Dynamics of quantum correlations in BECs from first principles

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First-principles simulations: Preview

1. How the simulations work

   (a few equations)

2. 1D gas dynamics: correlation waves

   (pictures)

3. 3D gas dynamics: BEC collision

   (pictures)

4. 1D gas thermodynamics

   (pictures)

Interacting Bose gas model

$$\widehat{H} = \int d^3\mathbf{x} \left\{ -\frac{\hbar^2}{2m} \widehat{\Psi}^\dagger(\mathbf{x})\, \nabla^2 \widehat{\Psi}(\mathbf{x}) \quad + \quad \frac{g}{2}\, \widehat{\Psi}^\dagger(\mathbf{x})\, \widehat{\Psi}^\dagger(\mathbf{x})\, \widehat{\Psi}(\mathbf{x})\, \widehat{\Psi}(\mathbf{x}) \right\}$$

- $\widehat{\Psi}(\mathbf{x})$ is the anihilating Bose field operator at point $\mathbf{x}$.
- This is the usual cold dilute boson gas.
- Can add *external potential, losses*, or *non-local interactions*:
  $\frac{1}{2}\int d^3\mathbf{y}\, U(\mathbf{x}-\mathbf{y})\, \widehat{\Psi}^\dagger(\mathbf{x})\, \widehat{\Psi}^\dagger(\mathbf{y})\, \widehat{\Psi}(\mathbf{x})\, \widehat{\Psi}(\mathbf{y})$
  if we like.
- We go to a lattice with spacing $\Delta\mathbf{x}$:
  $\Delta\mathbf{x}$ less than healing length ξ,
  $\Delta\mathbf{x}$ more than s-wave scattering length a_s.

First principles: direct method

State:

$$\hat{\rho} = \sum_{\tilde{n}\tilde{m}} C_{\tilde{n}\tilde{m}}\, e^{i\theta_{\tilde{n}\tilde{m}}}\, |\tilde{n}\rangle\langle\tilde{m}|$$

Each configuration:

$$\tilde{n} = \{\ldots, n_{(x,y,z)}, \ldots\}$$

- $|\tilde{n}\rangle$, $|\tilde{m}\rangle$ are number states. At each point $\mathbf{x}$ there are exactly $n_{\mathbf{x}}$ atoms.
- About N^M configurations $\tilde{n}$ for N particles on M lattice points.
- Real variables $C_{\tilde{n}\tilde{m}}$ and $\theta_{\tilde{n}\tilde{m}}$. One for *each configuration*.
- For macroscopic N you can't even *store* this, let alone do dynamics.

First principles: positive P method

$$\widehat{\rho} = \int P(\widetilde{\alpha},\widetilde{\beta}) \, \|\widetilde{\alpha}\rangle\langle\widetilde{\beta}\| \, e^{\widetilde{\alpha}\cdot\widetilde{\beta}^*} \, d\widetilde{\alpha} \, d\widetilde{\beta}$$

- $P(\widetilde{\alpha},\widetilde{\beta})$ is real & positive: A probability.
- $\|\widetilde{\alpha}\rangle$, $\|\widetilde{\beta}\rangle$ are coherent states
- Variables are continuous.
- There are only $2M$ complex variables, however many particles.
- Can sample this on a computer. The more samples, the better accuracy.

$$\hat{\rho} = \sum_{\tilde{n}\tilde{m}} C_{\tilde{n}\tilde{m}}\, e^{i\theta_{\tilde{n}\tilde{m}}}\, |\tilde{n}\rangle\langle\tilde{m}|$$

- Configurations discrete, basis orthogonal
  $\hookrightarrow$ Heaps of variables (several for each *configuration*)

- Deterministic.

$$\hat{\rho} = \int P(\tilde{\alpha}, \tilde{\beta})\, \| \tilde{\alpha}\rangle\langle\tilde{\beta} \|\, e^{\tilde{\alpha}\cdot\tilde{\beta}^*}\, d\tilde{\alpha}\, d\tilde{\beta}$$

- Configurations continuous, basis non-orthogonal
  $\hookrightarrow$ Few variables (several for each *lattice point*)

- Stochastic.

Dynamical equations

$$\frac{d\alpha(\mathbf{x})}{dt} = i\frac{\hbar}{2m}\nabla^2\alpha(\mathbf{x}) - i\left(\frac{g}{\hbar\Delta V}\right)\alpha(\mathbf{x})^2\,\beta(\mathbf{x})^* + i\sqrt{\frac{ig}{\hbar\Delta V}}\,\alpha(\mathbf{x})\,\xi(\mathbf{x})$$

Plus identical form for $\frac{d\beta(\mathbf{x})}{dt}$ but with independent noise.

- Just mean field GP equations plus noise.
- $\xi(\mathbf{x})$ is a real Gaussian noise

$$\langle\, \xi(\mathbf{x},t)\,\xi(\mathbf{y},t')\,\rangle = \delta(t-t')\,\delta_{\mathbf{x},\mathbf{y}}$$

- ΔV is the volume per lattice point
- Full quantum evolution.

1D BEC dynamics

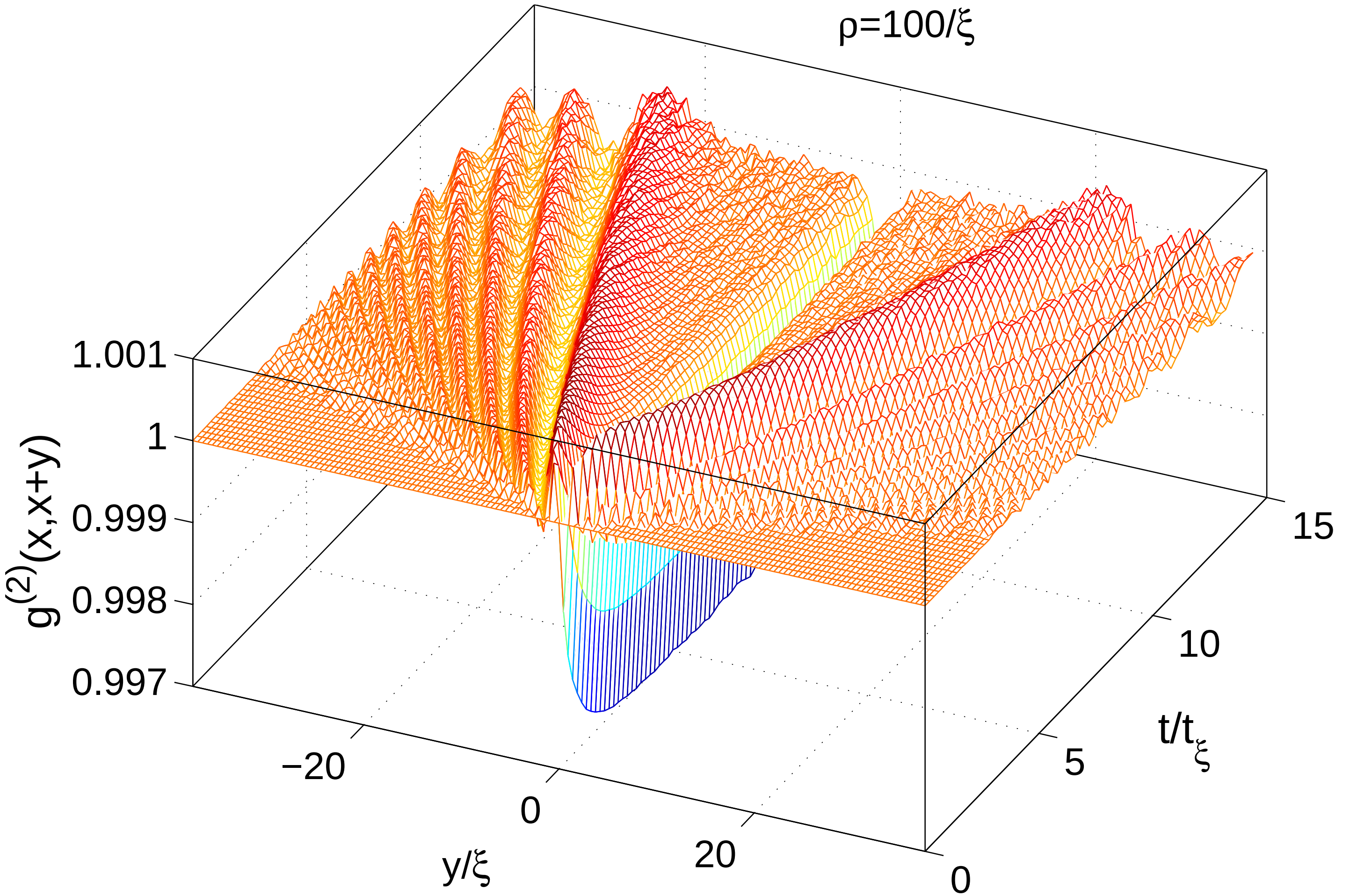
What goes on in a BEC when the interaction strength changes?

Basic model:

- At $t \leq 0$: Uniform non-interacting BEC.
- $t > 0$ Repulsive interactions turned on.
- Achieved by e.g.
  - Exploiting a Feshbach resonance
  - OR: changing transverse width

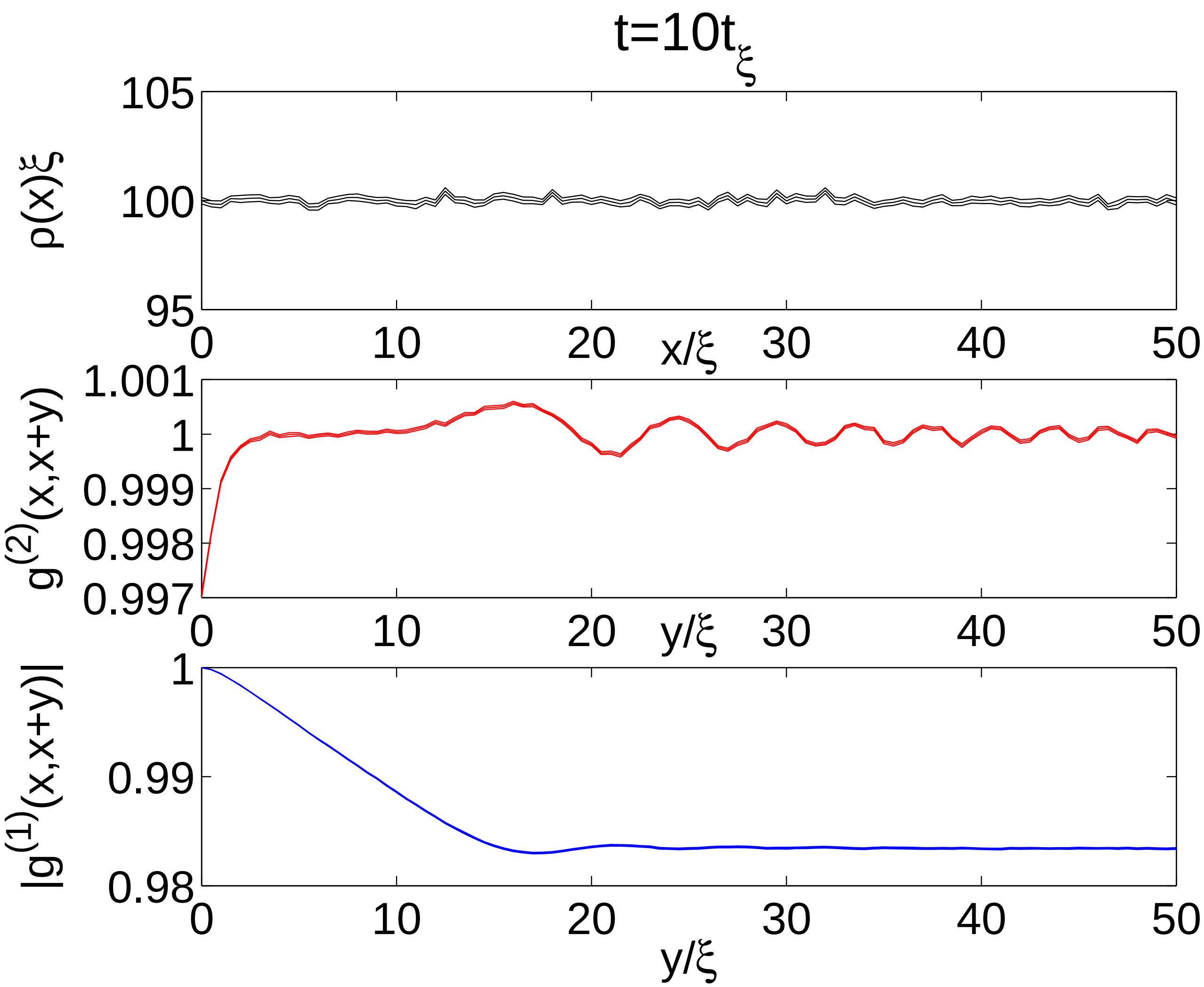
positive P simulation

$$g^{(2)}(x,x+y) = \frac{\langle\ \widehat{\Psi}^{\dagger}(x)\ \widehat{\Psi}^{\dagger}(x+y)\ \widehat{\Psi}(x)\ \widehat{\Psi}(x+y)\ \rangle}{\langle\ \widehat{\Psi}^{\dagger}(x)\ \widehat{\Psi}(x)\ \rangle \langle\ \widehat{\Psi}^{\dagger}(x+y)\ \widehat{\Psi}(x+y)\ \rangle}$$



$\xi = \hbar/\sqrt{2m\rho g}$ is the healing length $\qquad t_{\xi} = \hbar/2\rho g = m\xi^2/\hbar$ is a healing "time"

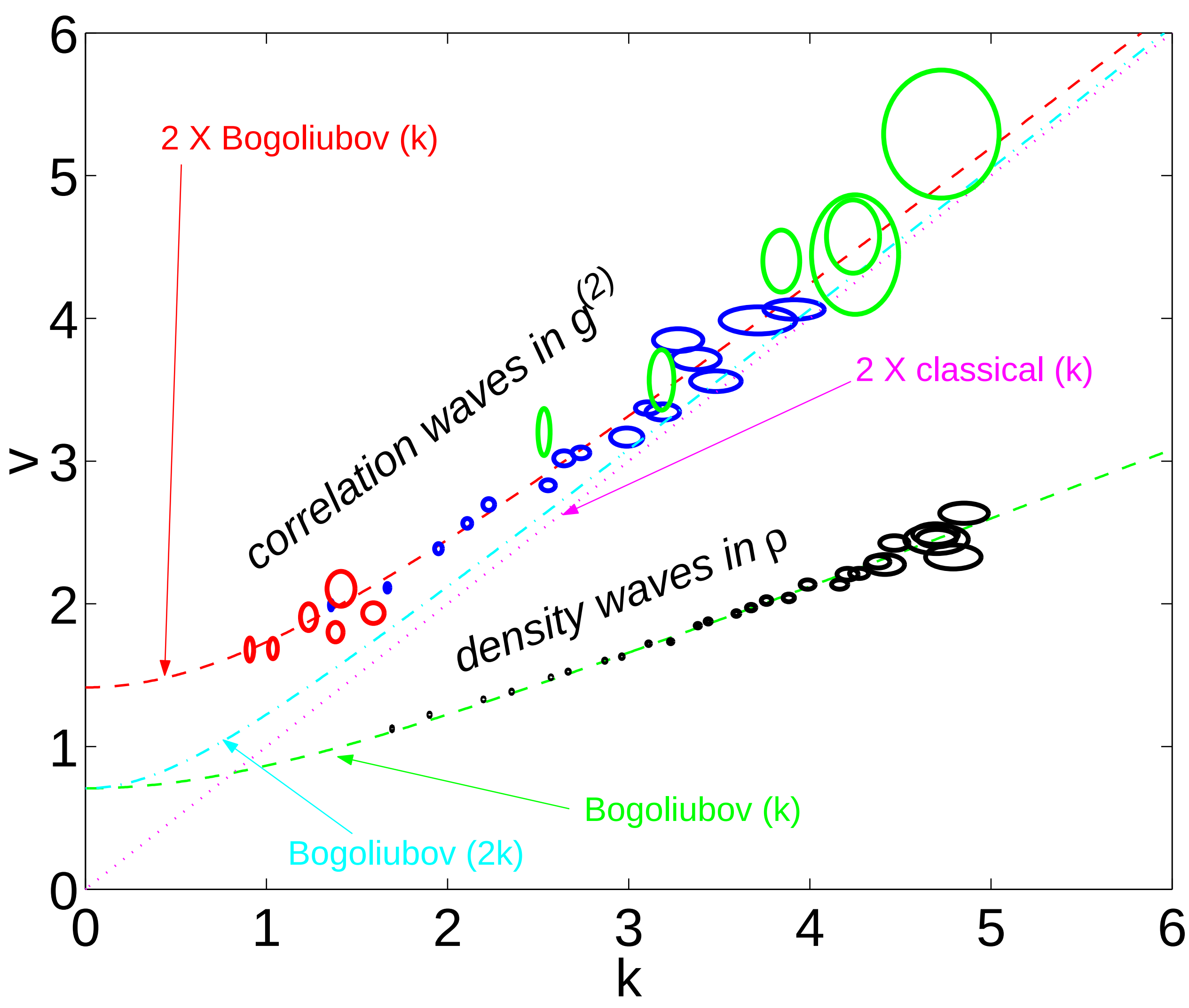
Detail: Structure only in correlations



Correlation values scale as:

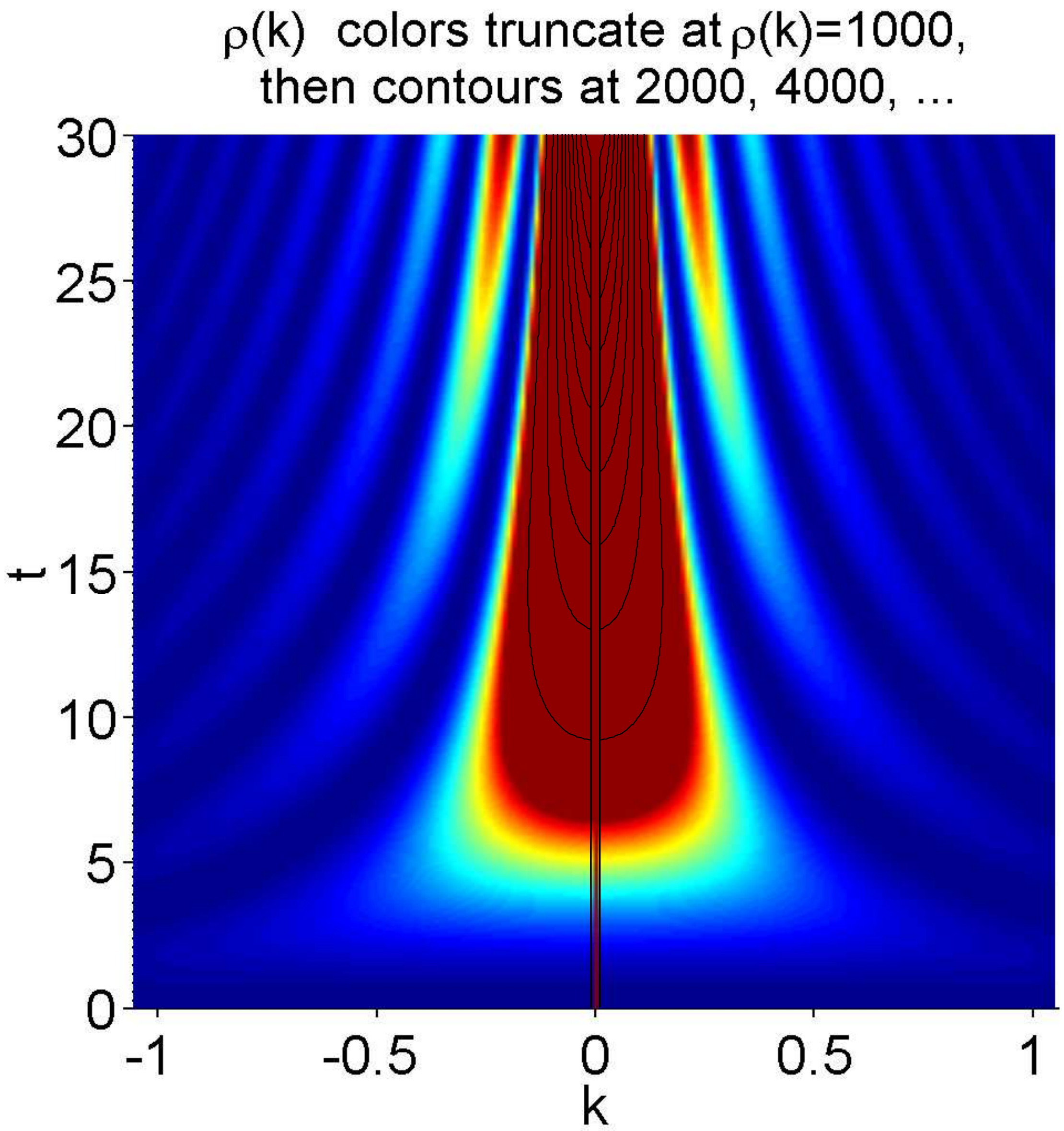
$$[g^{(n)} - 1] \propto \frac{1}{\rho\xi} \propto \sqrt{\frac{a_s}{\rho\sigma}}$$

Double Bogoliubov velocity



Dimensionless units: $v^2 = k^2 + 1/2$

Velocity distribution **(Bogoliubov calculation)**



Could this be observed in present experiments?

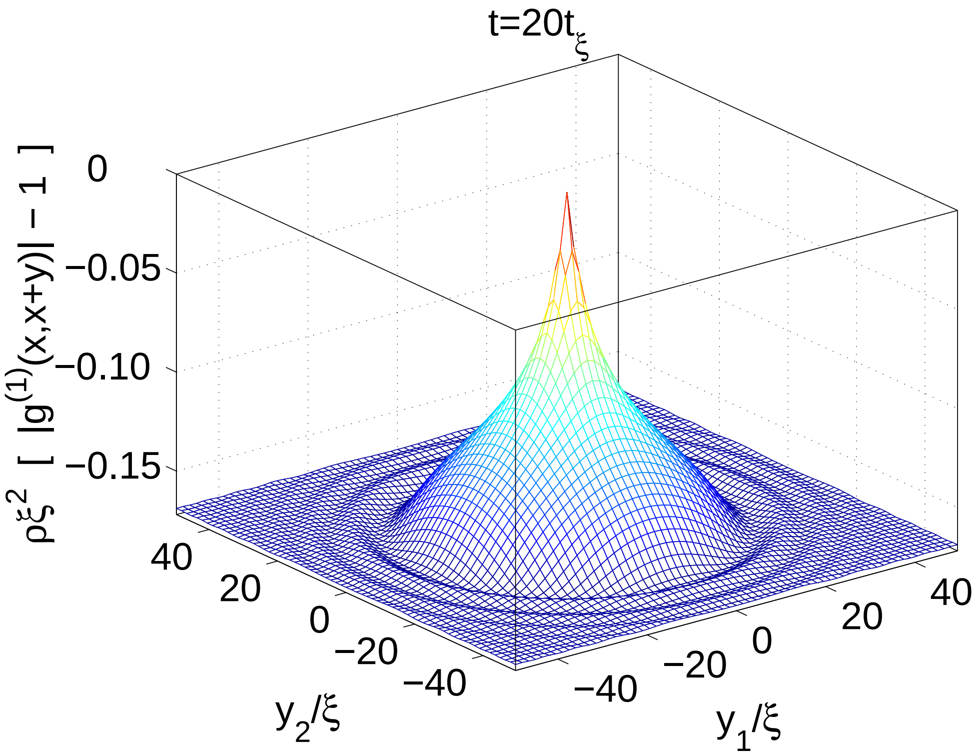
e.g. After initial disturbance:

— Change a_s back to ≈ 0,

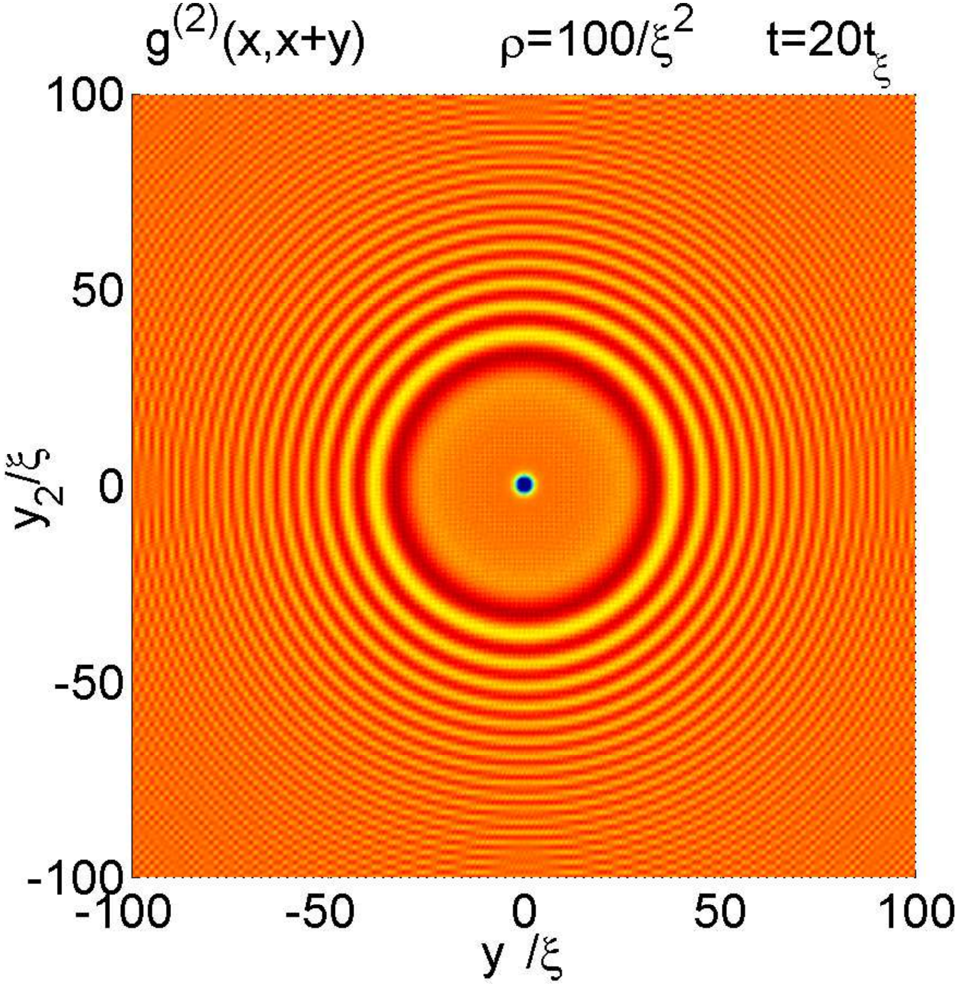
— Or release narrow sides of trap.

Then observe free-flight velocity distribution.

2D Gas (Bogoliubov calculation)

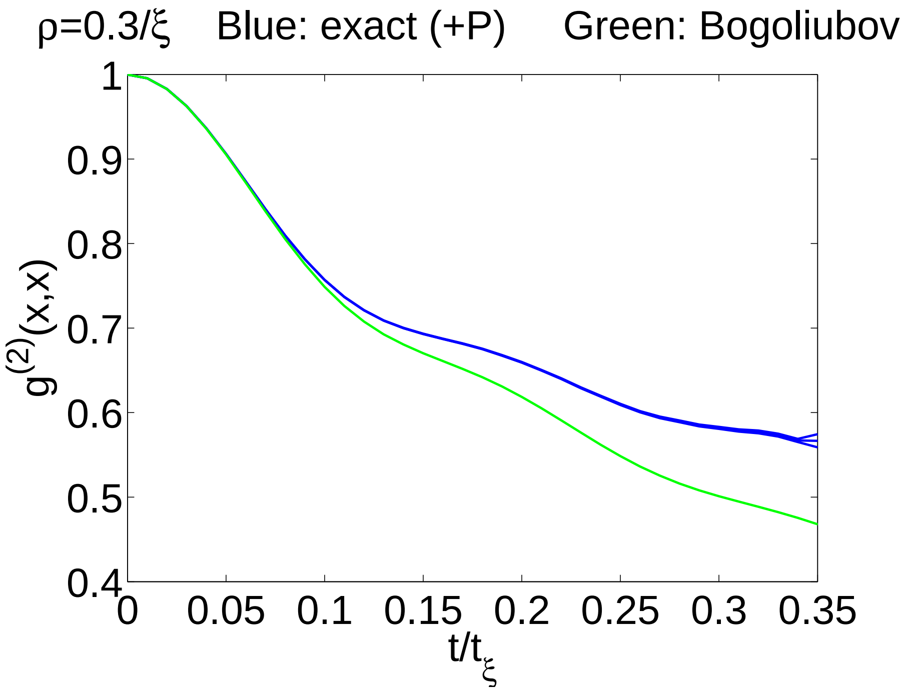


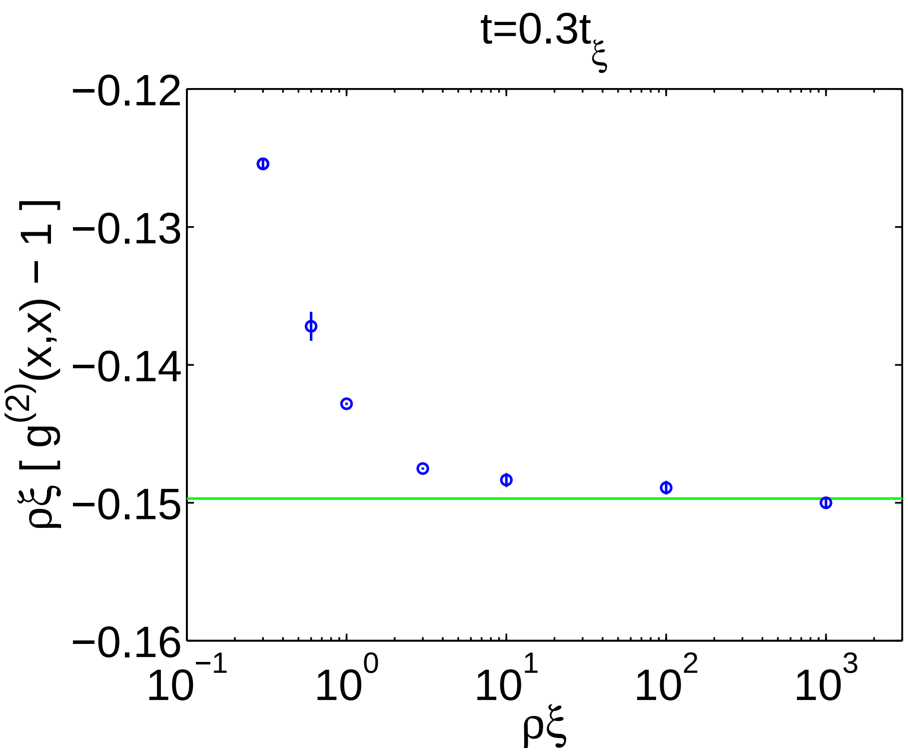
$|g^{(1)}|$



$g^{(2)}$

First-principles / Bogolibbov





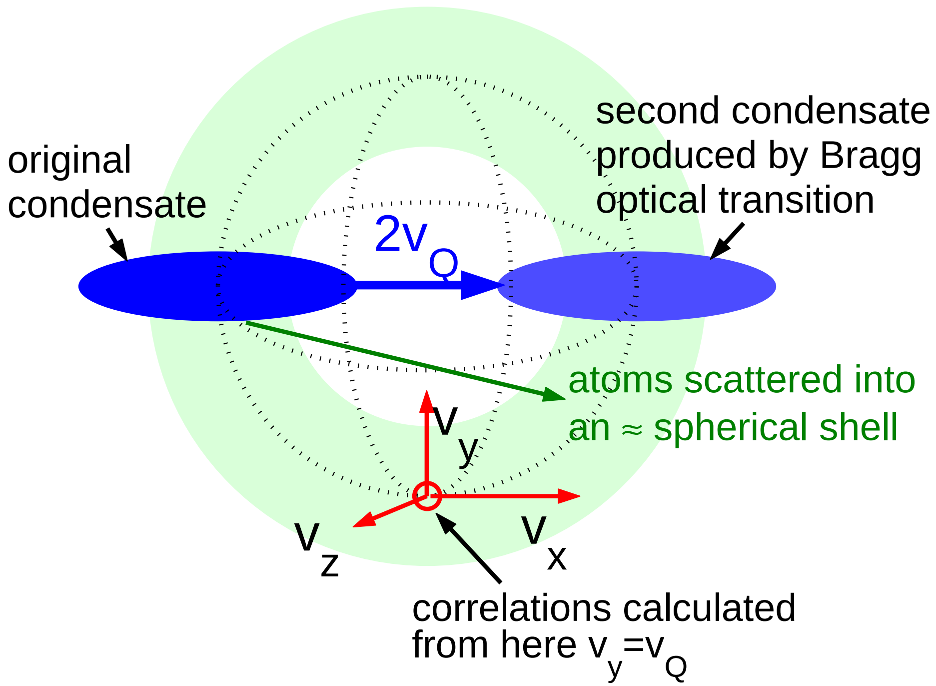
Discrepancies appear due to strong interactions when

$$\rho\xi \lesssim \mathcal{O}(1)$$

i.e. one or less atoms per healing length.

BEC collision in 3D

How do the scattered atoms behave?



—150000 atoms of $^{23}\mathrm{Na}$ in a BEC.

—Initial trap $f = 20 \times 80 \times 80\mathrm{Hz}$

—Trap turned off at $t \geq 0$

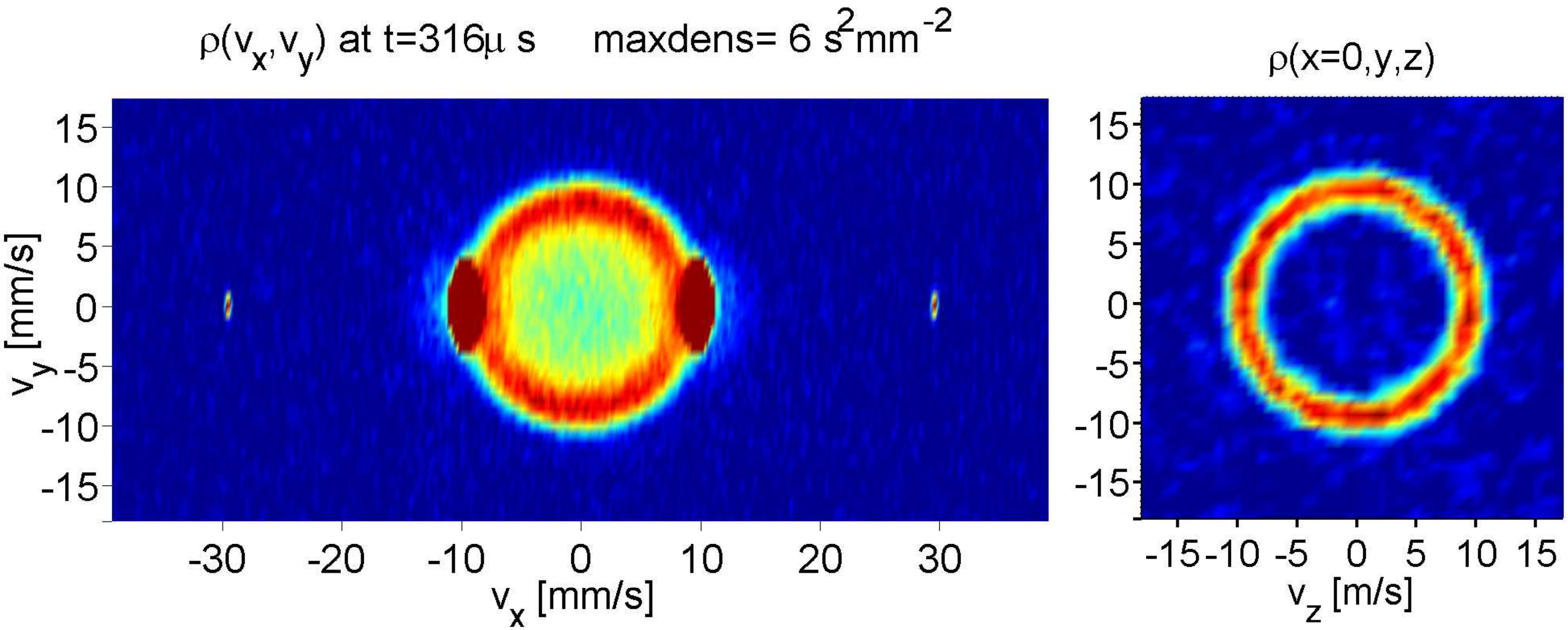
—At $t = 0$ Bragg laser pulse gives coherent kick $2\mathrm{v_Q} = 20\mathrm{mm/s}$ to 50% of atoms

—Initial conditions: assume $T \approx 0$

Similar setup to MIT experiment Vogels *et al* PRL **89**, 020401 and approximate calculation Norrie *et al* PRL **94**, 040401.

(experiment had 30 million atoms, and also four-wave mixing)

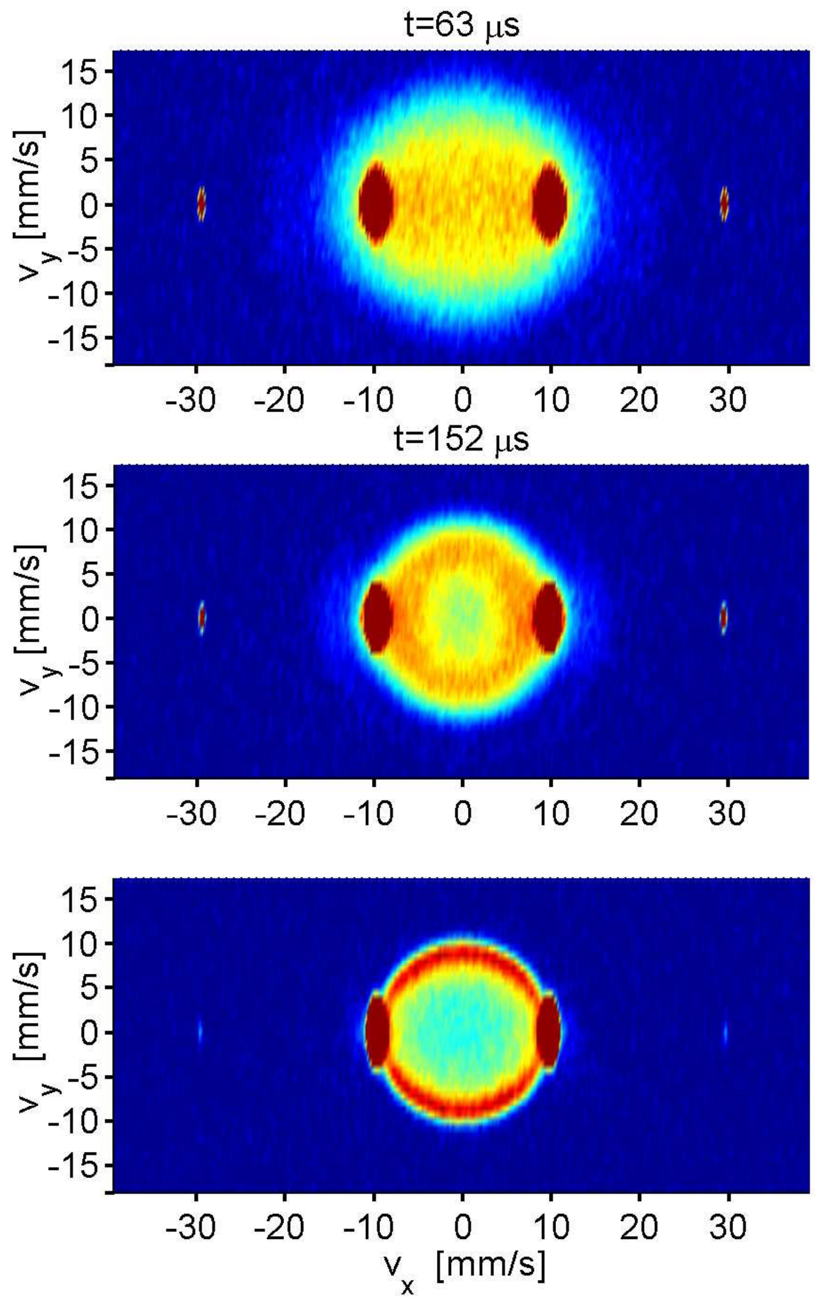
Velocity distribution after 316μs



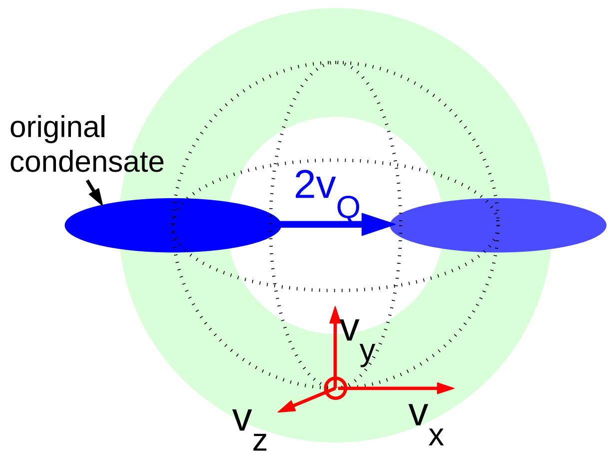
$N = 150000$ atoms on a $432 \times 50 \times 50$ lattice

$\Longrightarrow$ *Hilbert space of* $\approx 10^{5\times10^6}$ *dimensions!*

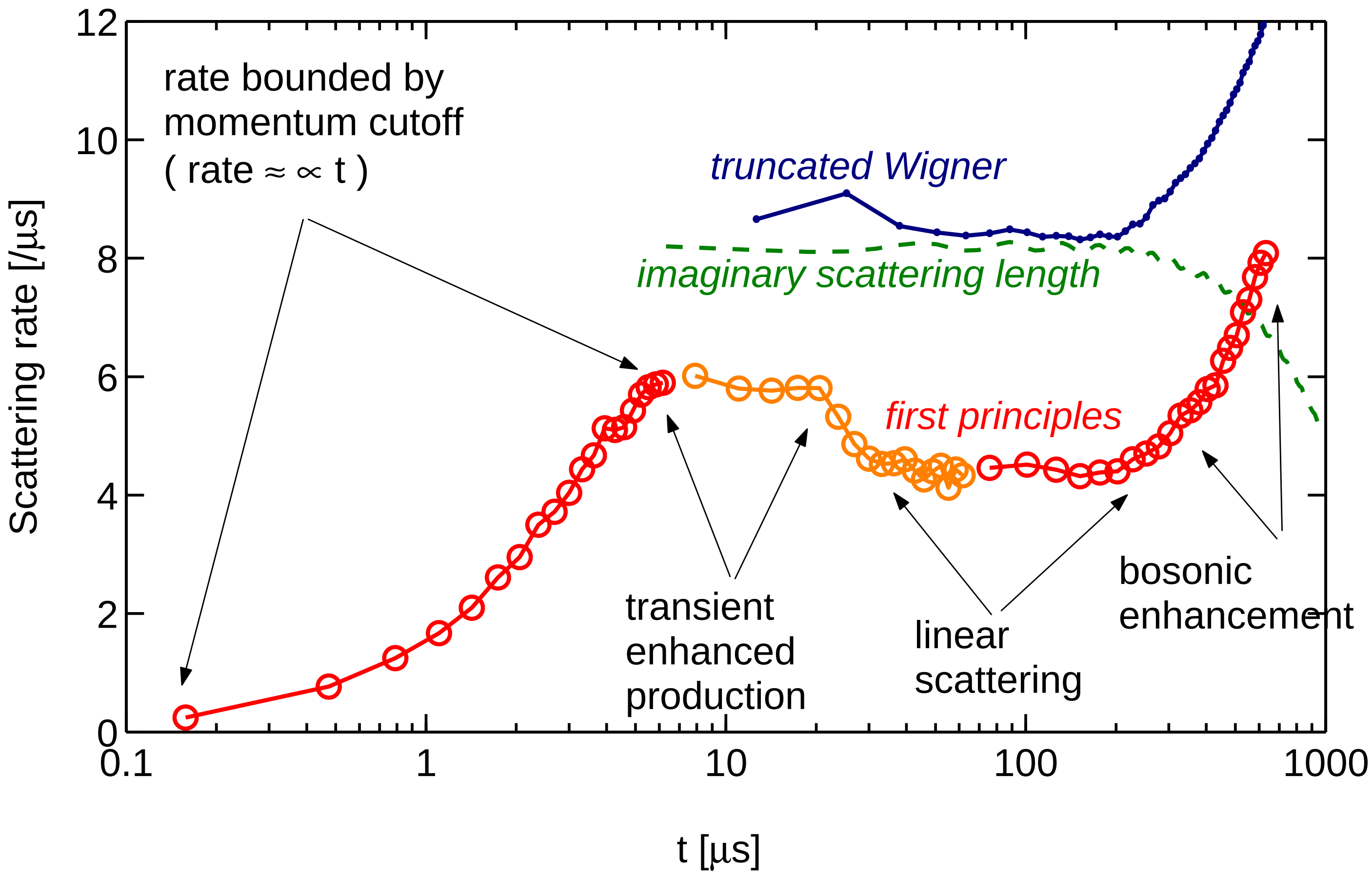
This is the largest system I know of for which quantum dynamics has been calculated from first principles.



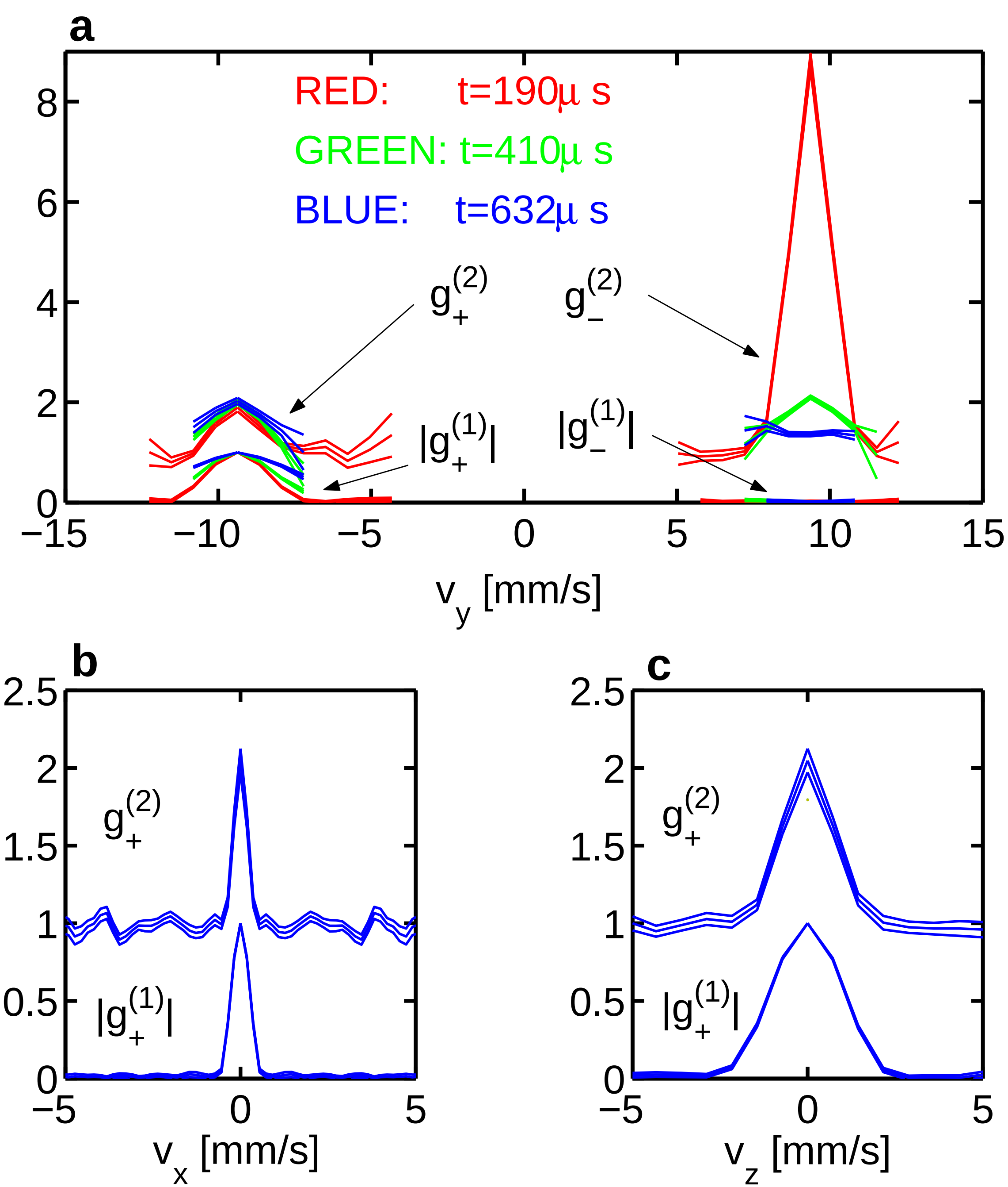
Evolution of Velocity distribution



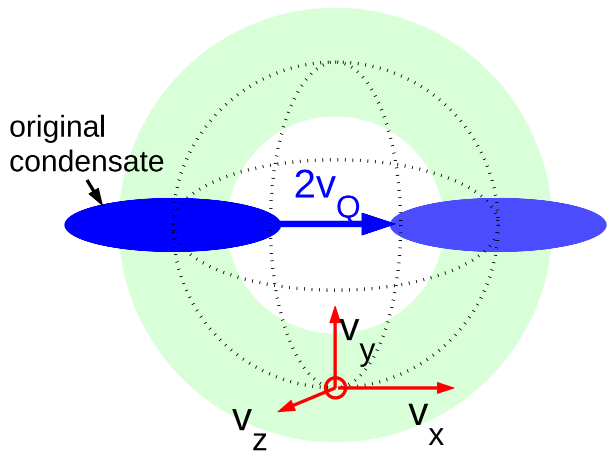
Scattering rate



In this regime the standard approximate methods appear to agree rather “qualitatively”.



Evolution of Correlations among scattered atoms

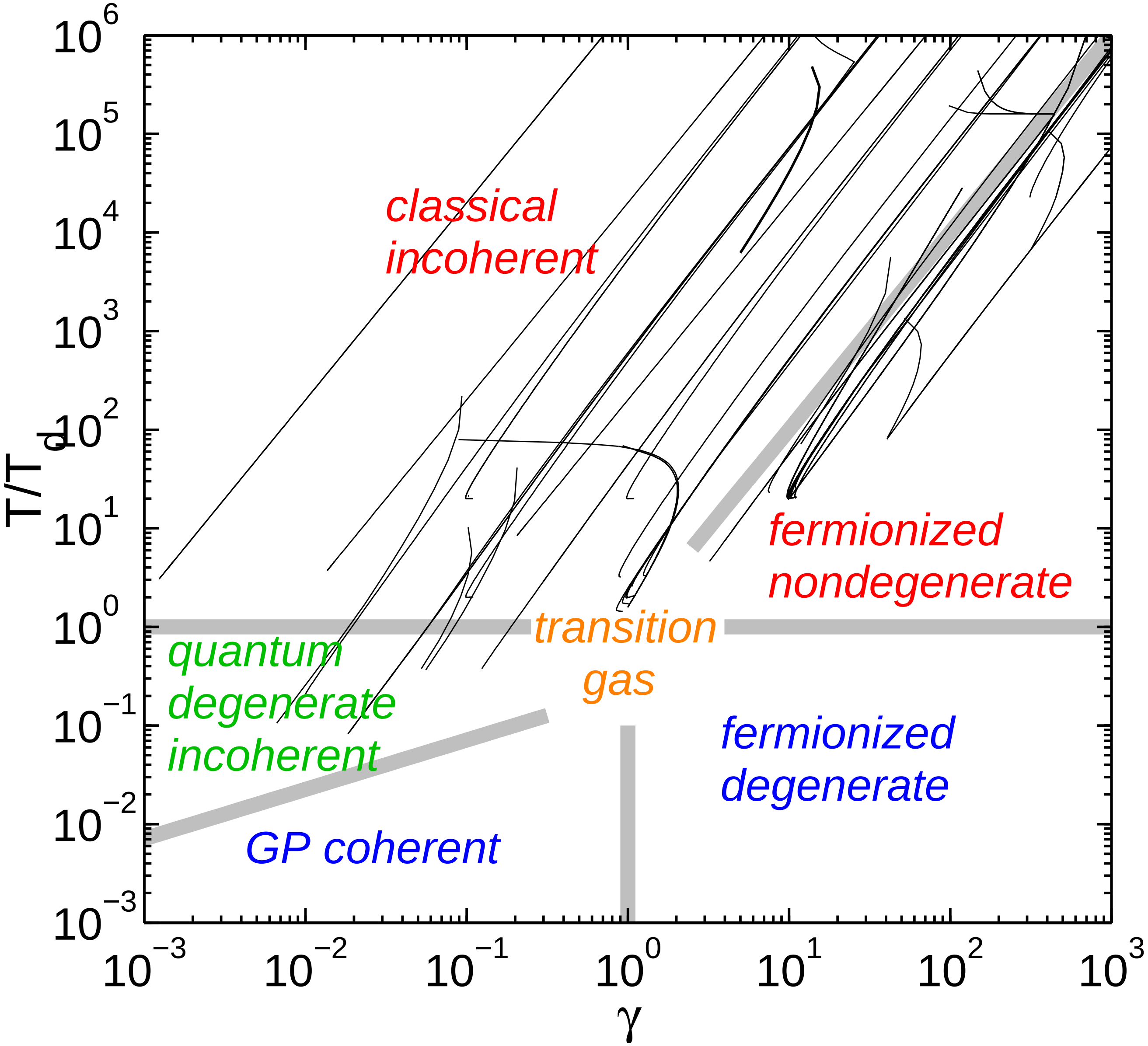


1D Bose gas thermodynamics

Correlations in a grand canonical ensemble

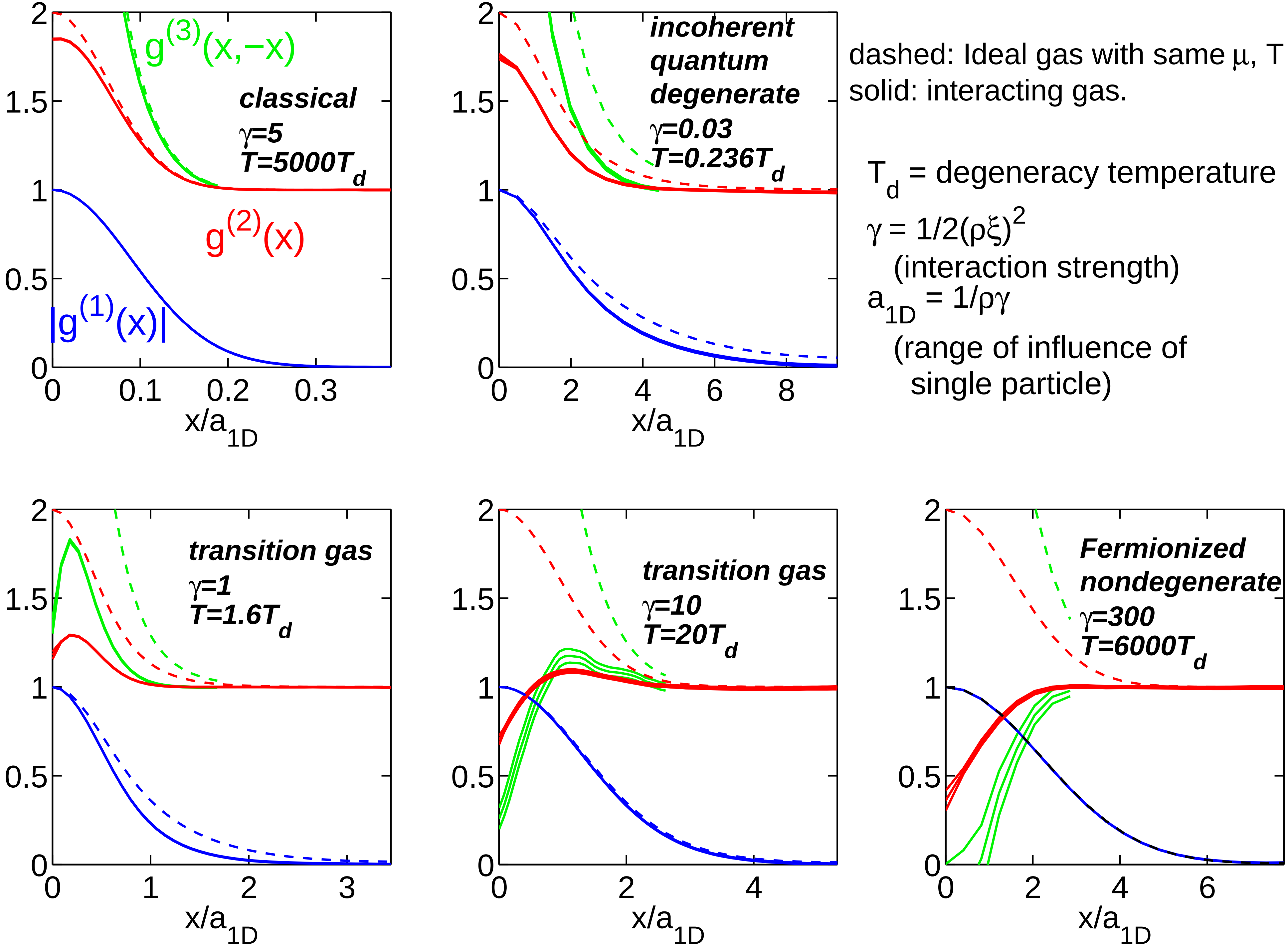
Model:

- Uniform 1D interacting gas.
- In a thermal and diffusion bath: T, μ.
- Two parameters:
  - $\widetilde{T} = T/T_d$ where $T_d =$ degeneracy temperature.
  - $\gamma = 1/2(\rho\xi)^2$ interaction strength.
- Simulation in *imaginary time:* $t \to it$, $\quad \xi(x) \to \sqrt{i}\,\xi(x)$.



Regimes attained

"Imaginary time" paths shown



g(3)(x,−x)
classical
γ=5
T=5000Td
g(2)(x)
|g(1)(x)|
x/a1D
incoherent
quantum
degenerate
γ=0.03
T=0.236Td
x/a1D
dashed: Ideal gas with same μ, T
solid: interacting gas.
Td = degeneracy temperature
γ = 1/2(ρξ)2
(interaction strength)
a1D = 1/ργ
(range of influence of
single particle)
transition gas
γ=1
T=1.6Td
x/a1D
transition gas
γ=10
T=20Td
x/a1D
Fermionized
nondegenerate
γ=300
T=6000Td
x/a1D

Thankyou

References:

- cond-mat/0507023
  (All the simulations)
- *cond-mat/0412174*
  (1D dynamics — correlation waves)
- *Phys. Rev. Lett. 92, 040405 (2004)*
  (1D thermodynamics)