Quantum dynamics of evaporatively cooled Bose-Einstein condensates

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Simulation of evaporative cooling

- initially a hot multimode system
- interacting particles in a finite trap
- quantum fluctuations important near critical point
- what state does the evaporation process lead to?

  $\Longrightarrow$ Is it really in thermal equilibrium?
  $\Longrightarrow$ Must solve a quantum many-body problem in the time-domain!

- use quantum phase-space methods (quasi-probabilities)

  $\Longrightarrow$ retains quantum features
  $\Longrightarrow$ allows multimode simulation

A quantum simulation?

- "Can a quantum system be probabilistically simulated by a classical (probabilistic, I'd assume) universal computer? ...If you take the computer to be the classical kind I've described so far, (...) and there're no changes in any laws, and there's no hocus-pocus, the answer is certainly, No!" (Richard P. Feynman[1])

- "Hence the implications of Feynman's argument seems to be that we really cannot simulate quantum dynamics on a local classical computer... Actual calculations involve only a few particles and very short propagations." (David M. Cerperle [2])

- "The equivalent to Molecular Dynamics (Quantum Molecular Dynamics) does not exist in any practical sense... One is forced to either simulate very small systems (i.e. less than five particles) or to make serious approximations." (David M. Cerpele [3])

[1] *Simulating Physics with Computers*, International Journal of Theoretical Physics **21**, 467 (1982)

[2] *The Simulation of Quantum Systems*, Address at receiving the Feenberg Medal

[3] *Lectures on Quantum Monte Carlo*, May 1996

+P representation

- expand quantum density matrix $\hat{\rho}$ in off-diagonal coherent state projection operators:

$$\hat{\rho} = \int P(\psi_1, \psi_2) \frac{|\psi_1\rangle \langle\psi_2|}{\langle\psi_2|\psi_1\rangle} \mathcal{D}\psi_1 \mathcal{D}\psi_2$$

- $|\psi_i\rangle$ are coherent states of the atomic many-body operators
- $\mathcal{D}\psi_1$, $\mathcal{D}\psi_2$ are the functional integration measures
- $P(\psi_1, \psi_2)$ is a positive distribution function which exists for all density matrices
- when the boundary terms in the integration vanish, P is governed by a Fokker-Planck equation (FPE)

+P Equations

- the FPE leads to two stochastic phase-space equations:

$$i\hbar\frac{\partial\psi_j}{\partial t} = [-\hbar^2\nabla^2/2m + V(\mathbf{x}) - i\hbar\Gamma(\mathbf{x})/2 + U\psi_j\psi^*_{3-j} + \sqrt{i\hbar U}\xi_j(t,\mathbf{x})]\psi_j(t,\mathbf{x})$$

where:

- $j = 1, 2$; $m =$ atomic mass
- $V(\mathbf{x}) =$ trapping potential
- $\Gamma(\mathbf{x}) =$ loss rate
- $U =$ atom-atom coupling
- $\xi_j(t,\mathbf{x}) =$ stochastic term
- $\langle\psi^*_2\psi_1\rangle = \left\langle\hat{\Psi}^+_2\hat{\Psi}_1\right\rangle =$atom density

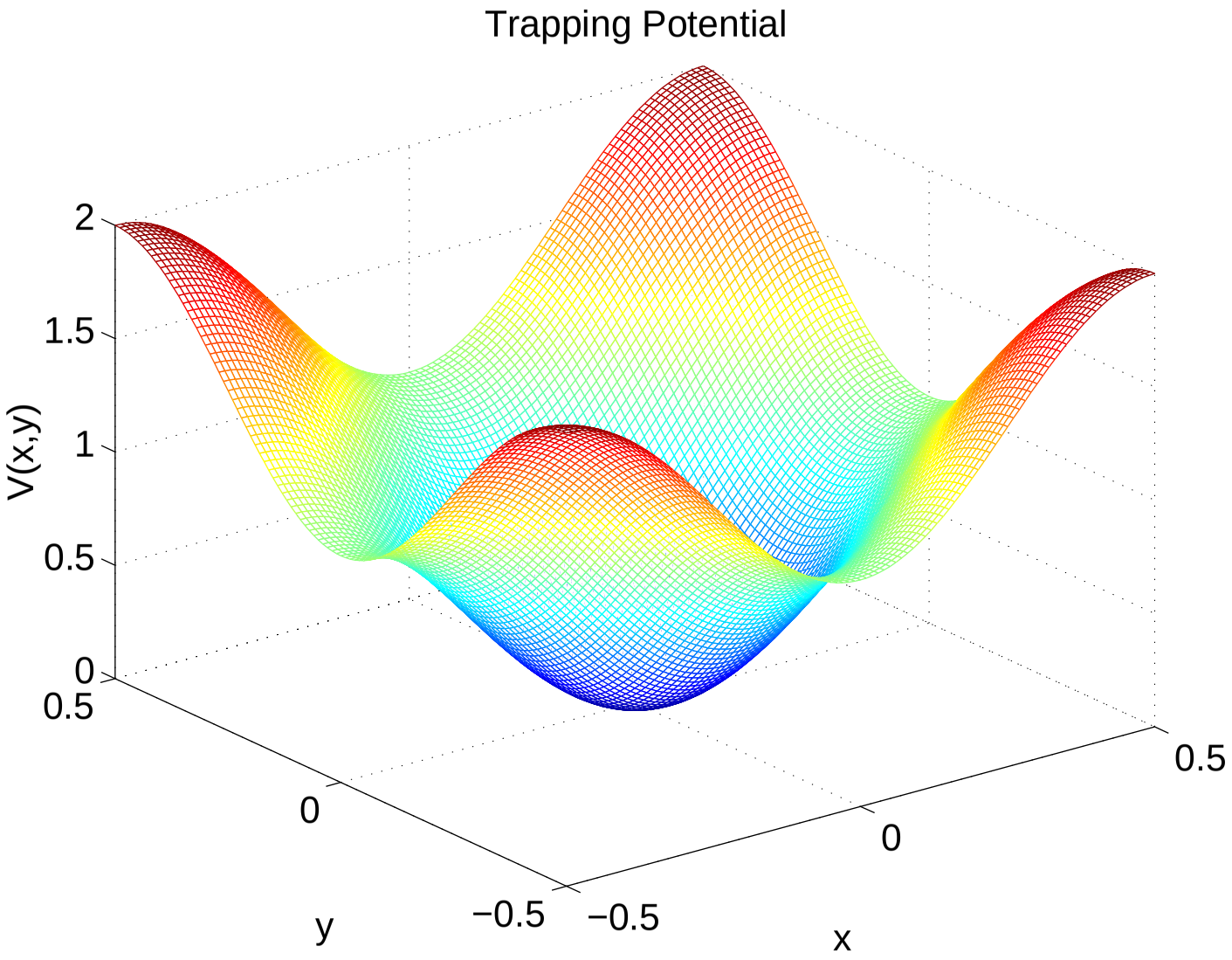
Correlations

- all quantum effects enter through the real stochastic noise terms $\xi_j(t, \mathbf{x})$
- without these, the equations correspond to the approximate classical mean-field equations
- the noise terms are independent, Gaussian, and delta-correlated in space and time:

$$\langle \xi_i(t, \mathbf{x}) \xi_j(t', \mathbf{x}') \rangle = \delta_{ij} \delta(\mathbf{x} - \mathbf{x}') \delta(t - t')$$

Potentials

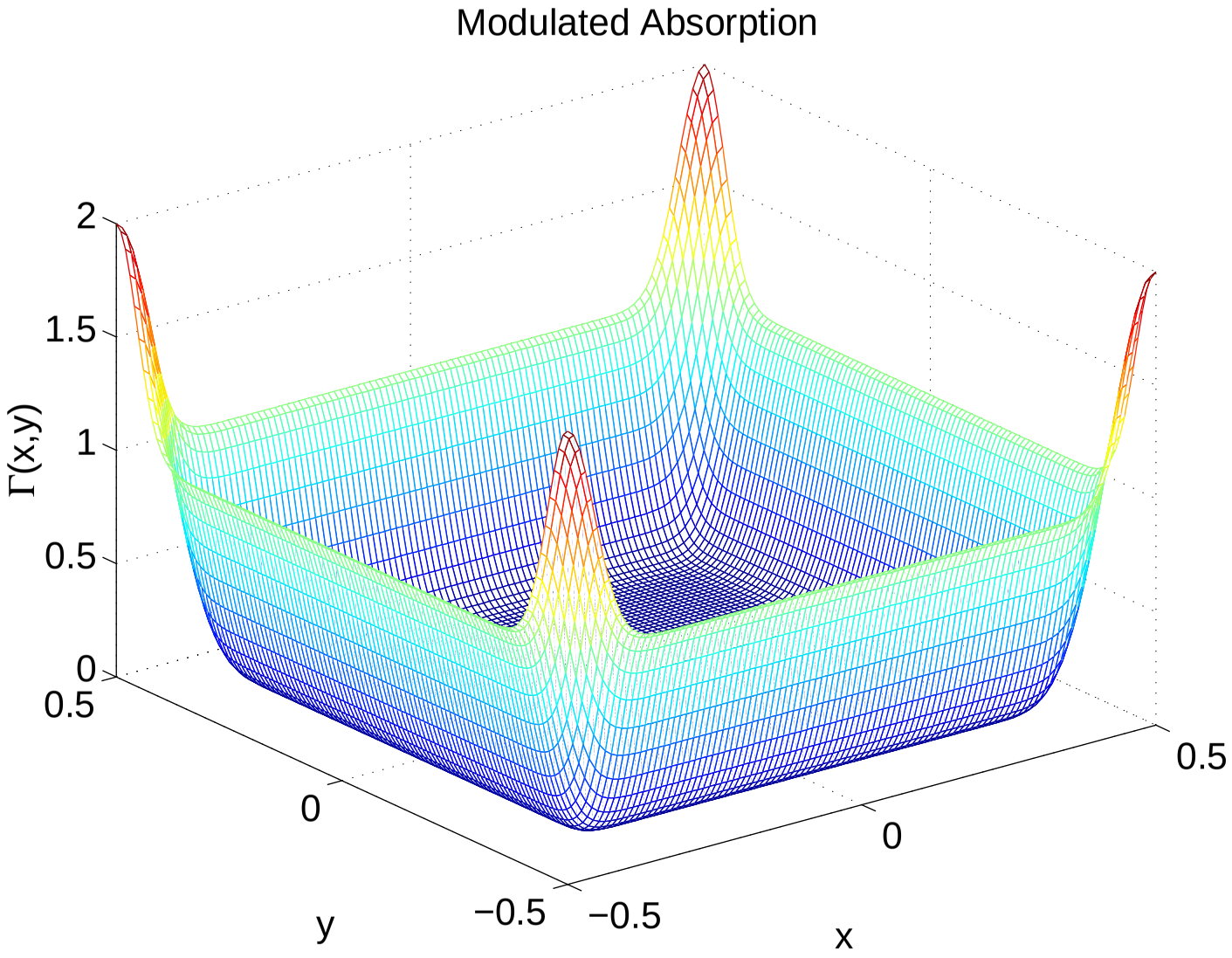
- $V(\mathbf{x},t) = (1-\alpha t)V_{max}\Sigma_{j=1}^{d}[\sin(\pi x_j/L_j)]^2$



- the trap walls are lowered over time

Atom loss

- hot atoms near the edge of the trap escape
- absorption: $\Gamma(\mathbf{x}) = \Gamma_{max} \Sigma_{j=1}^{d} [\sin(\pi x_j / L_j)]^{50}$



Initial Conditions

- the precise initial conditions are not expected to be very significant
- subsequent quantum noise dominates initial thermal noise
- the simplest possible choice is made: a high-temperature Bose-Einstein grand canonical ensemble
- in this initial state, no account is taken of the trapping or interparticle potentials

Parameters

- try to choose parameters used in the experiments
- however computational constraints on the lattice size

  $\Longrightarrow$ limited number of atoms
  $\Longrightarrow$ limited to either narrow deep traps, or wide shallow traps

- go for a compromise:
  - $a_0 = 0.6nm$; trap size $\simeq 10\mu m$
  - initial temperature $T_0 = 2.4 \times 10^{-7} K$
  - initial number of atoms $N_0 \simeq 500$ in 2d
  - initial number of atoms $N_0 \simeq 15000$ in 3d

Evaporative cooling dynamics

- have done 1d, 2d and 3d simulations
- final distribution in k-space is tall (intense) and narrow, because of:
  - ramped potential
  - thermalising effect of collisions
- quantum effects dominate for for these parameters
- high atom loss rate initially

  $\Longrightarrow$ change trap shape

  $\Longrightarrow$ alter evaporative cooling procedure

Figure 2

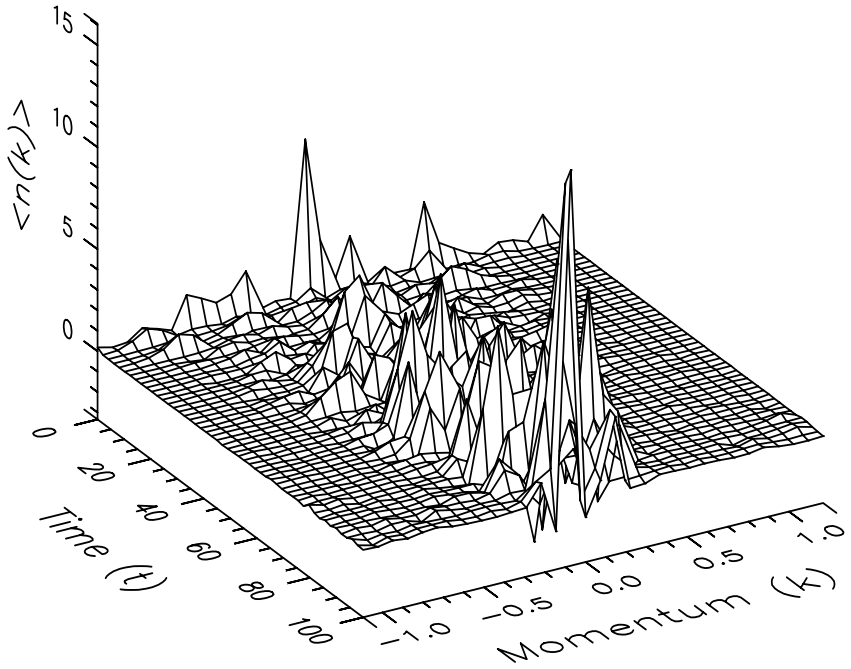
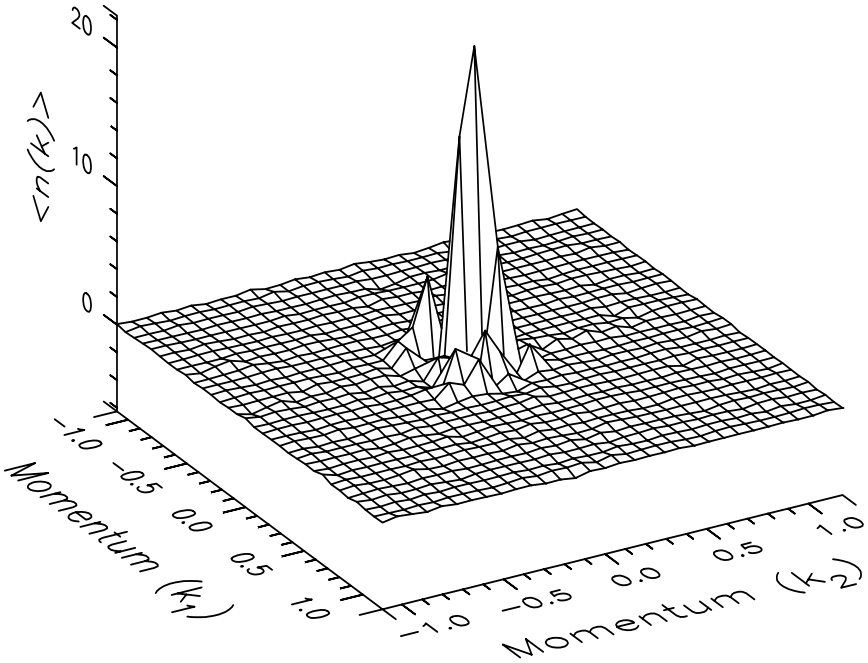
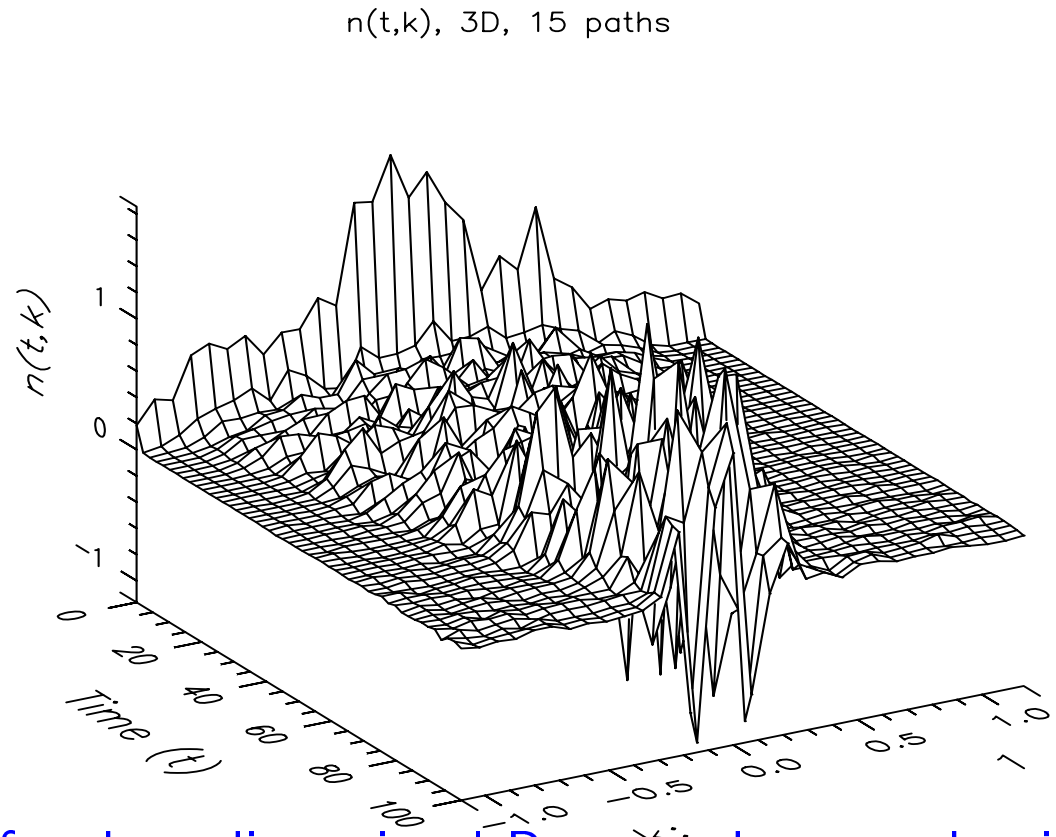


Figure 3

t = 100



Three dimensional simulation - evolution of the momentum distribution during a single trajectory.

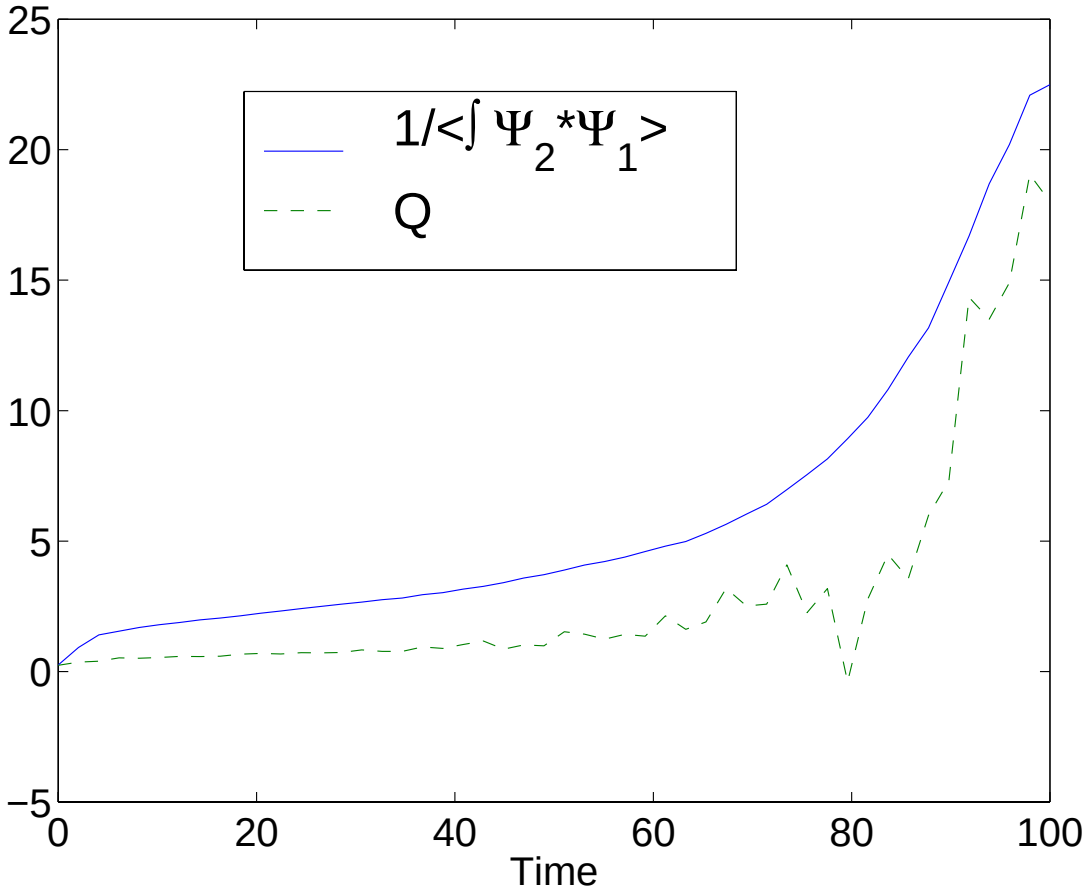


Simulation of a three-dimensional Bose condensate, showing the ensemble average (15 paths) atom density $\langle n(k) \rangle$ along one dimension in Fourier space versus time.

Confinement Measure

- measurable (physical) quantities given by ensemble average
- want to measure the occupied volume in k-space
- use higher order correlations to do this
- define confinement parameter:

$$Q = \frac{\int dk \, \langle \psi_1(\mathbf{k}) \psi_1(\mathbf{k}) \psi_2^*(\mathbf{k}) \psi_2^*(\mathbf{k}) \rangle}{\left(\int dk \, \langle \psi_1(\mathbf{k}) \psi_2^*(\mathbf{k}) \rangle \right)^2 x_0^3}$$



Simulation of a three-dimensional Bose condensate, showing the ensemble average evolution (11 paths) of the confinement parameter Q.

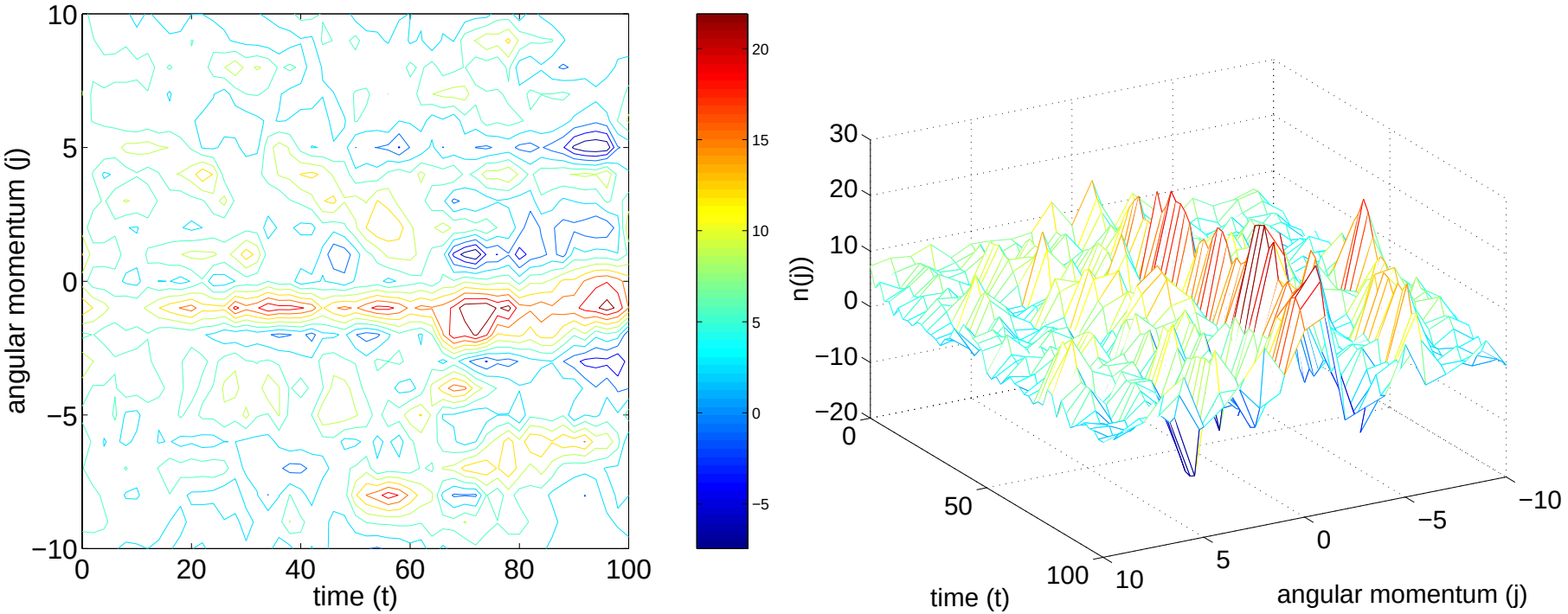
Angular Momentum

- nonzero final (angular) momentum $\Longrightarrow$ vortices
- calculate evolution of angular momentum distribution
- occupation of angular modes is given by:

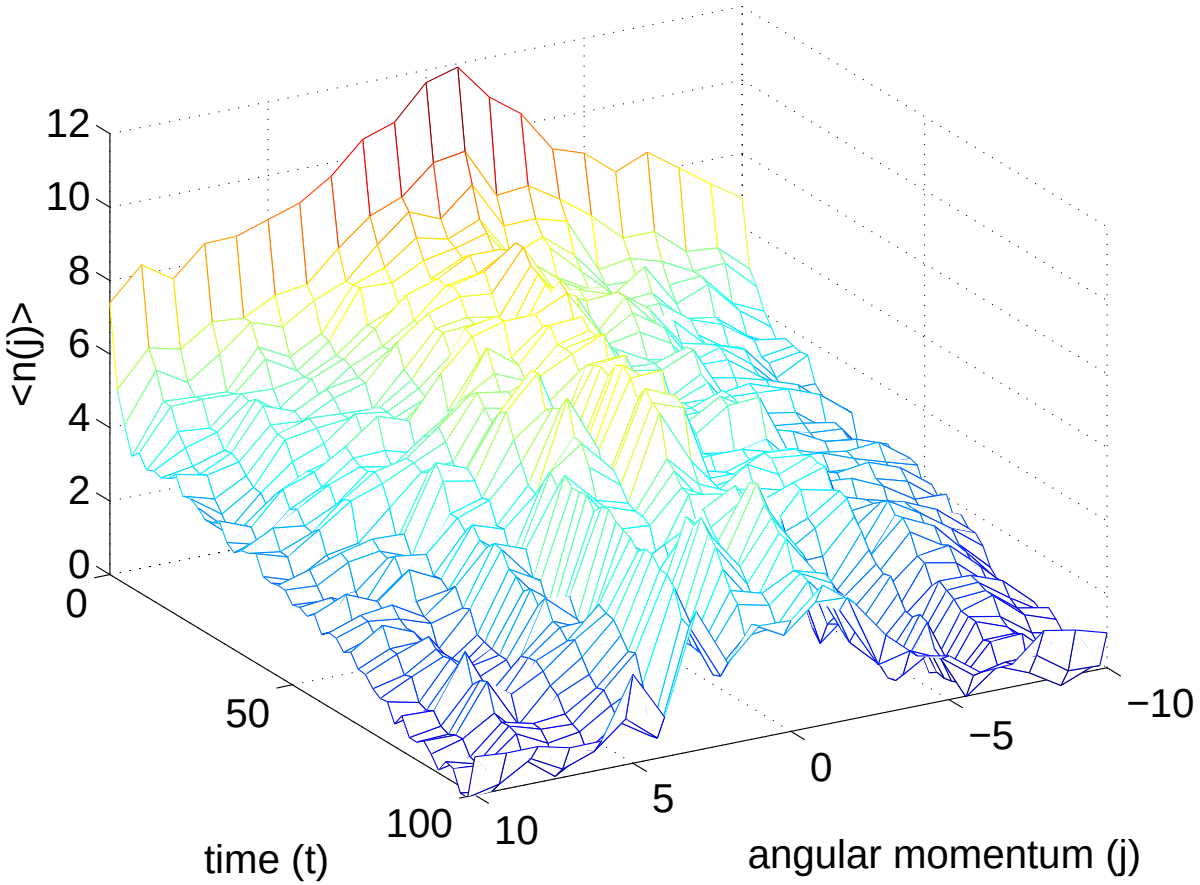
$$\langle n(j)\rangle = \sum_n \langle \hat{\Psi}_{jn} \hat{\Psi}^*_{jn}\rangle$$

where

- n is the index for the radial modes
- j is the index for the angular modes



Angular momentum distribution $n(j)$, during the condensation of a two-dimensional BEC.



Ensemble average of the angular momentum distribution $\langle n(j) \rangle$, during the condensation of a two-dimensional BEC.

Conclusions

- first principles quantum simulation of BEC
- $10,000$ atoms (initially) in 32000 trap modes; up to 200 atoms in condensate
- difficult - not impossible with classical computers
- physics: evaporative cooling with variable potential
- condensate can form in excited mode
- can spontaneously form metastable vortices