(x) - \frac{\hbar^2}{2m}\nabla^2 + g\,\psi(x)\phi(x)^* + \sqrt{i\hbar g}\,\xi(x)\right]\psi(x) \\ i\hbar\frac{d}{dt}\phi(x) &= \left[V_{\text{ext}}(x) - \frac{\hbar^2}{2m}\nabla^2 + g\,\phi(x)\psi(x)^* + \sqrt{i\hbar g}\,\zeta(x)\right]\phi(x) \end{aligned}$$

The $\xi(x,t)$ and $\zeta(x,t)$ are delta-correlated independent noise fields with variances:

$$\langle\xi(x,t)\xi(x',t')\rangle = \langle\zeta(x,t)\zeta(x',t')\rangle = \delta(t-t')\delta^d(x-x')$$

Differences to GP:

- noise
- *two* complex fields
- ψ and ϕ coupled by nonlinear terms

Is this a “free lunch”?

- No processes discarded $\Longrightarrow$ “exact” to all orders of perturbation etc.

- Complexity of description (e.g. number of variables) grows only *linearly* with system size (number of bins/modes etc.): just have the fields $\psi(x)$ and $\phi(x)$

- Simple to implement: (repeatedly integrate GP equation with fresh noises and add it all up)

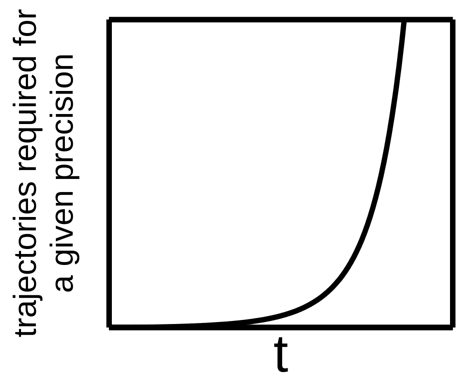
- All observables can in principle be computed via: $\langle \widehat{\Psi}^\dagger(x)^n \widehat{\Psi}(y)^m \rangle \equiv \langle \phi(x)^{*n} \psi(y)^m \rangle_S$

BUT

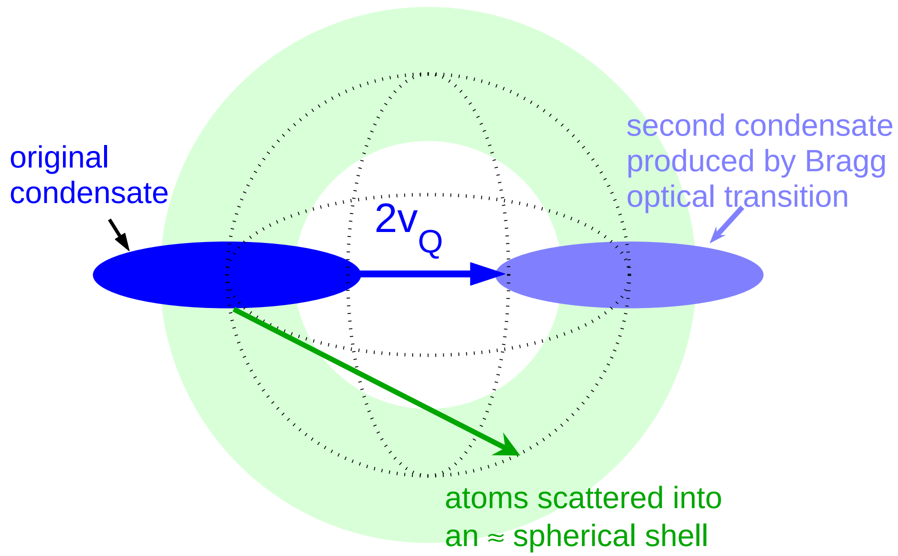
- Over time, nonlinearity amplifies the noise:

- $\Longrightarrow$ Time for which you can simulate is limited.

[PD & Drummond, J. Phys. A **39**, 1163 (2006)]



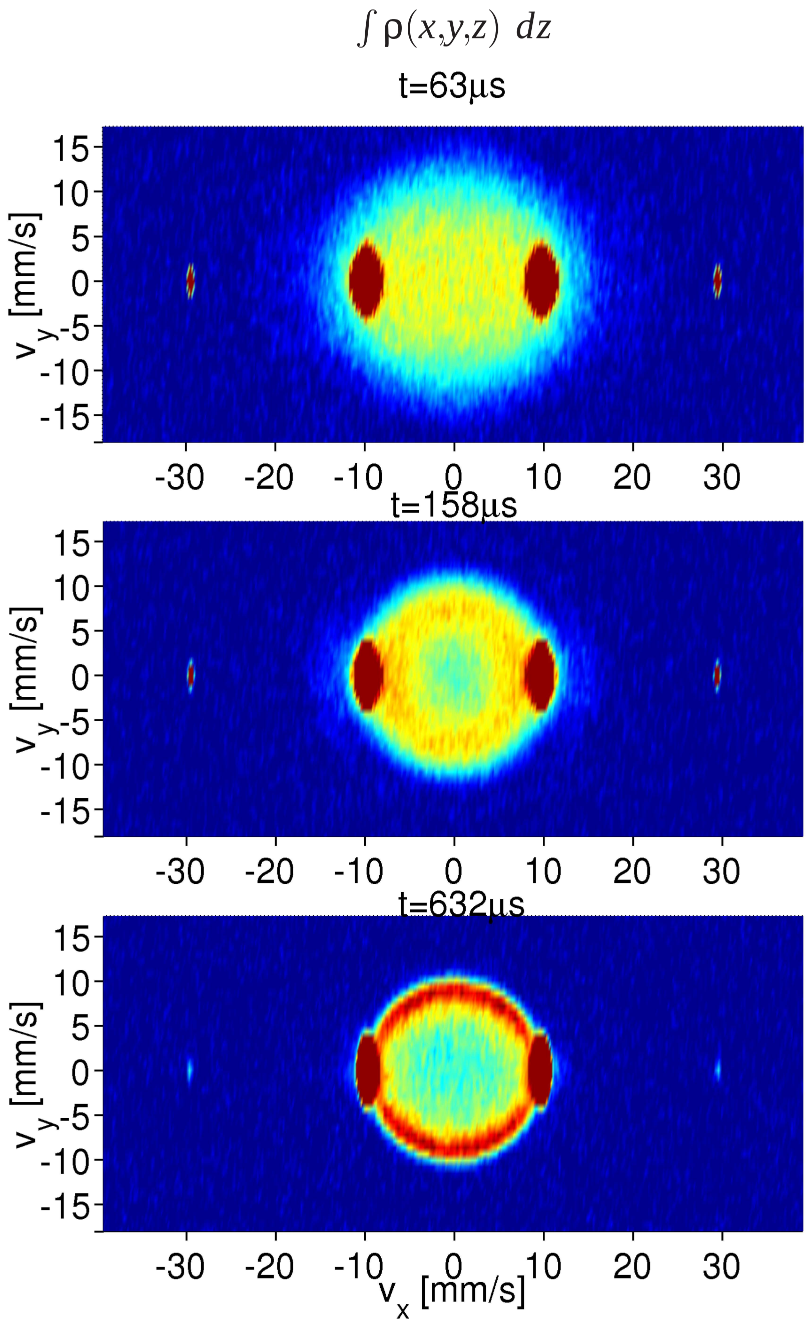
BEC collision



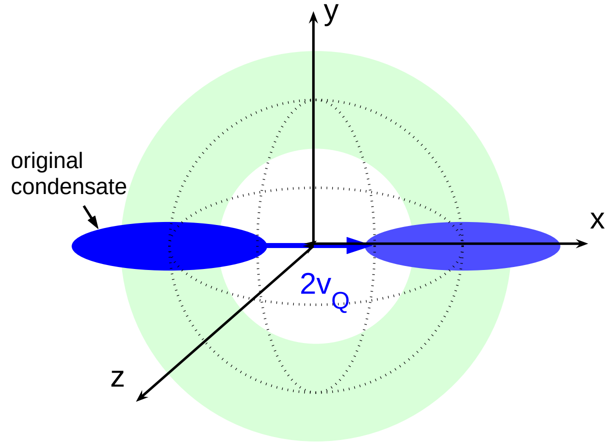
- 150,000 atoms of $^{23}\mathrm{Na}$ in a BEC.
- Initial trap $f = 20 \times 80 \times 80\mathrm{Hz}$.
- Trap turned off at $t \geq 0$
- At $t = 0$ Bragg laser pulse gives a coherent kick $2\mathrm{v_Q} \approx 19.64\mathrm{mm/s}$ to 50% of the atoms.
- Collision well above sound velocity (3.1 mm/s in center of cloud)

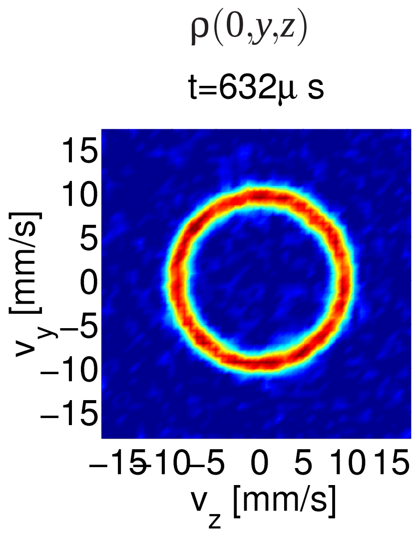
- Similar setup to experiments at MIT ($^{23}\mathrm{Na}$ – with 3×10^7 atoms) [Vogels *et al.* PRL **89**, 020401 (2002)], and Orsay ($^{3}\mathrm{He}$) [Perrin *et al.* arXiv:0704.3047]
- Initial conditions used here at $t = 0$ were $T \approx 0$ and a coherent GP ground state (realistically one has, for $T \approx 0.4T_c$, quantum depletion $\approx$ 1%, which is negligible)
- Theory includes: [Bach *et al.* PRA **65**, 063605 (2002), Zin *et al.* PRL **94**, 200401 (2005)](Bogoliubov expansion), [Norrie *et al.* , PRL **84**, 040401 (2005); PRA **73**, 043617(2006)](truncated Wigner), [PD & Drummond, PRL **98**, 120402 (2007)](here)

Scattered atoms



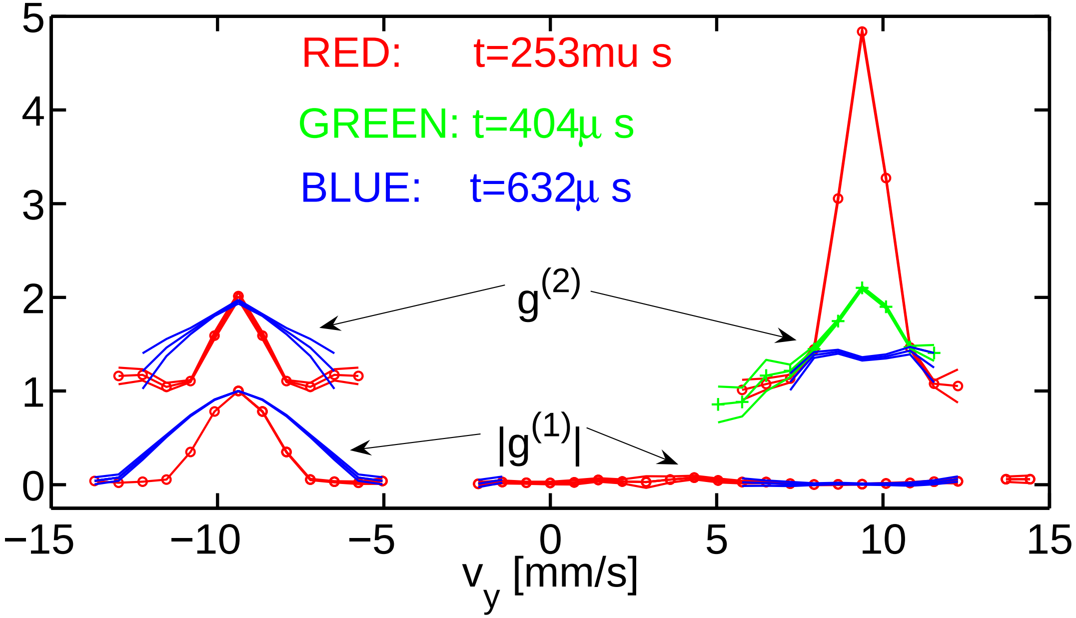
note: color scale varies

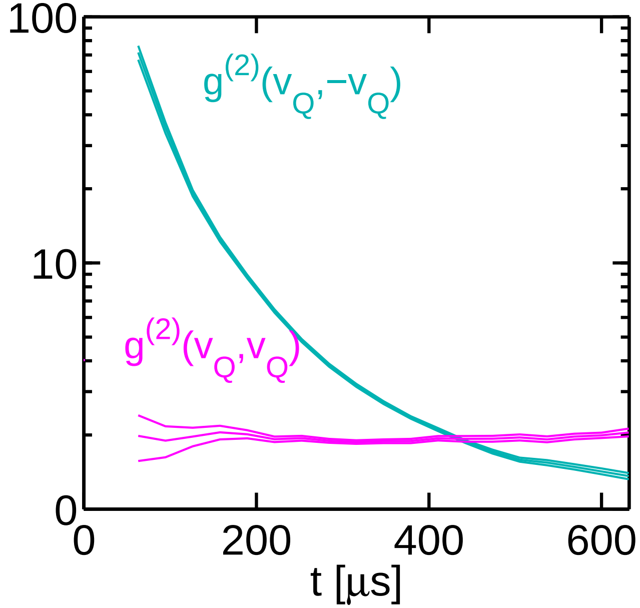




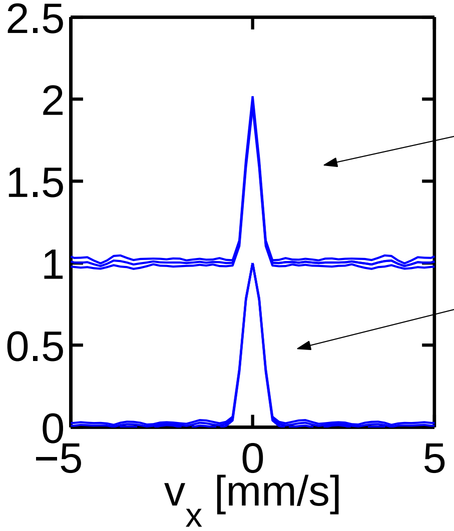
Correlations

radial velocity correlations

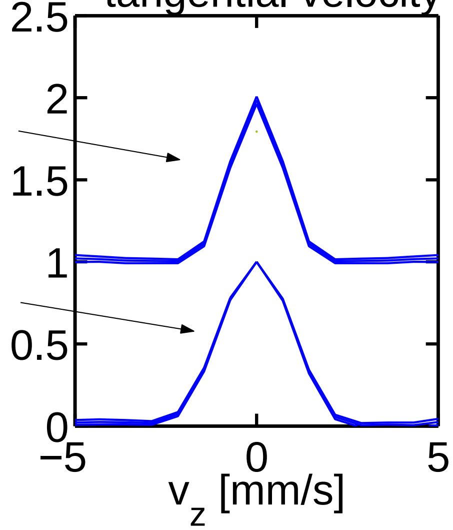




axial velocity

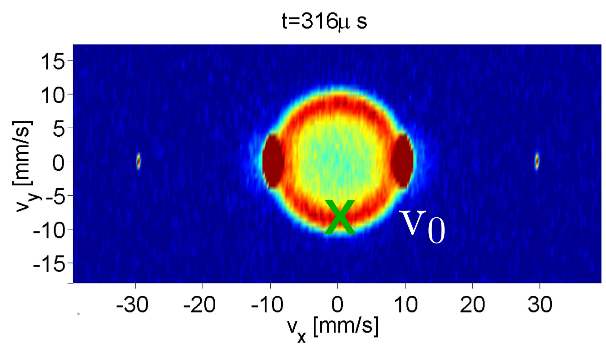


tangential velocity

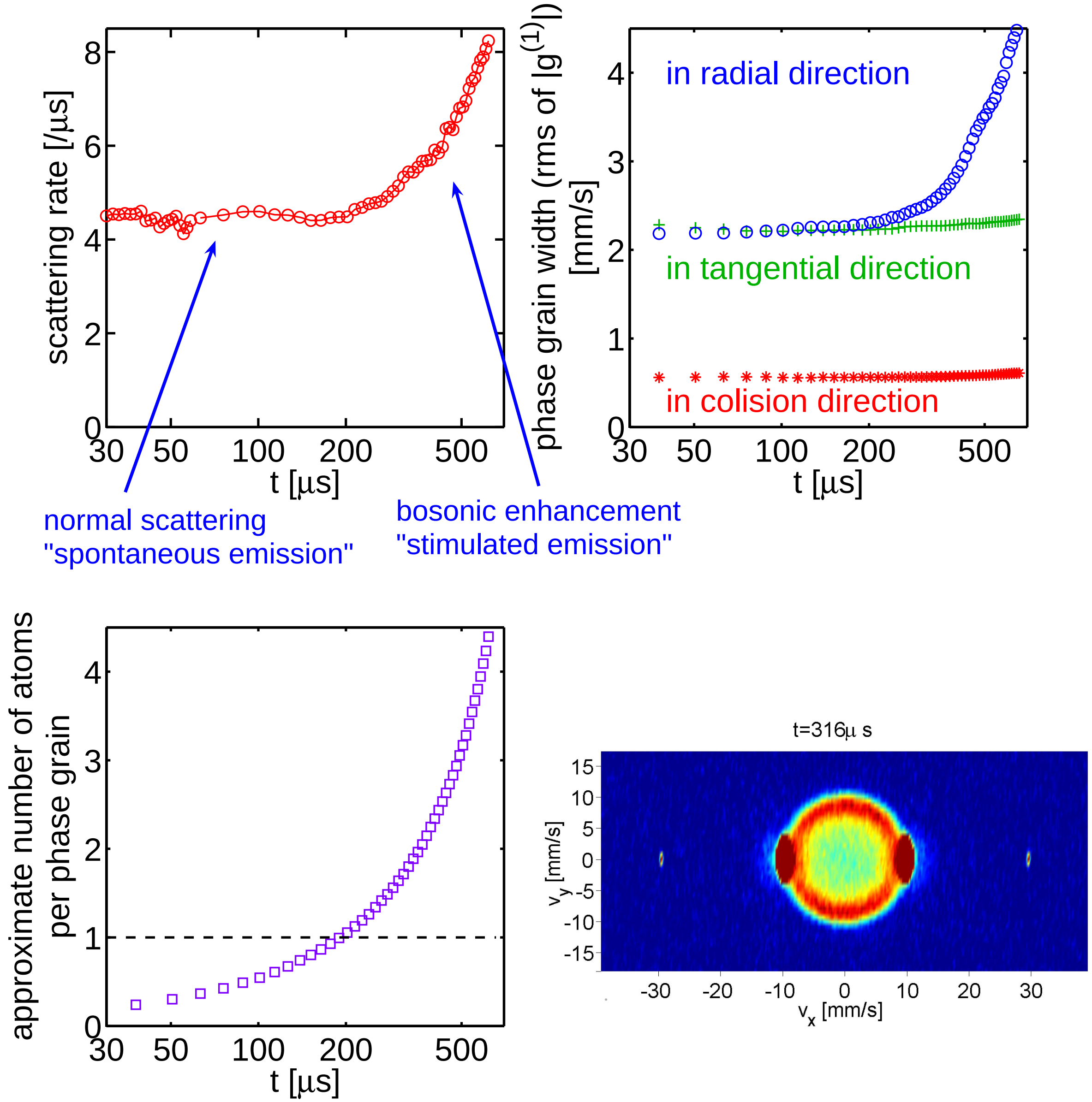


$$g^{(1)} = \langle \widehat{\Psi}^\dagger(\mathrm{v}_0)\widehat{\Psi}(\mathrm{v})\rangle / \sqrt{\rho(\mathrm{v}_0)\rho(\mathrm{v})}$$

$$g^{(2)} = \langle \widehat{\Psi}^\dagger(\mathrm{v}_0)\widehat{\Psi}^\dagger(\mathrm{v})\widehat{\Psi}(\mathrm{v})\widehat{\Psi}(\mathrm{v}_0)\rangle / \rho(\mathrm{v}_0)\rho(\mathrm{v})$$



Phase grains and Bose enhancement



Conclusions

- Full quantum dynamics of an interacting Bose gas can be simulated efficiently; However — *for a limited time only.*

- Formulation is rather simple : two coupled GP equations + noise.

- Atoms scattered in a collision of BECs display rich dynamics and correlations

- Their dynamics undergo a qualitative change once “phase grains” become occupied by more than one particle.