First-principles simulations of interacting Bose gases

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Outline

- The model: Quantum Bose gas with local two-particle collisions.
- When might we want first principles calculations?
- How to overcome the Hiblert space complexity problem to simulate a many-body system.
- How it is done using the positive P representation (from quantum optics).
- Show some simulation results.

Bose gas model: Field Hamiltonian

Spatial position is $\mathbf{x}$
$\widehat{\Psi}(\mathbf{x})$ destroys Boson at $\mathbf{x}$
$\widehat{\Psi}^\dagger(\mathbf{x})$ createsBoson at $\mathbf{x}$
$\langle\widehat{\Psi}^\dagger(\mathbf{x}\widehat{\Psi}(\mathbf{x})\rangle$ is the density at $\mathbf{x}$.

$$\widehat{H} = \int d\mathbf{x}\Bigg\{$$

Kinetic energy

$$\frac{\hbar^2}{2m}\frac{\partial\widehat{\Psi}^\dagger(\mathbf{x})}{\partial\mathbf{x}}\frac{\partial\widehat{\Psi}(\mathbf{x})}{\partial\mathbf{x}}$$

Two-body interactions

$$+ \quad \frac{1}{2}\int d\mathbf{y}U(\mathbf{x}-\mathbf{y})\widehat{\Psi}^\dagger(\mathbf{x})\widehat{\Psi}^\dagger(\mathbf{y})\widehat{\Psi}(\mathbf{x})\widehat{\Psi}(\mathbf{y})$$

External potential (e.g. trap)

$$+ \quad V_{\text{ext}}(\mathbf{x})\widehat{\Psi}^\dagger(\mathbf{x})\widehat{\Psi}(\mathbf{x})\Bigg\}$$

Bose gas model: Dynamics

State: Density matrix $\widehat{\rho}$.

Master equation (Linblad form):

$$\begin{aligned}\frac{\partial\widehat{\rho}}{\partial t} &= \frac{1}{i\hbar}\left[\widehat{H},\widehat{\rho}\right] \\ &\quad -\frac{1}{2}\int d\mathbf{x}\sum_j\left\{\widehat{L}_j^\dagger\widehat{L}_j\widehat{\rho}+\widehat{\rho}\widehat{L}_j^\dagger\widehat{L}_j-2\widehat{L}_j\widehat{\rho}\widehat{L}_j^\dagger\right\}\end{aligned}$$

e.g. interaction with heat bath. $\overline{n}\,(T)$ particles per bath mode:

$$\begin{aligned}\widehat{L}_1(\mathbf{x}) &= \widehat{\Psi}(\mathbf{x})\sqrt{\gamma(\mathbf{x})\,(1+\overline{n}\,(T))} \\ \widehat{L}_2(\mathbf{x}) &= \widehat{\Psi}^\dagger(\mathbf{x})\sqrt{\gamma(\mathbf{x})\,\overline{n}\,(T)}.\end{aligned}$$

What can this model describe?

- Cold gas of alkali-metal atoms
  - in a trap (3D,2D,1D)
  - free
- Bose-Einstein Condensate (BEC) when very cold
- Interactions with an environment. e.g. loss of atoms at the edge of the trap.
  - Evaporative cooling
  - Coherent out-coupling (atom laser)
- interacting BECs
- Bosons in a lattice potential

When do we want first-principles calculations?

- If system is very hot, can use thermodynamics **non-coherent**

- If system is very cold, all atoms are in one **coherent** orbital (BEC), and can use mean field theory

$$\widehat{\Psi} \to \psi$$

- If it is a bit hotter can use perturbation theory around the mean field

$$\widehat{\Psi} \to \psi(1 + \epsilon\widehat{c} + \dots)$$

- If both coherent and non-coherent processes are important and coupled to each other, then neither approach works well, and a first-principles method is desirable. e.g.
  - Formation of BEC under evaporative cooling.
  - Collision of BECs
  - BEC near critical temperature.

Lattice

- For computer simulations need to approximate space as a lattice with volume $\Delta\mathbf{x}$ at each lattice point.

- At each point

$$\widehat{\Psi}(\mathbf{x}) \to \frac{\widehat{a}_{\mathbf{x}}}{\sqrt{\Delta\mathbf{x}}}.$$

- $\widehat{a}_{\mathbf{x}}$ and $\widehat{a}^{\dagger}_{\mathbf{x}}$ are anihilation/creation operators like in quantum optics.

- For cold alkali metal gases (e.g. BEC) can use

$$U(\mathbf{x}-\mathbf{y}) \to g\,\delta(\mathbf{x}-\mathbf{y})$$

Hilbert space complexity problem

Brute force does not work for many-body systems, as everyone knows.

- Supose we have a lattice with 5 points ($not\ very\ big!$)
- And there are 10 atoms.
- The basis at each lattice point x can consist of $|n_x\rangle_x$ with n_x atoms ($n_x \leq 10$).
- The full density matrix is

$$\widehat{\rho} = \sum_{n_x, m_x} C_{n_x, m_x} \otimes_x |n_x\rangle_x \langle m_x|_x$$

- There are $\approx 1.3 \times 10^{10}$ complex coefficients C_{n_x, m_y} to store in memory.
- **Number of coefficients grows as e^N with N lattice points.**

A fix: phase space representations

$$\widehat{\rho} = \int P(\overrightarrow{v})\ |\psi(\overrightarrow{v})\rangle\ \langle\phi(\overrightarrow{v})|\ d\overrightarrow{v}$$

$$|\psi(\overrightarrow{v})\rangle = \bigotimes_x |\psi(\overrightarrow{v}_x)\rangle_x \,.$$

- Local off-diagonal operator $|\,\psi\,\rangle_x \langle\,\phi\,|_x$ at each lattice point x

- Each local basis state $|\,\psi(\overrightarrow{v}_x)\,\rangle_x$ depends on a set of continuous variables $\overrightarrow{v}_x$

- $P(\overrightarrow{v})$ is a distribution of the variables $\overrightarrow{v}_x$ which specify the separable off-diagonal operators $|\,\psi\,\rangle\langle\,\phi\,|$.

Statistical interpretation

If P is real and positive then it is a distribution of the variables $\overrightarrow{v}$. Taking S samples,

$$\widehat{\rho} \approx \frac{1}{S} \sum_{j=1}^{S} \left| \psi(\overrightarrow{v}^{(j)}) \right\rangle \left\langle \phi(\overrightarrow{v}^{(j)}) \right| .$$

when $\overrightarrow{v}^{(j)}$ is the jth sample of the distribution $P(\overrightarrow{v})$.

- There is a small set number of variables in $\overrightarrow{v}^{(j)}$ per lattice point (usually two complex).
- **The number of variables in each sample grows only $\propto N$ with N lattice points.**
- Tractable for calculations.

Correspondences for evolution

For some kernels $\widehat{\Lambda}$, you can make the following $exact$ correspondences:

1. Master equation to equation for distribution P

$$\frac{\partial \widehat{\rho}}{\partial t} \leftrightarrow \frac{\partial P(\overrightarrow{v})}{\partial t}$$

2. to stochastic (i.e. noisy) equations for the kernel variables

$$\frac{\partial P}{\partial t} \leftrightarrow \frac{\partial \overrightarrow{v}}{\partial t}$$

These last equations for $\overrightarrow{v}$ can be applied separately to each sample $\overrightarrow{v}^{(j)}$.

Numerical procedure

- Approximate initial state $\widehat{\rho}(0)$ by taking S samples $\overrightarrow{v}^{(j)}$ according to the initial distribution $P(\overrightarrow{v}, 0)$.

- Evolve each sample according to the stochastic equations which correspond to the exact quantum evolution.

- Calculate observables by

$$\begin{aligned} \langle \widehat{O} \rangle &= \mathrm{Tr}\left[\widehat{\rho}\widehat{O}\right] \\ &\approx \frac{1}{S}\sum_{j=1}^{S} \Omega^{(j)} \left\langle \phi(\overrightarrow{v}^{(j)}) \right| \widehat{O} \left| \psi(\overrightarrow{v}^{(j)}) \right\rangle \end{aligned}$$

- As the number of samples grows, the observables are estimated with growing accuracy.

- Since the number of variables is $\propto N$ for N lattice points, can do first principles calculations of very large systems.

- BUT with limited precision.

Positive P distribution

Off-diagonal coherent state operators

$$|\alpha_x\rangle_x \langle\beta_x^*|_x$$

at each lattice point x, where

$$|\alpha_x\rangle = e^{-|\alpha_x|^2/2} e^{\widehat{a}_x^\dagger \alpha_x} |0\rangle$$

is the coherent state well known in quantum optics.

- $P(\alpha_x, \beta_x)$ is positive real, so stochastic interpretation is possible.
- stochastic equations for α_x and β_x can be obtained for our interacting Bose gas model.
- e.g. number of particles at lattice point x is

$$\langle \widehat{a}_x^\dagger \widehat{a}_x \rangle \approx \frac{1}{S} \sum_{j=1}^{S} \mathrm{Re}\left\{ \alpha_x^{(j)} \beta_x^{(j)} \right\}$$

Why use coherent states?

Suppose we use instead a number state operator

$$|n\rangle \langle m|$$

at each lattice point, where $|n\rangle$ means there are precisely n atoms. This does not work because:

- e.g. number of particles at the lattice point is

$$\langle \widehat{a}^\dagger \widehat{a} \rangle = \langle m| \widehat{a}^\dagger \widehat{a} |n\rangle$$

- Most density matrix samples are off-diagonal ($m \neq n$)
- So, most samples contribute $zero$ to the observable calculations.
- Lots of computer time, no result.

Coherent states work because

$$\langle \beta^*| \widehat{a}^\dagger \widehat{a} |\alpha\rangle \neq 0$$

and each sample contributes.

Equations

Just as an example:

$$\begin{aligned}
\frac{d\alpha_x}{dt} &= -i\omega_{xy}\alpha_y - i\frac{g}{\Delta x}\alpha_x^2\beta_x - \frac{\gamma_x}{2}\alpha_x + i\alpha_x\sqrt{\frac{ig}{\delta x}}\,\xi_x(t) \\
\frac{d\beta_x}{dt} &= i\omega_{xy}^*\beta_y + i\frac{g}{\Delta x}\alpha_x\beta_x^2 - \frac{\gamma_x}{2}\beta_x + \beta_x\sqrt{\frac{ig}{\delta x}}\,\tilde{\xi}_x(t).
\end{aligned}$$

- ω_{xy} contain kinetic interactions
- ω_{xx} contain external potential and kinetic interactions
- γ_x is loss to a $T = 0$ heat bath
- g is the inter-atom collision strength
- Δx is the lattice spacing
- $\xi(t)$ and $\tilde{\xi}(t)$ are gaussian random noises of variance 1. Independent at each time step.

Too good to be true?

- The equations for α_x and β_x are unstable.

- Straightforward simulation does not last long before precision is lost.

- Can develop equivalent but more stable equations using "stochastic gauge" method.
  Phys. Rev. A **66**, 033812 (2002)
  J. Opt. B. **5**, S281 (2003)
  Phys. Rev. Lett. **92**, 040405 (2004)

- I won't go into this because it becomes rather technical.

- But will show some simulation results.

Thermodynamics

- Environment at temperature $T = 1/k_B\tau$ and chemical potential $\mu(T)$.

- Density matrix:

$$\widehat{\rho}(\tau) = \exp\left[\left(\mu(\tau)\widehat{N} - \widehat{H}\right)\tau\right].$$

- Particle number

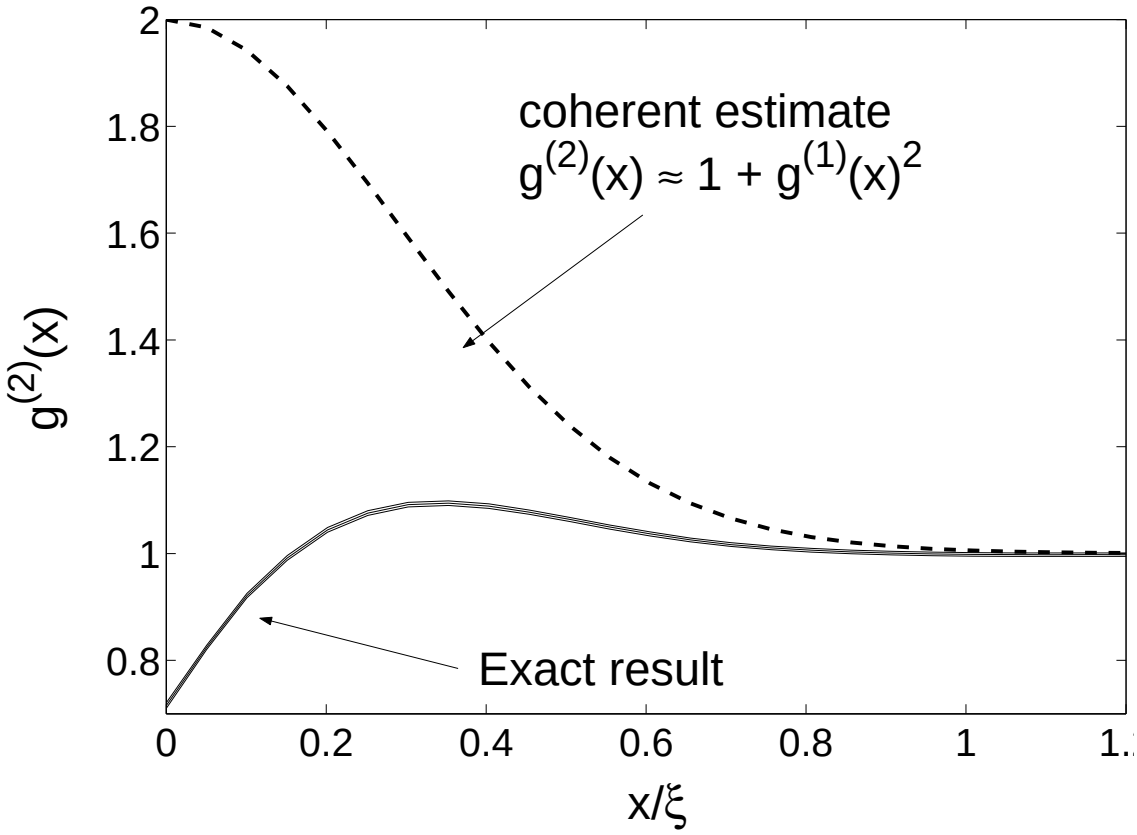
$$\widehat{N} = \int d\mathbf{x}\widehat{\Psi}^\dagger(\mathbf{x})\widehat{\Psi}(\mathbf{x}).$$

- Master equation:

$$\frac{\partial\widehat{\rho}(\tau)}{\partial\tau} = -\left[\widehat{H} - \frac{\partial(\tau\mu(\tau))}{\partial\tau}\widehat{N}\right]\widehat{\rho}.$$

- $\widehat{\rho}(0)$ is known ($T \to \infty$), so can start there, and integrate master equation to obtain grand canonical ensemble at finite temperature.

1D Bose gas: spatial correlations



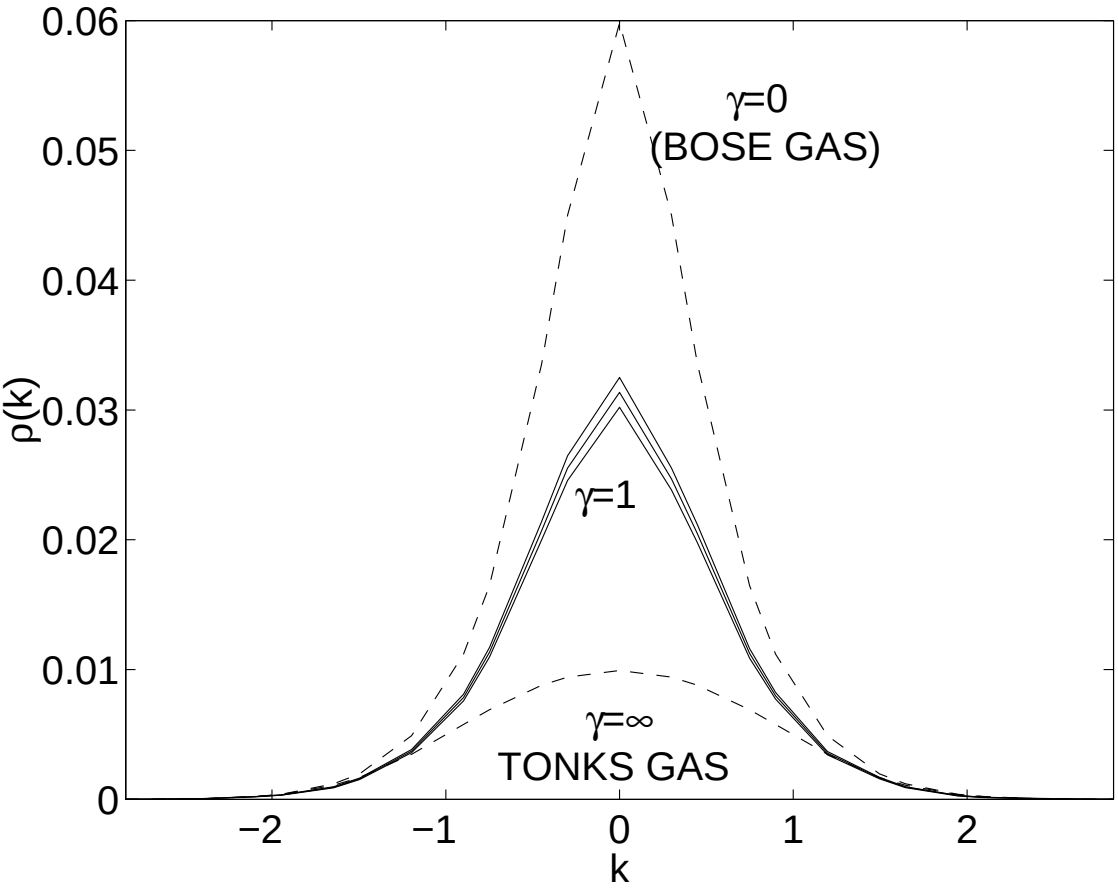
$$g^{(2)}(x) = \frac{\langle : \widehat{n}(0)\widehat{n}(x) : \rangle}{\langle \widehat{n}(0) \rangle \langle \widehat{n}(x) \rangle}$$

with density $\widehat{n}(x)$.

Collision strength $\gamma = \frac{mg}{n\hbar^2} = 10$
(Ideal gas $\gamma \to 0$, hard sphere gas $\gamma \to \infty$).

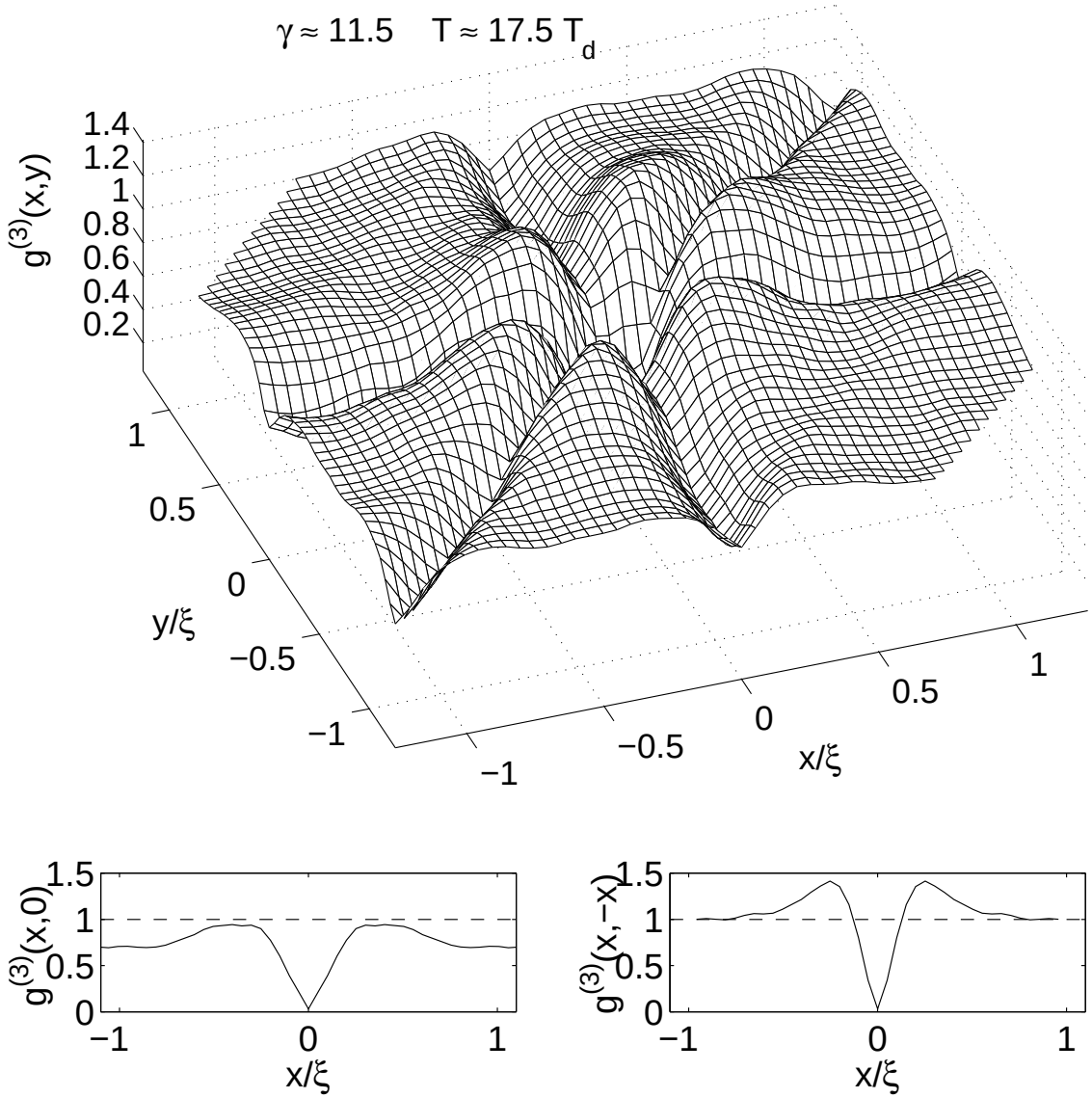
Temperature $T = 10T_d$,
(quantum degeneracy temperature $k_B T_d = \frac{2\pi\hbar^2 n^2}{m}$).

1D Bose gas: momentum distribution



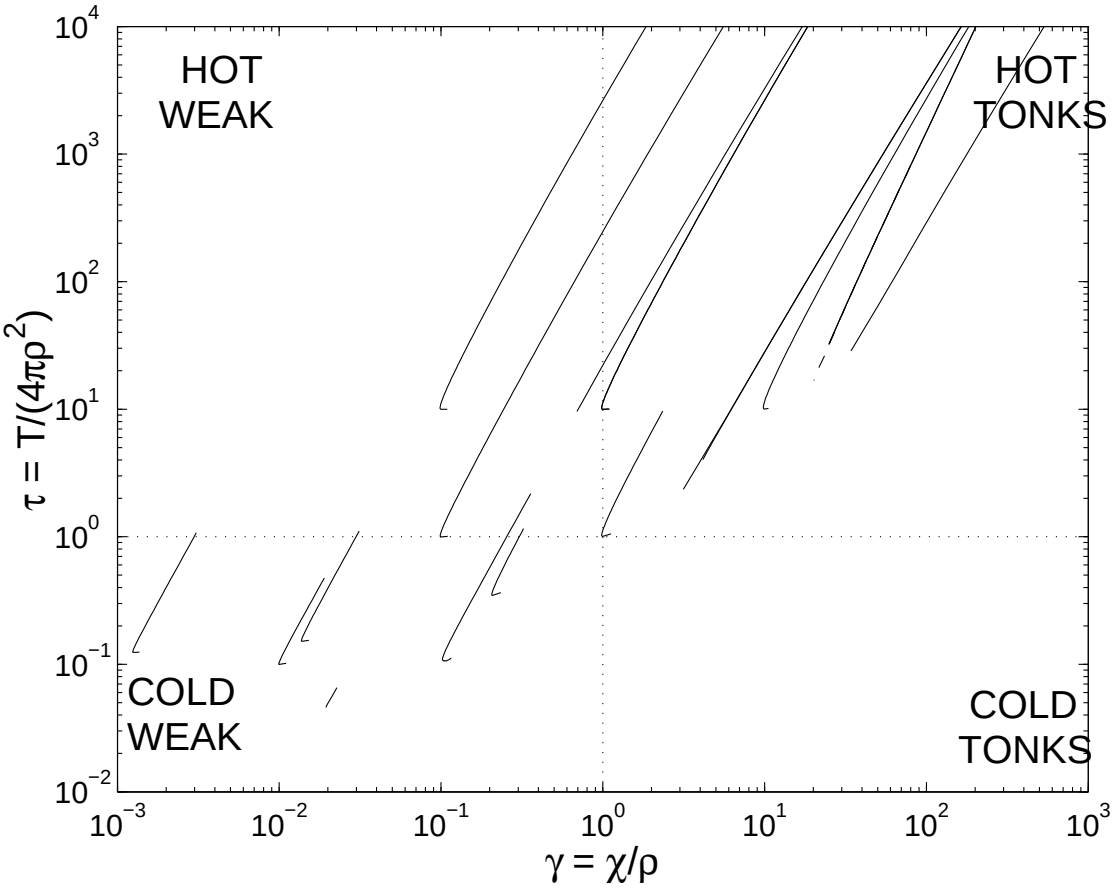
$$\gamma = T_d = 1$$

1D Bose gas: three-particle correlations

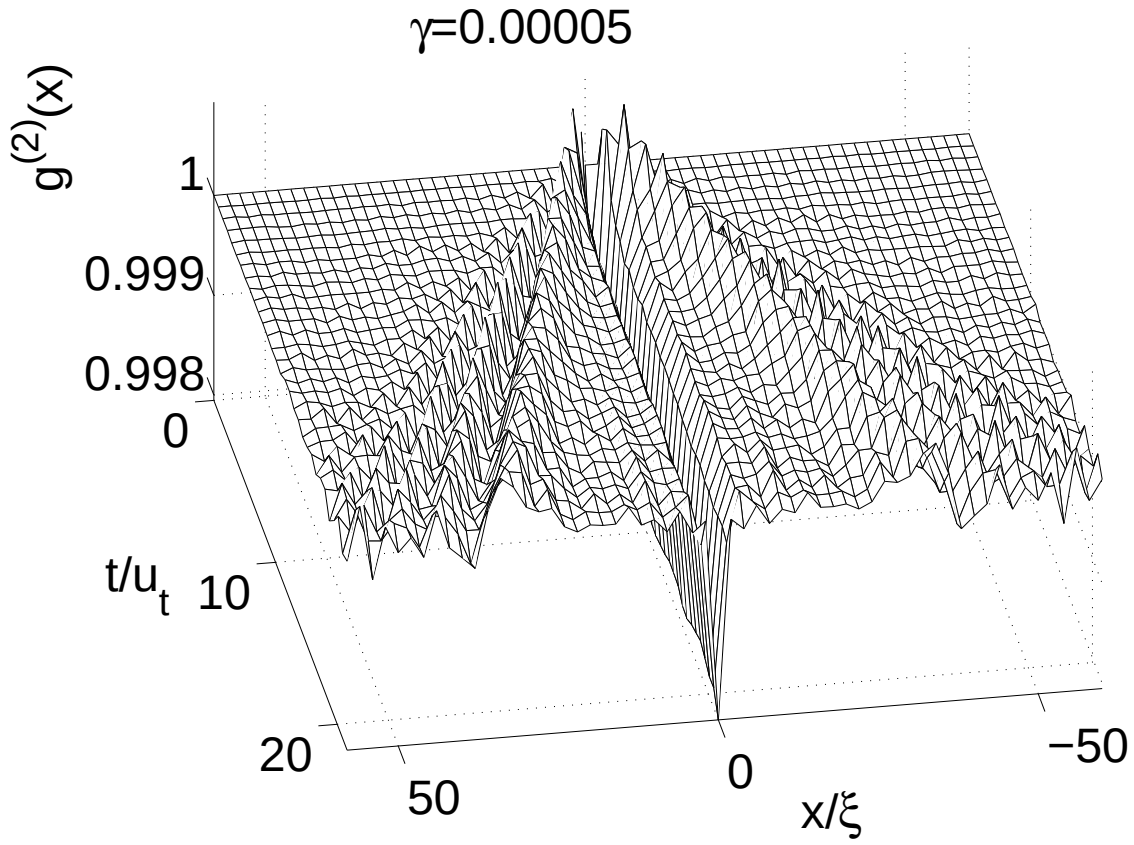


$$g^{(3)}(x,y) = \frac{\langle : \widehat{n}(0)\widehat{n}(x)\widehat{n}(y) : \rangle}{\langle \widehat{n}(0) \rangle \langle \widehat{n}(x) \rangle \langle \widehat{n}(y) \rangle}$$

1D Bose gas: Simulation Range

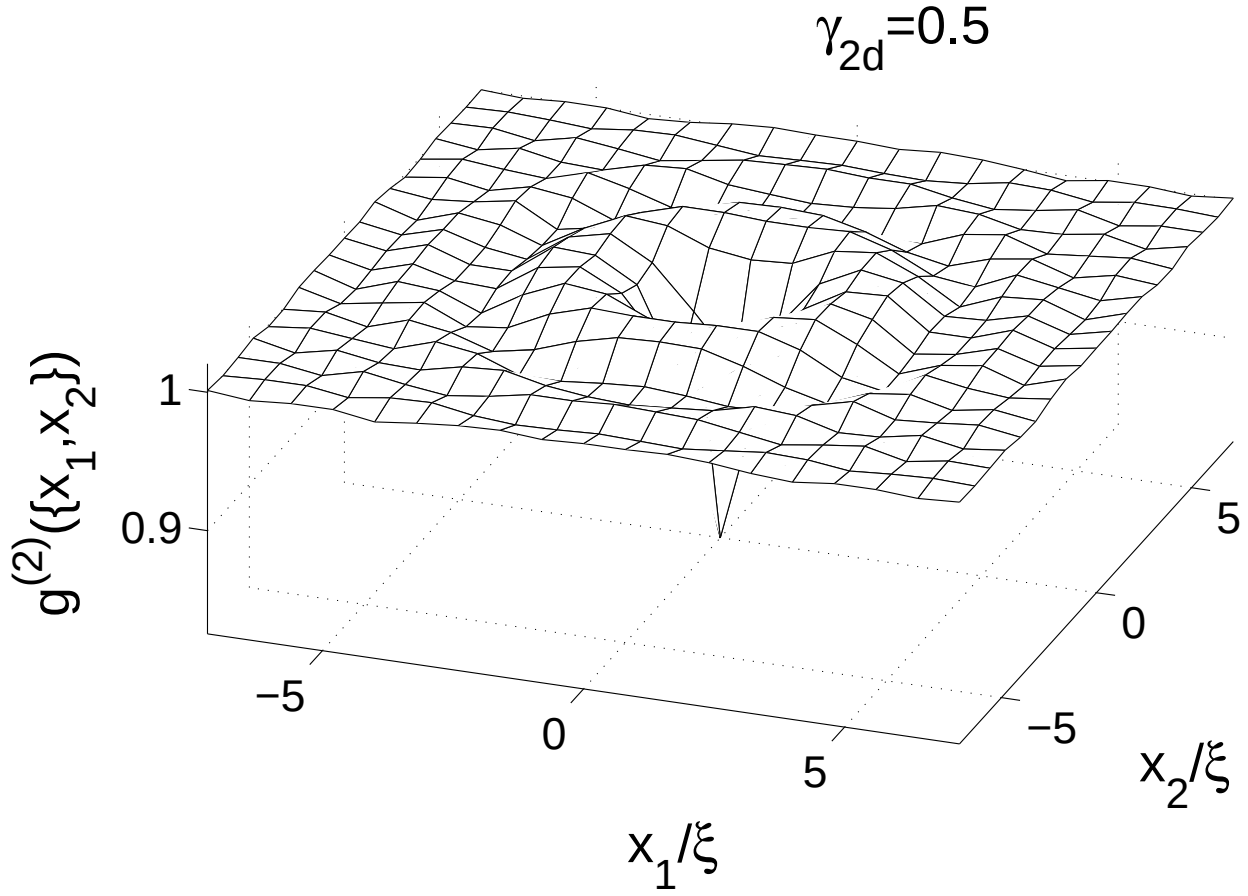


Propagation of correlations in 1D condensate



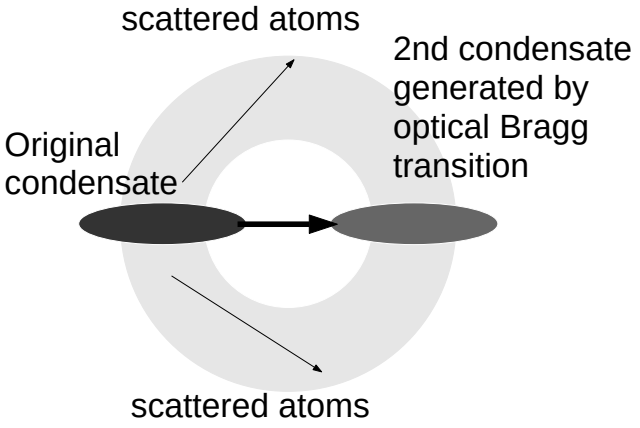
- Initially: coherent wavefunction — effectively interaction zero.
- Subsequently: rise in intereaction to finite levels induces a correlation on interatomic scales.
- e.g. change in scattering length due to Feschbach resonance.

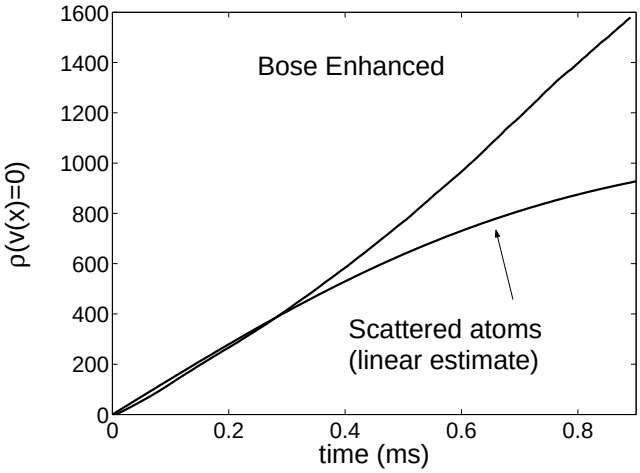
In two dimensions



$$g^{(2)}(\{x_1, x_2\}) = \frac{\langle : \widehat{n}(\{0,0\})\widehat{n}(\{x_1, x_2\}) : \rangle}{\langle \widehat{n}(\{0,0\}) \rangle \langle \widehat{n}(\{x_1, x_2\}) \rangle}$$

Bose enhancement of scattered atoms in moving condensates





- Collaboration with Marek Trippenbach, and Jan Chwedeńczuk, Warszawa.
- Three-dimensional simulation
- ^{23}Na.
- Parameters as in Vogels,Xu&Ketterle[PRL **89**, 020401], but with less atoms (150 000 rather than 30 000 000).