First-principles quantum simulations of interacting Bose gases

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Model

Hamiltonian density:

$$\widehat{H} = \frac{\hbar^2}{2m}\nabla\widehat{\Psi}^\dagger\nabla\widehat{\Psi} + V(x)\widehat{\Psi}^\dagger\widehat{\Psi} + \frac{g}{2}\widehat{\Psi}^{\dagger 2}\widehat{\Psi}^2$$

Boson creation operators $\widehat{\Psi}^\dagger(x)$ at x.

Method

Gauge P representation[?]

$$\widehat{\rho} = \int G(\vec{v})\,\Omega \bigotimes_x \widehat{\Lambda}_x\, d\vec{v}$$

- Probability distribution G of variables $\vec{v} = \{\Omega, \vec{\alpha}(\vec{x}), \vec{\beta}(\vec{x})\}$ which specify operators $\widehat{\Lambda}_x$ at each lattice point x.
- Complex weight Ω.
- At each lattice point x, LOCAL coherent state operator:

$$\widehat{\Lambda}_x = |\alpha(x)\rangle\langle\beta^*(x)|$$

- 2 complex variables per lattice point.
- Describes *any* quantum state.
- Correspondences:
  1. Master equation for $\widehat{\rho}$.
  2. $\rightarrow$ Fokker-Planck equation for G.
  3. $\longrightarrow$ Stochastic equations for $\vec{v}$.
- Quantum observables correspond to appropriate averages of variables $\vec{v}$.

Dynamics

Just Gross-Pitaevskii equations plus Gaussian noise

$$\frac{d\alpha(x)}{dt} = -i\hbar\sum_y \omega_{xy}\,\alpha(y) - \frac{ig}{\Delta x}\alpha(x)^2\beta(x) + i\sqrt{\frac{ig}{\Delta x}}\,\alpha(x)\,\xi_1(x,t)$$

And $\frac{d\beta(x)}{dt} = \frac{d\alpha^*(x)}{dt}$ but with $\alpha^* \leftrightarrow \beta$ and new noise ξ_2.

- $\xi_j(x,t)$ are independent Gaussian noises of variance $1/\Delta t$ for each x, t, j.
- Linear couplings ω_{xy} between x and y contain kinetics and external potential.

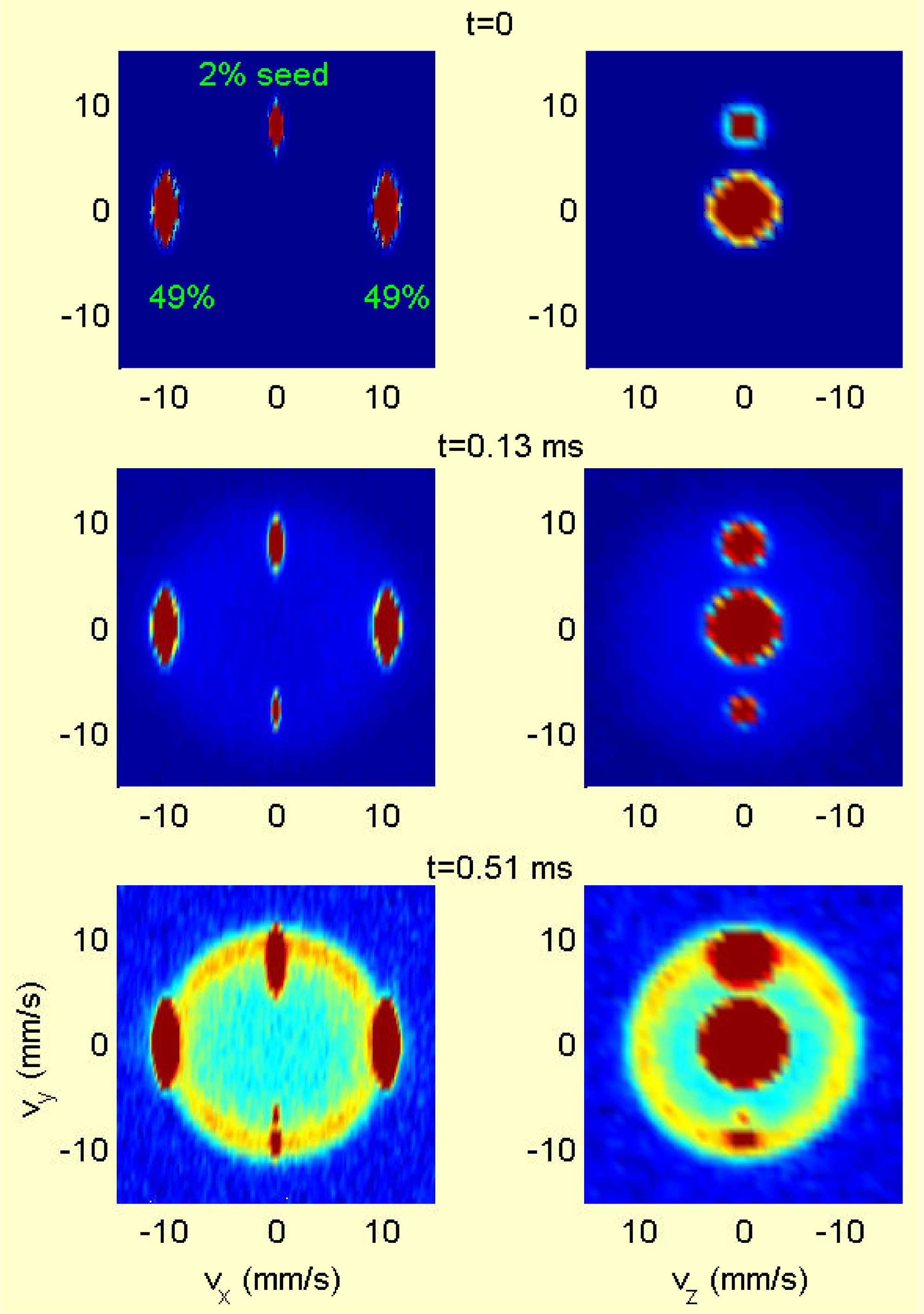
Simulation properties

- Number of equations linear in lattice size. $\longrightarrow$ TRACTABLE!
- No linearization. No truncation of any kind. Full quantum evolution.
- Applies to open and closed systems.
- Any observables can be calculated.
- Parallel algorithm easily implemented.

3D Colliding BECs

- 150000 atoms.
- No truncation or linearization.
- Collision along cigar-shaped trap in direction x.
- 4-wave mixing as per Vogels *et al*[?] experiment (but less atoms).

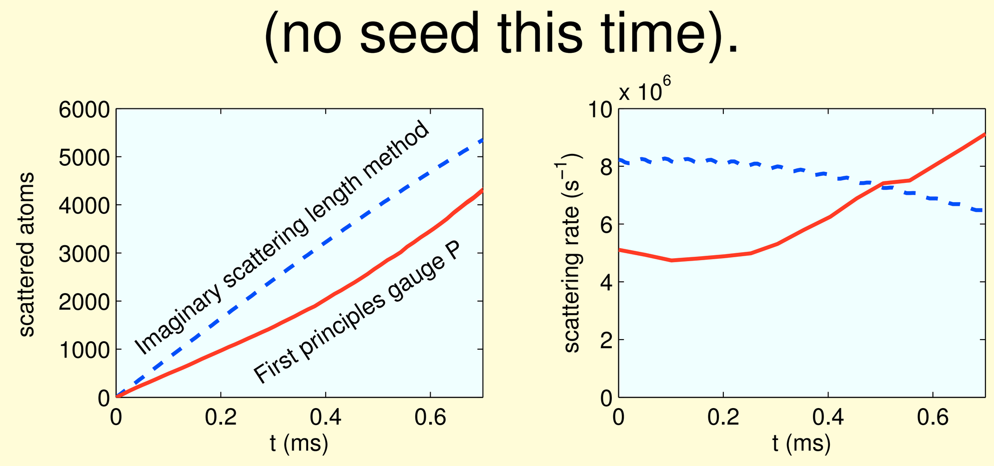
Velocity distribution evolution.



- Both coherent and incoherent scattering important.

Scattering into initially empty modes

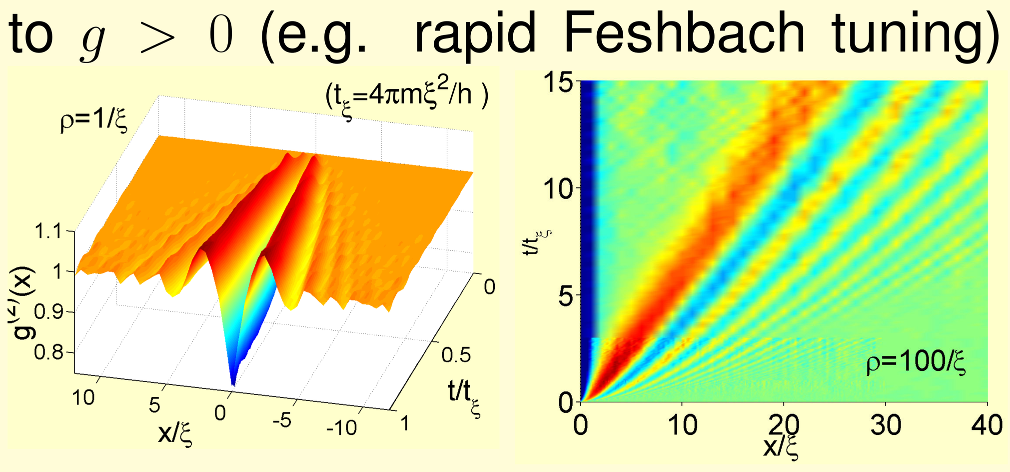
(no seed this time).



- Beginnings of coherent scattering into initially empty modes visible.

Correlation waves

- 1D uniform gas.
- Evolution after disturbance at $t = 0$ in the form of a change from $g = 0$ to $g > 0$ (e.g. rapid Feshbach tuning)



- Wave behaviour not visible in density — *only in correlations*.

Thermodynamics

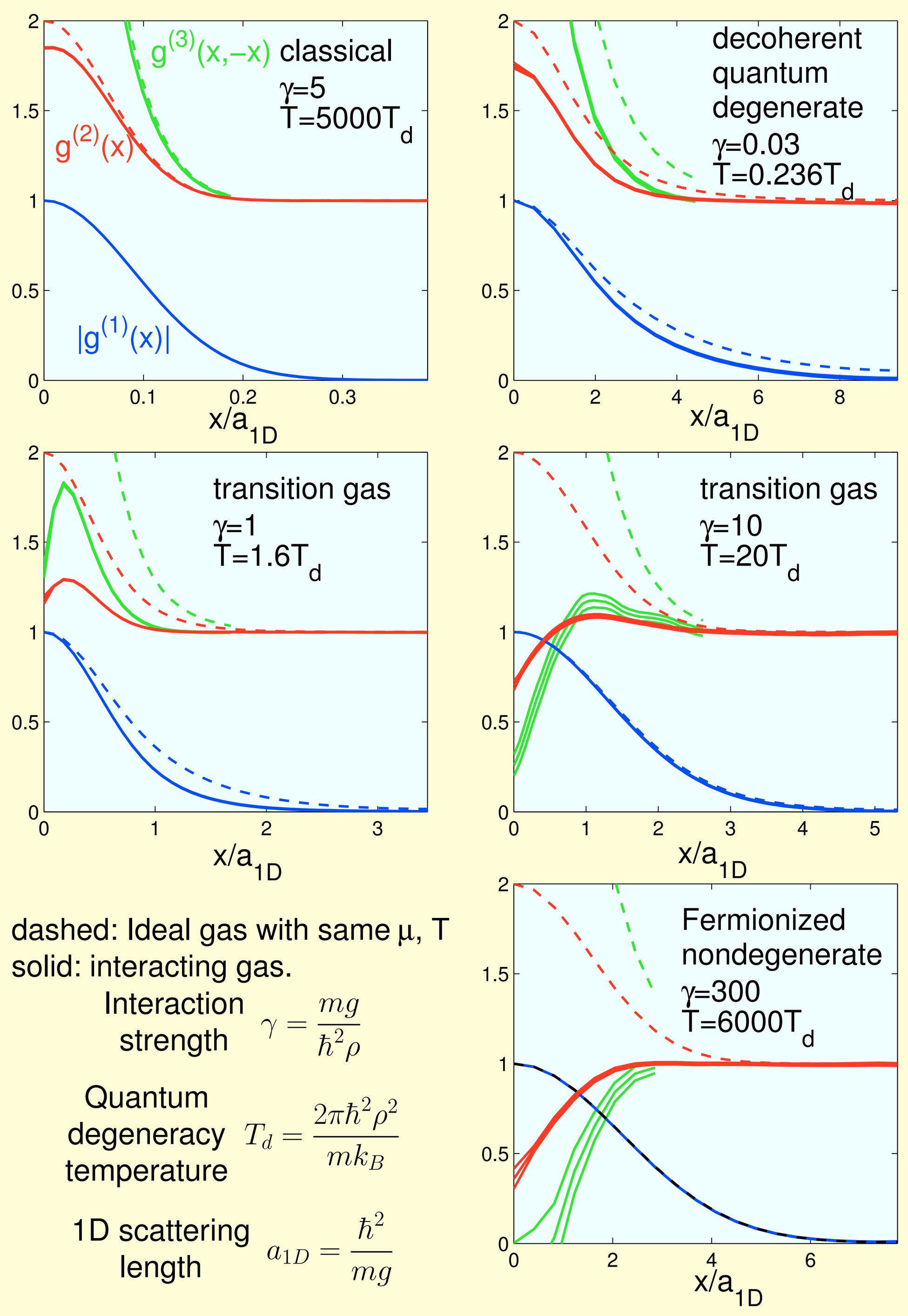
Grand canonical ensemble

- Similar to dynamics but in "imaginary time" $\tau = 1/k_BT$
- Evolution of weight Ω.
- Initial (high T) condition: $\widehat{\rho}(0) = \widehat{I}$

$$\frac{d\widehat{\rho}}{d\tau} = -\frac{1}{2}\left[\widehat{H} - \widehat{N}\frac{\partial\mu}{\partial\tau},\ \widehat{\rho}\right]_+$$

1D uniform gas[?]

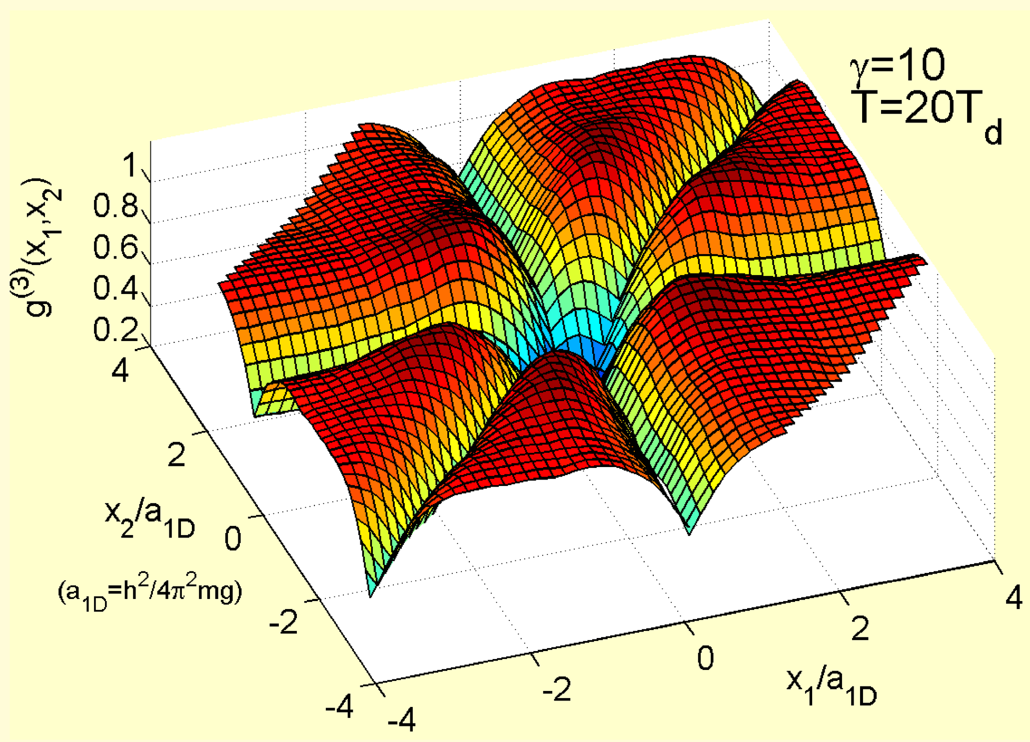
Spatial correlations (1st–3rd order) In various regimes



We find that a Preferred interparticle distance $\mathcal{O}(a_{1D})$ arises in transition gas regime.

Three-point correlations

$$g^{(3)}(x_1,x_2) = \frac{1}{\rho^3}\left\langle \widehat{\Psi}^\dagger(0)\widehat{\Psi}^\dagger(x_1)\widehat{\Psi}^\dagger(x_2)\widehat{\Psi}(0)\widehat{\Psi}(x_1)\widehat{\Psi}(x_2)\right\rangle$$



References

[1] P. D. Drummond and P. Deuar, J. Opt. B-Quant. and Semi-class. Opt. **5**, S281 (2003).

[2] P. D. Drummond, P. Deuar, and K. V. Kheruntsyan, Phys. Rev. Lett. **92**, 040405 (2004).

[3] J. M. Vogels, K. Xu, and W. Ketterle, Phys. Rev. Lett. **89**, 020401 (2002).