First-principles simulations of interacting Bose gases using stochastic gauges

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Many-body simulation scheme

$$\widehat{\rho} = \int P(\overrightarrow{v})\, \widehat{\Lambda}(\overrightarrow{v})\, d\overrightarrow{v}$$
$$\approx \sum_{j=1}^{\mathcal{S}\gg 1} \widehat{\Lambda}(\overrightarrow{v}^{(j)})$$

- Sample initial state $\widehat{\rho}(0)$ with $\mathcal{S}$ operators $\widehat{\Lambda}(\overrightarrow{v}^{(j)})$.
- Evolve each set of variables $\overrightarrow{v}^{(j)}$ according to stochastic equations which correspond to master equation for $\widehat{\rho}$.
- Calculate observables along the way using $\overrightarrow{v}$, and then average.

To be tractable, need to split into N subsystems:

$$\widehat{\Lambda} \propto \bigotimes_{i=1}^{N} \widehat{\lambda}(\overrightarrow{v}_i)$$

then the number of variables $\propto N$.

Interacting Bose gas

$$
\begin{aligned}
\widehat{H} &= \int d\mathbf{x} \Bigg\{ \frac{\hbar^2}{2m} \frac{\partial \widehat{\Psi}^\dagger(\mathbf{x})}{\partial \mathbf{x}} \frac{\partial \widehat{\Psi}(\mathbf{x})}{\partial \mathbf{x}} \\
&\quad + \frac{1}{2} \int d\mathbf{y} U(\mathbf{x}-\mathbf{y}) \widehat{\Psi}^\dagger(\mathbf{x}) \widehat{\Psi}^\dagger(\mathbf{y}) \widehat{\Psi}(\mathbf{x}) \widehat{\Psi}(\mathbf{y}) \\
&\quad + V_{\mathrm{ext}}(\mathbf{x}) \widehat{\Psi}^\dagger(\mathbf{x}) \widehat{\Psi}(\mathbf{x}) \Bigg\}
\end{aligned}
$$

- For cold alkali-metal gases use $U(\mathbf{x}-\mathbf{y}) = g\delta(\mathbf{x}-\mathbf{y})$.

- Extended interactions $U \neq \delta$ pose no problem, but slow calculation down.

- Dynamics:

$$
\frac{\partial \widehat{\rho}}{\partial t} = -\frac{i}{\hbar} \left[\widehat{H}, \widehat{\rho} \right] + \text{environment}
$$

Gauge P representation

$$\widehat{\Lambda} = \Omega \bigotimes_{\mathbf{x}} \frac{|\alpha_{\mathbf{x}}\rangle_{\mathbf{x}} \langle \beta^*_{\mathbf{x}}|_{\mathbf{x}}}{\langle \beta^*_{\mathbf{x}} | \alpha_{\mathbf{x}} \rangle}$$

- $|\alpha_{\mathbf{x}}\rangle_{\mathbf{x}}$ is a coherent state at lattice position $\mathbf{x}$.
- Ω is a complex weight
- Thsi is like the positive P representation, but with a global weight.
- Equations are similar to Gross-Pitaevskii form, plus noise.
- Observables estimated by weighted averages of α, β. e.g.

$$\langle \widehat{\Psi}^\dagger(\mathbf{x}) \widehat{\Psi}(\mathbf{x}) \rangle = \frac{\langle \Omega \alpha_{\mathbf{x}} \beta_{\mathbf{x}} \rangle_{\mathrm{stoch}}}{d\mathbf{x} \, \langle \Omega \rangle_{\mathrm{stoch}}}$$

- All/any observables can be calculated from single simulation.

1D uniform gas thermodynamics

- Simple model, but not many exact results:
  1. Energy, density, pressure: Yang&Yang (1968)
  2. Local correlations $g^{(2)}(0)$, $g^{(3)}(0)$: Gangardt, Shlyapnikov, Kheruntsyan, Drummond (2003)

- Grand canonical ensemble:

$$\widehat{\rho} \propto \exp\left[\frac{\widehat{N}\mu - \widehat{H}}{k_B T}\right]$$

- Equation ($t = 1/k_B T$):

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

- Initial condition:

$$\widehat{\rho}(t=0) \propto \widehat{I}$$

Stabilization with gauges

- Positive P equations for α, β were unstable

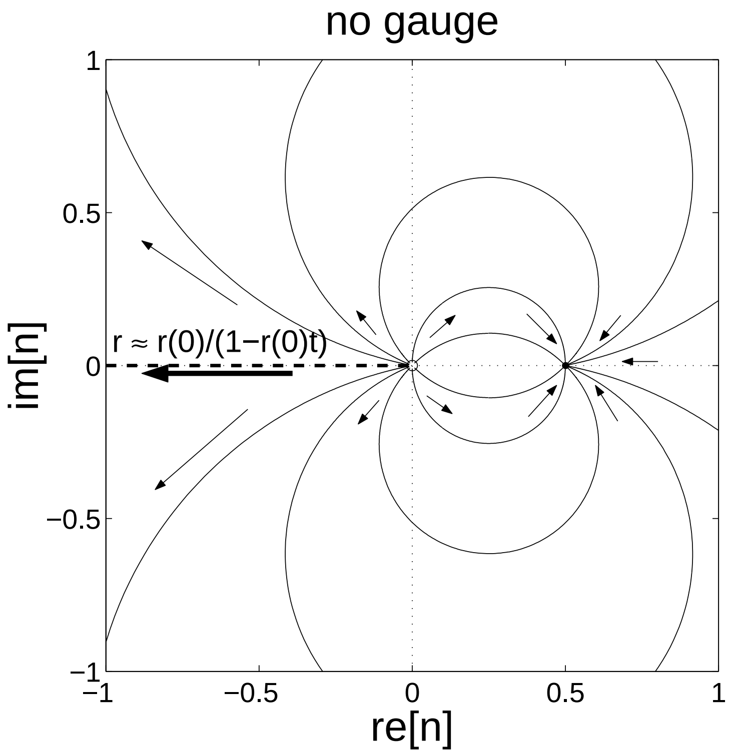
- But due to the weight Ω we have extra freedom to:

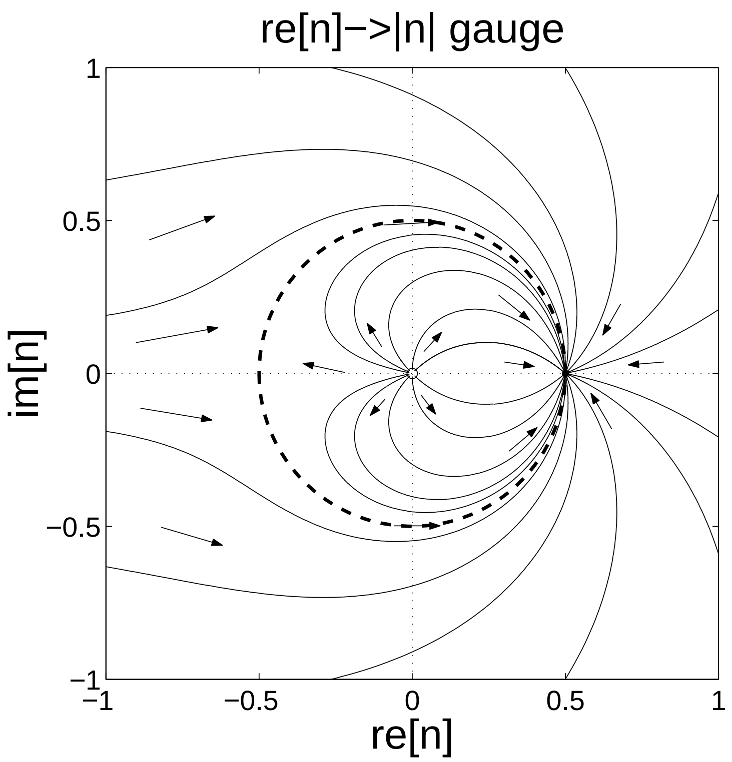
  1. Change deterministic evolution of α, β (arbitrarily) to make it stable.
  2. Compensate by modifications of weight.

- Form of changes:

$$
\begin{aligned}
\dot{\overrightarrow{\alpha}} &= \overrightarrow{A} + B\left(\overrightarrow{\xi} - \overrightarrow{\mathcal{G}}\right) \\
\dot{\overrightarrow{\beta}} &= \overrightarrow{A'} + B'\left(\overrightarrow{\xi}' - \overrightarrow{\mathcal{G}}'\right) \\
\dot{\Omega} &= \Omega\left(\overrightarrow{\mathcal{G}} \cdot \overrightarrow{\xi} + \overrightarrow{\mathcal{G}'} \cdot \overrightarrow{\xi}'\right)
\end{aligned}
$$

The $\overrightarrow{\mathcal{G}}$, $\overrightarrow{\mathcal{G}}'$ are arbitrary (gauge) functions.
The $\overrightarrow{\xi}$, $\overrightarrow{\xi}'$ are gaussian noises.


no gauge
1
0.5
0
−0.5
−1
−1
−0.5
0
0.5
1
im[n]
re[n]
r ≈ r(0)/(1−r(0)t)


re[n]−>|n| gauge
1
0.5
0
−0.5
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−1
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0
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1
im[n]
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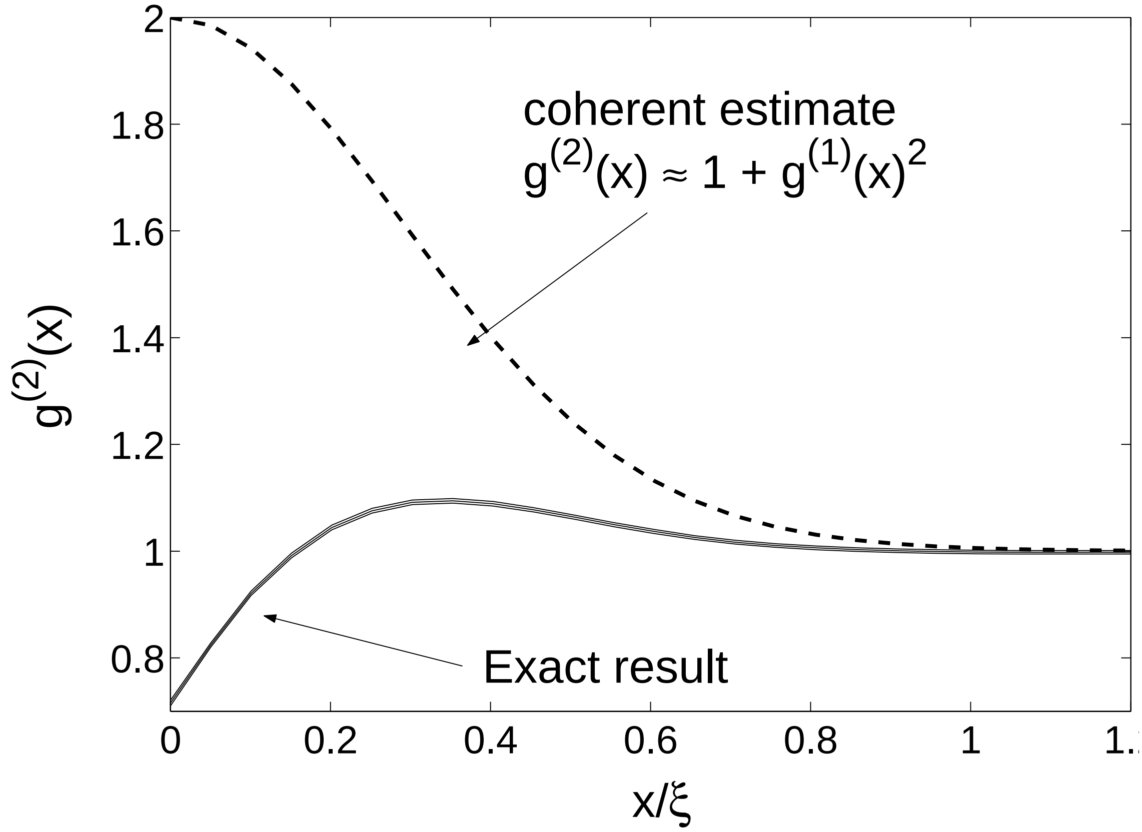
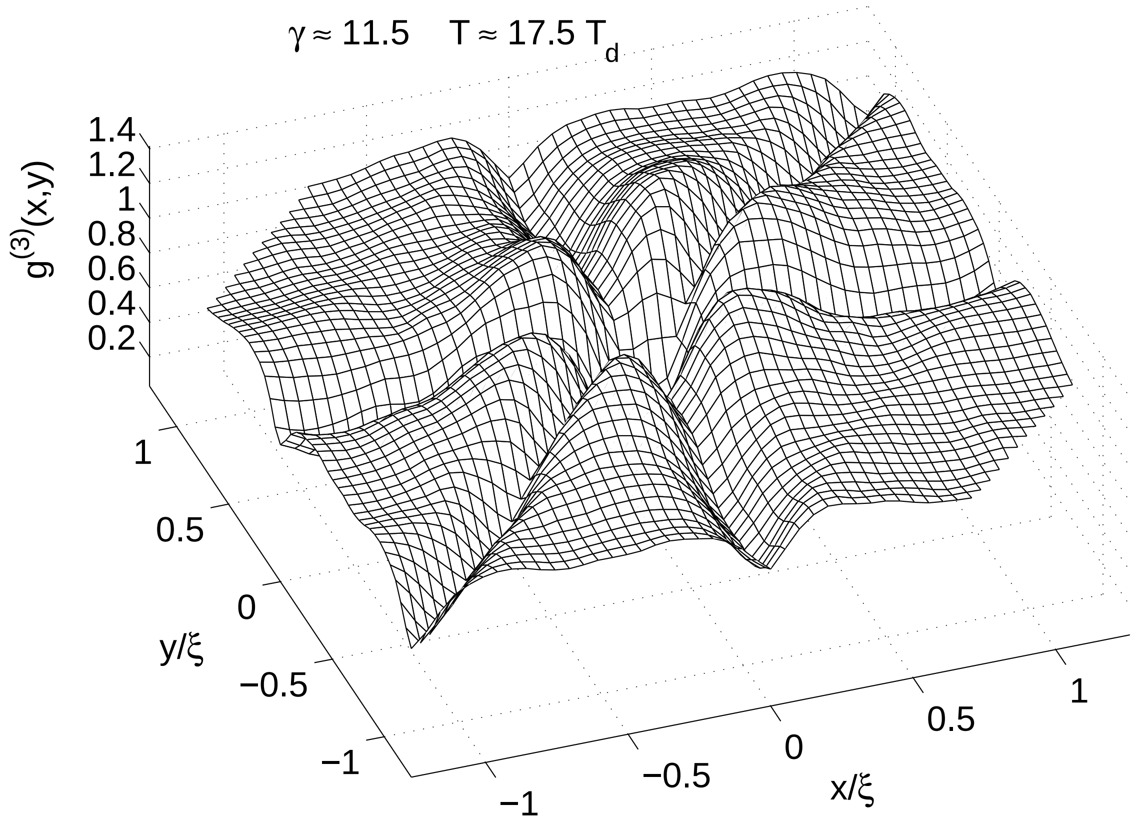


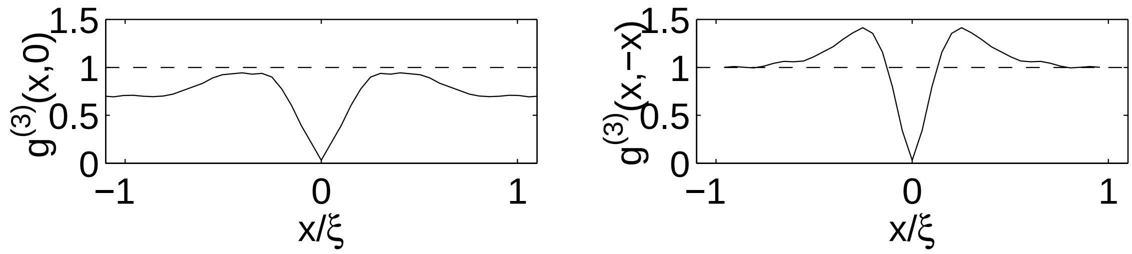
$$g^{(2)}(x) = \frac{\langle \widehat{n}(0)\widehat{n}(x)\rangle}{\langle \widehat{n}(0)\rangle\langle \widehat{n}(x)\rangle}$$

with density $\widehat{n}(x) = \widehat{\Psi}^\dagger(x)\widehat{\Psi}(x)$.

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

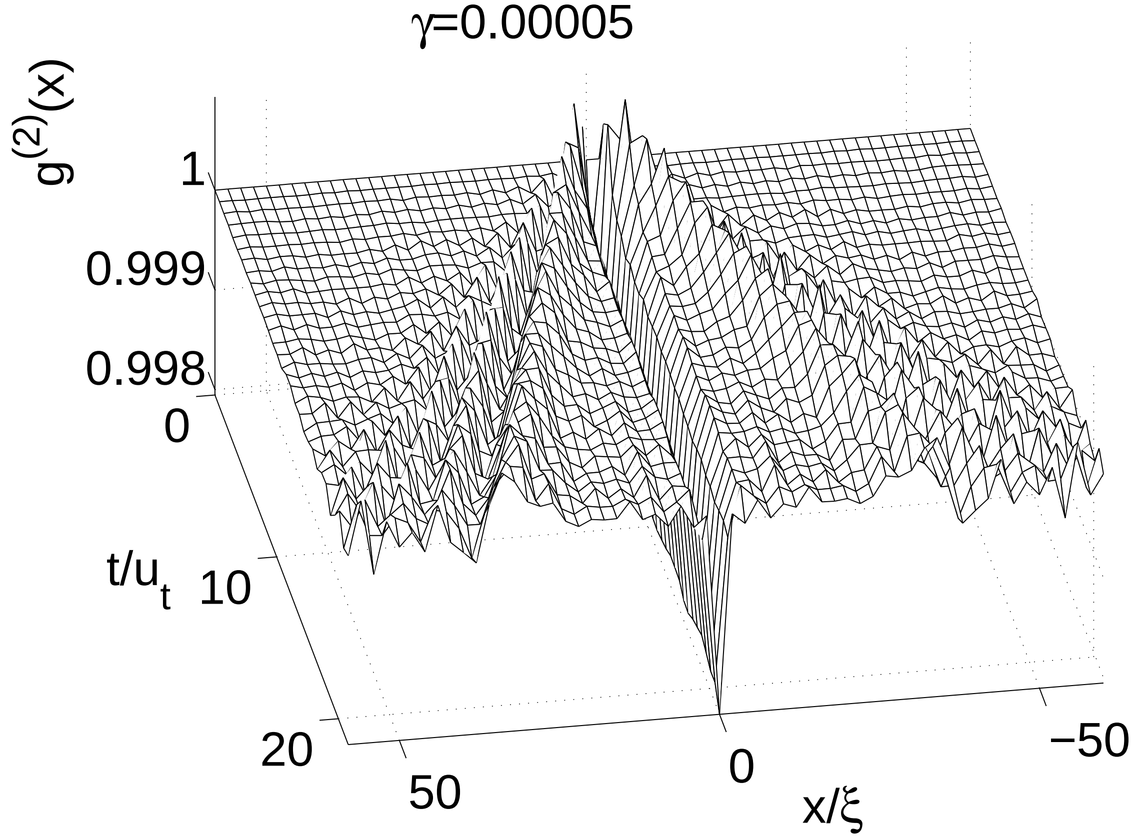
Temperature $T = 10T_d$,
(quantum degeneracy temperature $k_B T_d = \frac{2\pi\hbar^2 n^2}{m}$).





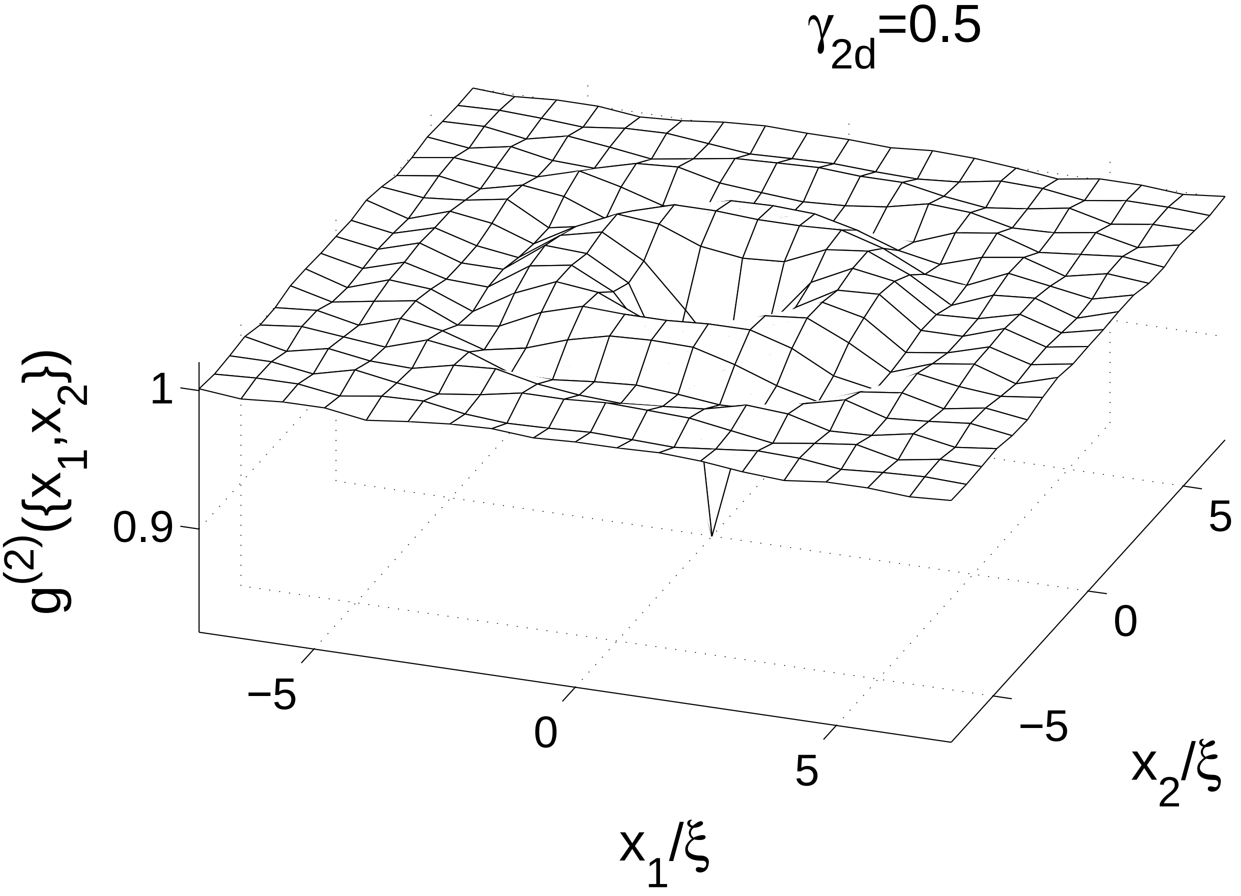
$$g^{(3)}(x,y) = \frac{\langle \widehat{n}(0)\widehat{n}(x)\widehat{n}(y)\rangle}{\langle \widehat{n}(0)\rangle\langle \widehat{n}(x)\rangle\langle \widehat{n}(y)\rangle}$$

Propagation of correlations in 1D condensate



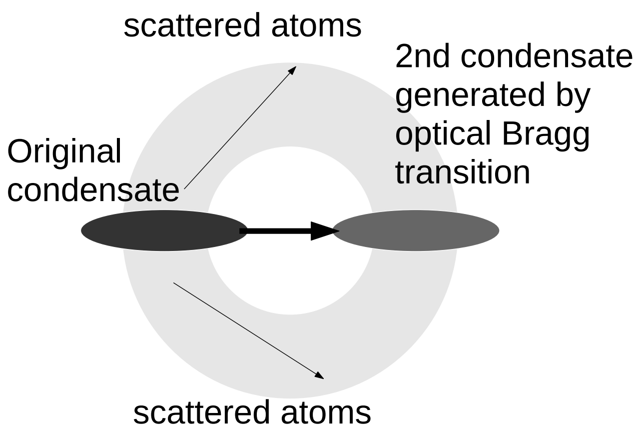
- Initially: coherent wavefunction — effectively interaction zero.
- Subsequently: rise in intereaction to finite levels induces a correlation on interatomic scales.
- e.g. change in scattering length due to Feschbach resonance.

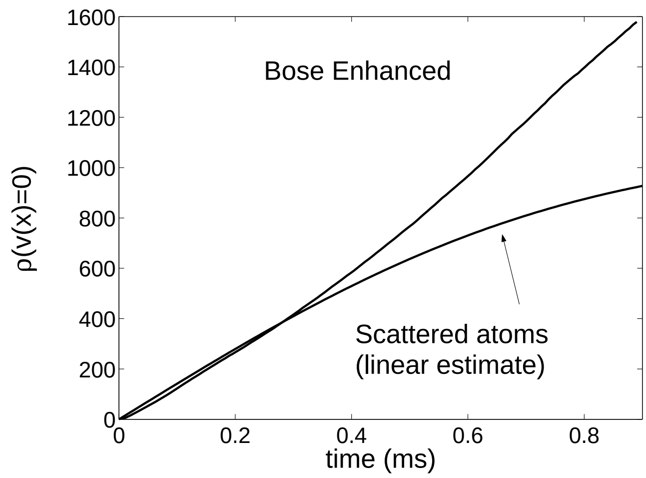
In two dimensions



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

Bose enhancement of scattered atoms in moving condensates





- Three-dimensional simulation
- ^{23}Na.
- Initial cloud: GP gound state with trap frequencies 20Hz, 80Hz, 80Hz.
- Parameters as in Vogels,Xu&Ketterle[PRL **89**, 020401], but with less atoms (150 000 rather than 30 000 000).

Thankyou