Direct Numerical Simulation of Gross-Pitaevskii Turbulence

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0 Abstract

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Gross-Pitaevskii (GP) equation describes the dynamics of low-temperature superfluids and Bose-Einstein Condensates (BEC). We performed a numerical simulation of turbulence obeying GP equation (Quantum turbulence). We report some preliminary results of the simulation.

Outline of the talk

1 Background (Statistical theory of turbulence)

2 Quantum turbulence

3 Numerical simulation

1 Background (Statistical theory of turbulence)

1.1 Governing equations of Turbulence (Classical)

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Navier-Stokes equations (in real space)

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} &= -\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{f}, \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned}$$

$\mathbf{u}(\mathbf{x},t)$:velocity field, $p(\mathbf{x},t)$: pressure field,
ν: viscosity, $\mathbf{f}(\mathbf{x},t)$: force field.

Navier-Stokes equations (in wave vector space)

$$\left(\frac{\partial}{\partial t} + \nu k^2\right) u^i_{\mathbf{k}} = \int d\mathbf{p}d\mathbf{q}\delta(\mathbf{k}-\mathbf{p}-\mathbf{q}) M^{iab}_{\mathbf{k}} u^a_{\mathbf{p}} u^b_{\mathbf{q}} + f^i_{\mathbf{k}}$$

$$M^{iab}_{\mathbf{k}} = -\frac{i}{2}\left[k_a D^{ib}_{\mathbf{k}} + k_b D^{ia}_{\mathbf{k}}\right], \qquad D^{ab}_{\mathbf{k}} = \delta_{ij} - \frac{k_i k_j}{k^2}.$$

Symbolically,

$$\left(\frac{\partial}{\partial t} + \nu L\right) u = Muu + f$$

1.2 Turbulence as a dynamical System

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Characteristics of turbulence as a dynamical system

- Large number of degrees of freedom
- Nonlinear (modes are strongly interacting)
- Non-equilibrium (forced and dissipative)

Statistical mechanics of thermal equilibrium states can not be applied to turbulence.

- The law of equipartition do not hold.
- Probability distribution of physical variables strongly deviates from Gaussian (Gibbs distribution).

1.3 Violation of equipartition (1)

Energy spectrum

$$E(k) = \frac{1}{2}\int d\mathbf{k}'\delta(|\mathbf{k}'| - k)|\mathbf{u}_{\mathbf{k}'}|^2$$

Inviscid truncated system (ITS)

- $\nu = 0$, $\mathrm{f} = \mathbf{0}$ (energy conserved system) and cutoff wavenumber k_c is introduced.
- The law of equipartition holds. $E(k) \propto k^2$.

Navier-Stokes turbulence (NS)

- Energy cascades from large scales to small scales.
- Kolmogorov spectrum $E(k) = C_k \epsilon^{2/3} k^{-5/3}$. ($\epsilon$, energy dissipation rate).

1.4 Violation of equipartition (2)

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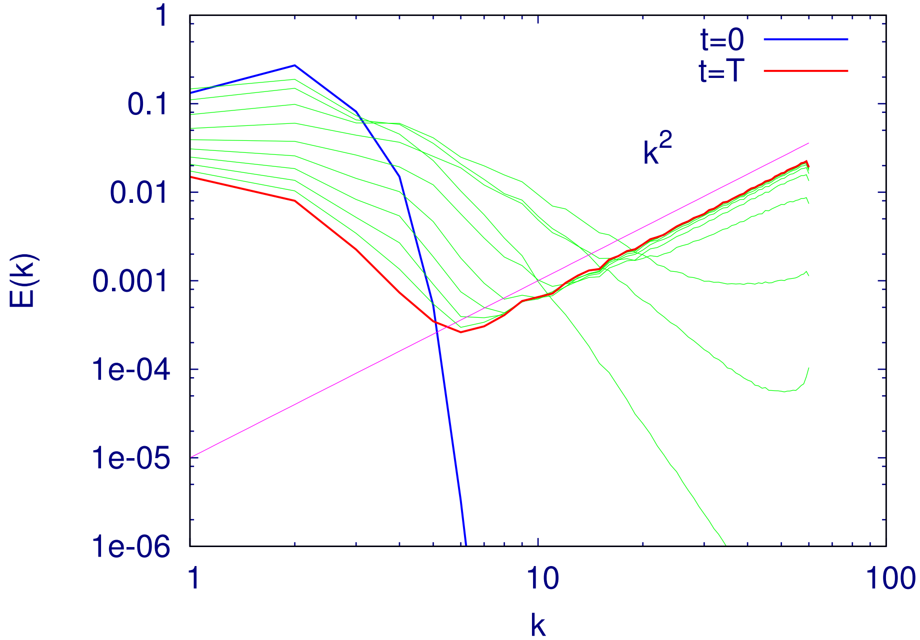
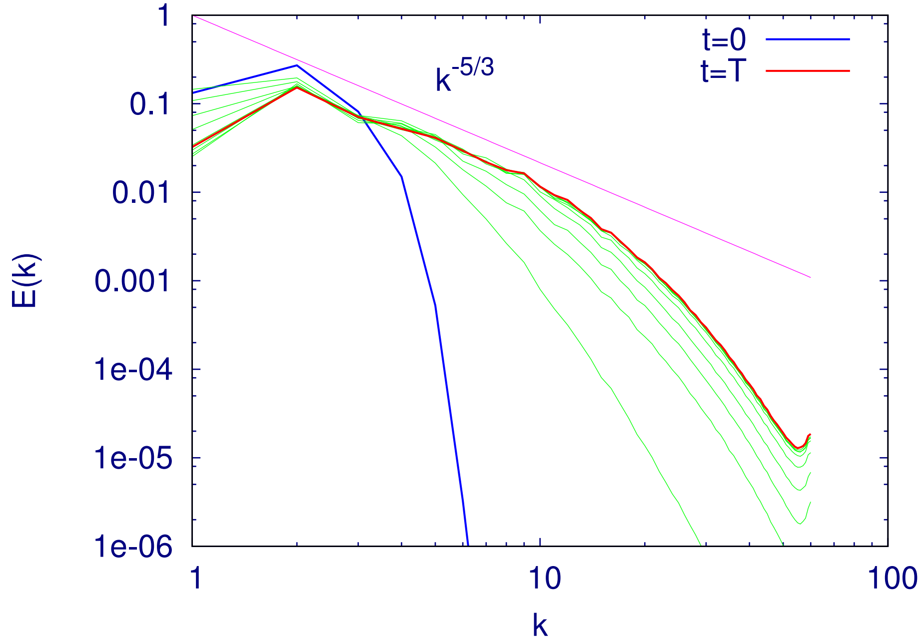
ITS ($\sim 128^3$ modes)



Forced NS ($\sim 128^3$ modes)

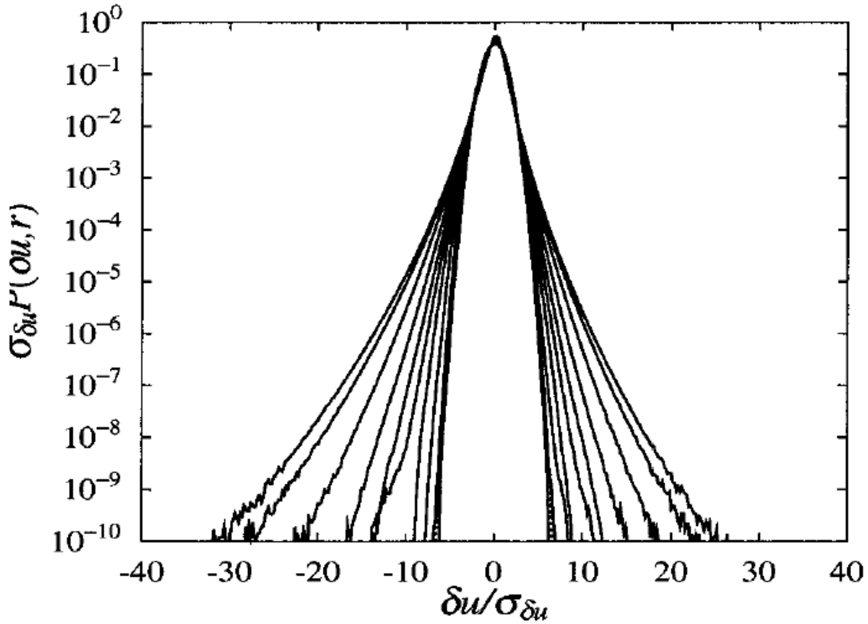


1.5 Non-Gaussianity

Longitudinal velocity increment

$$\delta u(r) = u^i(\mathbf{x} + r\mathbf{e}^i) - u^i(\mathbf{x})$$

Probability density function (PDF) of $\delta u(r)$ strongly deviates from Gaussian and has long tail for small r (intermittency).



Gotoh, Fukayama, and Nakano, Phys. Fluids **14**, 1065 (2002) cf. (for equilibrium states)

Thermodynamics

The macroscopic state is completely characterized by the free energy,

$$F(T, V, N).$$

Statistical mechanics

Macroscopic variables are related to microscopic characteristics (Hamiltonian).

$$F(T, V, N) = -kT \log Z(T, V, N)$$

Statistical theory of turbulence ?

What are the set of variables that characterize the statistical state of turbulence?

- ϵ? (Kolmogorov Theory ?)
- Fluctuation of ϵ? (Multifractal models?)

How to relate statistical variables to Navier-Stokes equations?

- Lagrangian Closures?

1.7 Classical Turbulence to Quantum Turbulence

The statistical theory of (classical) turbulence is far from complete (to our knowledge).

Why quantum turbulence ?

- Quantum turbulence may provide a test ground for the existing empirical theories for classical turbulence.
- Some new ideas may be obtained from the study of quantum turbulence.
  - Discrete structure of quantized vortex lines. Reconnection of the vortex line.

2 Quantum turbulence

2.1 Dynamics of order parameter

Hamiltonian of locally interacting boson field $\hat{\psi}(\mathbf{x}, t)$

$$\hat{H} = \int d\mathbf{x} \left[-\hat{\psi}^\dagger \frac{\hbar^2}{2m} \nabla^2 \hat{\psi} - \mu \hat{\psi}^\dagger \hat{\psi} + \frac{g}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \right]$$

μ : chemical potential, g: coupling constant

Heisenberg equation

$$i\hbar \frac{\partial \hat{\psi}}{\partial t} = -\left(\frac{\hbar^2}{2m} \nabla^2 + \mu \right) \hat{\psi} + g \hat{\psi}^\dagger \hat{\psi} \hat{\psi}$$

$$\hat{\psi} = \psi + \hat{\psi}', \qquad \psi = \langle \hat{\psi} \rangle$$

$\psi(\mathbf{x}, t)$: Order parameter

$\psi(\mathbf{x}, t) \sim O(N)$ (N: number density of all particles) for $T < T_c$.
Dynamics equations of ψ is obtained by neglecting $\hat{\psi}'$.

2.2 Governing equations of Quantum Turbulence

Gross-Pitaevskii (GP) equation

$$
\begin{aligned}
i\hbar \frac{\partial \psi}{\partial t} &= -\left(\frac{\hbar}{2m} \nabla^2 + \mu \right) \psi + g|\psi|^2 \psi, \\
\mu &= g\bar{n}, \qquad n = |\psi|^2
\end{aligned}
$$

$\bar{\cdot}$: volume average.

Normalization

$$
\tilde{\mathbf{x}} = \frac{\mathbf{x}}{L}, \qquad \tilde{t} = \frac{g\bar{n}}{\hbar} t, \qquad \tilde{\psi} = \frac{\psi}{\sqrt{\bar{n}}}
$$

Normalized GP equation

$$
i \frac{\partial \tilde{\psi}}{\partial \tilde{t}} = -\tilde{\xi}^2 \tilde{\nabla}^2 \tilde{\psi} - \tilde{\psi} + |\tilde{\psi}|^2 \tilde{\psi}, \qquad \left(\xi = \frac{\hbar}{\sqrt{2mg\bar{n}}}, \qquad \tilde{\xi} = \frac{\xi}{L} \right)
$$

ξ: Healing length ($\sim 0.5 \mathring{A}$ in Liquid ^{4}He)

Hereafter, $\tilde{\cdot}$ is omitted.

2.3 Superfluid velocity and quantized vortex line

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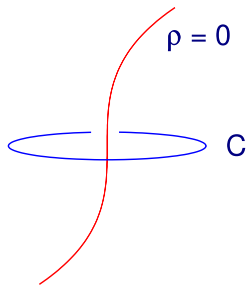
$$\psi(\mathbf{x}, t) = \sqrt{\rho(\mathbf{x}, t)} e^{i\varphi(\mathbf{x}, t)}, \qquad \mathbf{v}(\mathbf{x}, t) = 2\xi^2 \nabla \varphi(\mathbf{x}, t)$$

$$\begin{aligned} \frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \frac{\partial}{\partial t}\mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} &= -\nabla p_q \qquad \left(p_q = 2\xi^4 \rho - 2\xi^4 \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} \right) \end{aligned}$$

ρ : Superfluid (condensate) density
$\mathbf{v}$: Superfluid (condensate) velocity

Quantized vortex line ($\rho = 0$)

$$\begin{aligned} \omega &= \nabla \times \mathbf{v} = \mathbf{0} \quad (\text{for } \rho \neq 0) \\ \int_C d\mathbf{l} \cdot \mathbf{v} &= (2\pi n) 2\xi^2 \quad (n = 0, \pm 1, \pm 2 \cdots) \end{aligned}$$



2.4 Experiments

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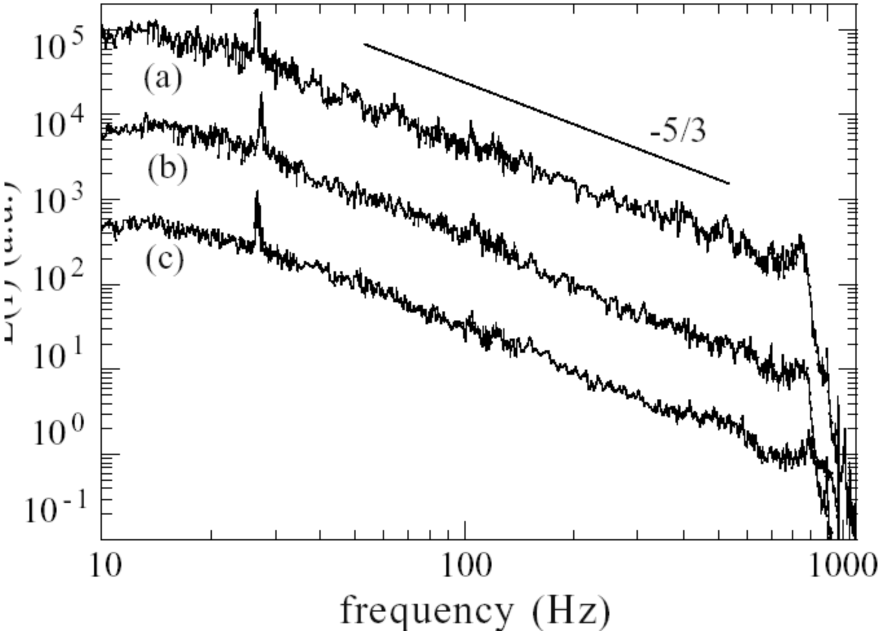
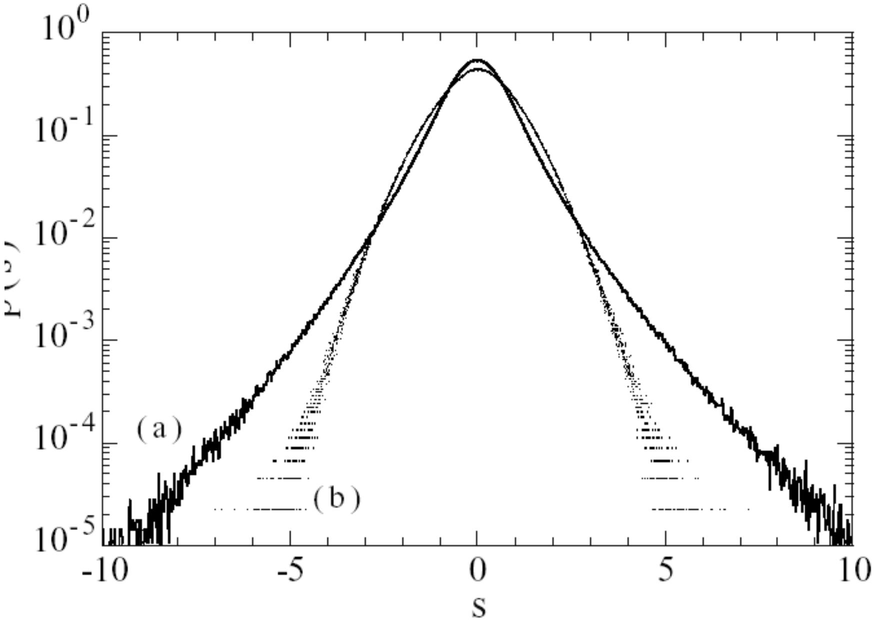
Maurer and Tabeling, Europhysics Lett. **4**3, 29 (1998)





- $k^{-5/3}$ spectrum is observed in superfluid turbulence (well below T_c).
- PDF of velocity increment

$$\delta u(r) = \delta u(\mathbf{x} + \mathbf{r}) - u(\mathbf{x})$$

deviates from Gaussian for small r (Intermittency).

2.5 Preceding Numerical Simulations

- Nore, Abid, and Brachet (1997), Abid *et al* (2003)
- Kobayashi and Tsubota (2005)
  - With dissipation and random forcing.

$$[i - \gamma(\mathbf{x}, t)] \frac{\partial}{\partial t}\psi(\mathbf{x}, t) = [-\nabla^2 - \mu(t) + g|\psi(\mathbf{x}, t)|^2]\psi(\mathbf{x}, t) + V(\mathbf{x}, t)\psi(\mathbf{x}, t)$$

(in non-normalized form)

  - $E^{\mathrm{wi}}(k) \sim k^{-5/3}$ is observed.

$$\mathbf{w} = \sqrt{\rho}\mathbf{v}$$

$E^{\mathrm{wi}}(k)$ is the energy spectrum related to the incompressible part of $\mathbf{w}$.

3 Numerical simulation

3.1 Dissipation and Forcing

GP equation (in wave vector space)

$$i\frac{\partial}{\partial t}\psi_{\mathbf{k}} = \xi^2 k^2 \psi_{\mathbf{k}} - \psi_{\mathbf{k}} + \int d\mathbf{p} d\mathbf{q} d\mathbf{r} \delta(\mathbf{k}+\mathbf{p}-\mathbf{q}-\mathbf{r}) \psi_{\mathbf{p}}^* \psi_{\mathbf{q}} \psi_{\mathbf{r}}$$
$$-i\nu k^2 \psi_{\mathbf{k}} + i\alpha_{\mathbf{k}} \psi_{\mathbf{k}}$$

- Dissipation
  - The normal viscosity type model. $\nu = \xi^2$ is chosen.
  - The dissipation term acts mainly in the high wavenumber range ($k \sim> 1/\xi$).
- Forcing (Pumping of condensates)

$$\alpha_{\mathbf{k}} = \begin{cases} \alpha & (k < k_f) \\ 0 & (k \geq k_f) \end{cases}$$

  - α is determined at every time step so as to keep $\bar{\rho}$ almost constant.
  - The forcing acts in the low wavenumber range $k < k_f$.

3.2 Simulation conditions

- $(2\pi)^3$ box with periodic boundary conditions.
- an alias-free spectral method with a Fast Fourier Transform.
- a 4th order Runge-Kutta method for time marching.
- Resolution $k_{\rm max}\xi = 3$.
- $\nu = \xi^2$.

N	$k_{\rm max}$	ξ	$\nu(\times 10^{-3})$	k_f	Δt	$\bar{\rho}$
128	60	0.05	2.5	2.5	0.01	0.998
256	120	0.025	0.625	2.5	0.01	0.999
512	241	0.0125	0.15625	2.5	0.01	0.998

3.3 Energy

Energy density per unit volume

$$E = E^{\rm kin} + E^{\rm int}$$

$$E^{\rm kin} = \frac{1}{V}\int d\mathbf{x}\xi^2|\nabla\psi|^2 = \int d\mathbf{k}\xi^2k^2|\psi_{\mathbf{k}}|^2 = \int dk E^{\rm kin}(k)$$

$$E^{\rm int} = \frac{1}{2V}\int d\mathbf{x}(\rho')^2 = \frac{1}{2}\int d\mathbf{x}|\rho'_{\mathbf{k}}|^2 = \int dk E^{\rm int}(k) \qquad (\rho' = \rho - \bar{\rho})$$

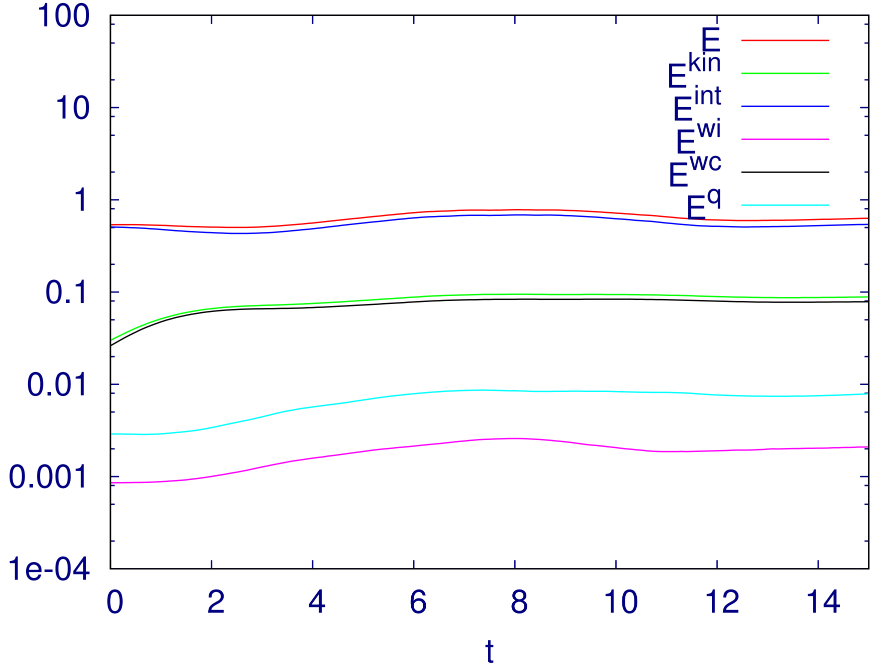
$$E^{\rm kin} = E^{\rm wi} + E^{\rm wc} + E^{\rm q}$$

$$E^{\rm wi} = \frac{1}{2V}\int d\mathbf{x}|\mathbf{w}^{\rm i}|^2 = \frac{1}{2}\int d\mathbf{k}|\mathbf{w}^{\rm i}_{\mathbf{k}}|^2 = \int dk E^{\rm wi}(k) \qquad \left(\mathbf{w} = \frac{1}{\sqrt{2}\xi}\sqrt{\rho}\mathbf{v}\right)$$

$$E^{\rm wc} = \frac{1}{2V}\int d\mathbf{x}|\mathbf{w}^{\rm c}|^2 = \frac{1}{2}\int d\mathbf{k}|\mathbf{w}^{\rm c}_{\mathbf{k}}|^2 = \int dk E^{\rm wc}(k)$$

$$E^{\rm q} = \frac{1}{V}\int d\mathbf{x}\xi^2|\nabla\sqrt{\rho}|^2 = \int d\mathbf{k}\xi^2k^2|(\sqrt{\rho})_{\mathbf{k}}|^2 = \int dk E^{\rm q}(k)$$

3.4 Energy in the simulation



- $E^{\mathrm{wc}} > E^{\mathrm{wi}}$. Different from Kobayashi and Tubota (2005).
- Dissipation and forcing are different from those of KT.

3.5 Energy spectrum

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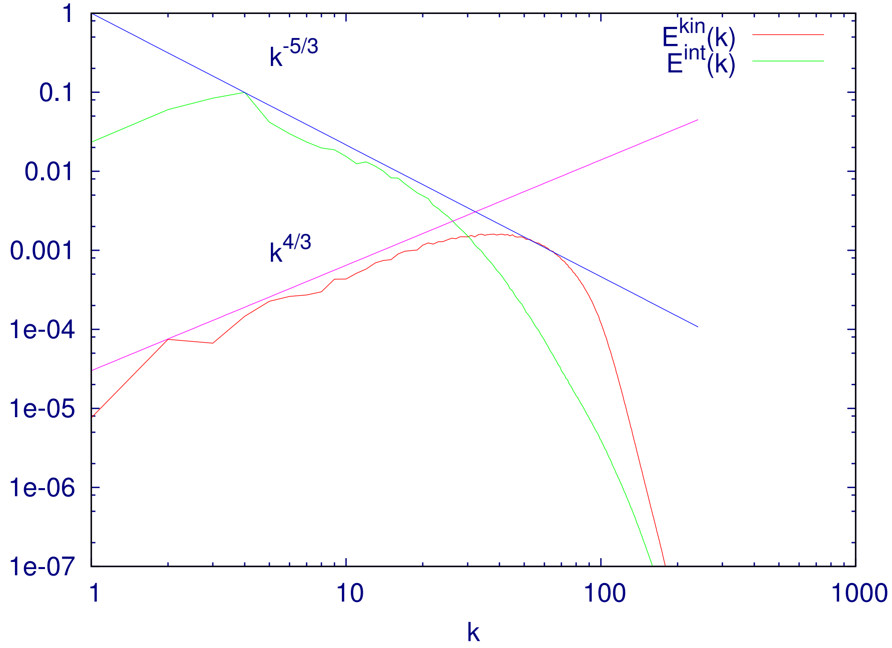

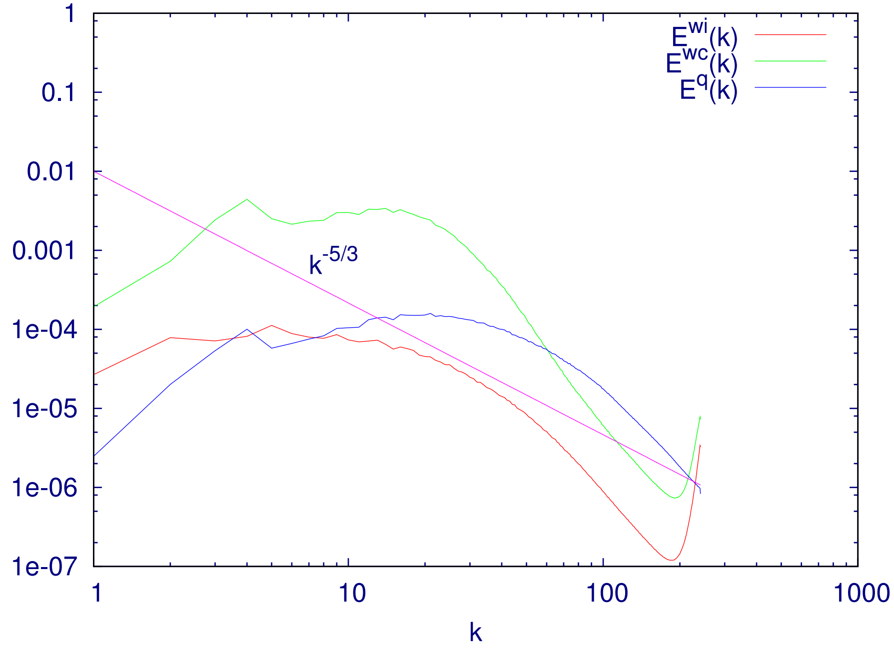

- $E^{\text{int}} \sim k^{-5/3}$, $E^{\text{kin}} \sim k^{4/3}$.
- $E^{\text{wi}} \sim k^{-5/3}$?

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3.6 PDF of the density field

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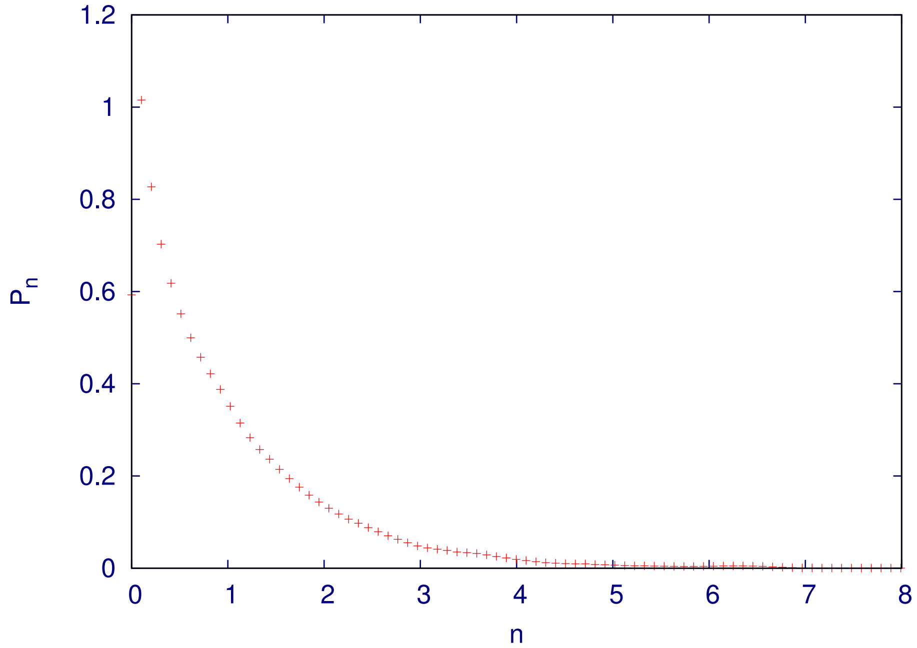
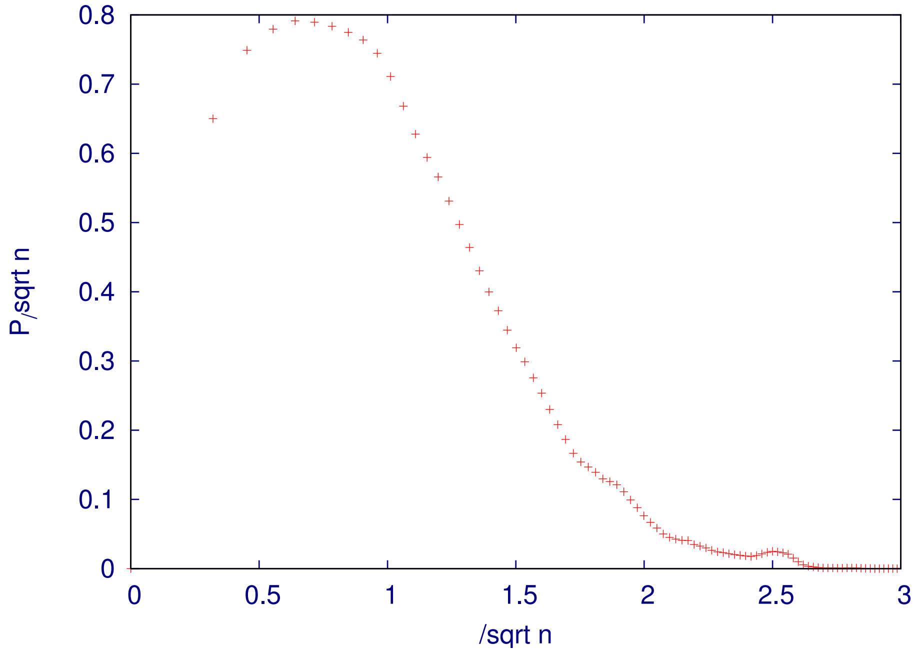
$$\rho(\mathbf{x}) = |\psi(\mathbf{x})|^2, \qquad \sqrt{\rho(\mathbf{x})} = |\psi(\mathbf{x})|$$



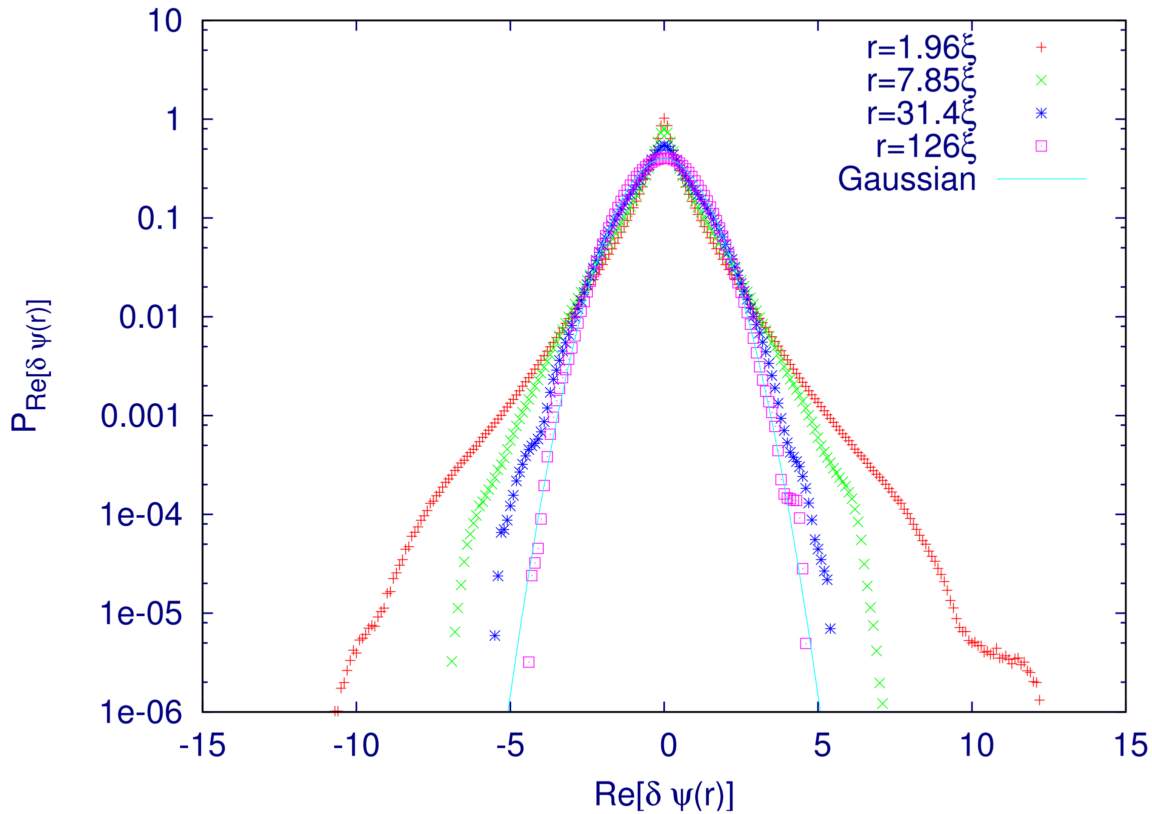


- The system is not nearly incompressible ($\rho \sim\neq$ const).
  - due to the non-separation of the scales ($L \sim 100\xi$) ?

3.7 PDF of order parameter increment

$$\delta\psi(\mathbf{r}) = \psi(\mathbf{x}+\mathbf{r}) - \psi(\mathbf{x})$$

PDF of $\mathrm{Re}[\delta\psi(r)]$



3.8 PDF of density increment

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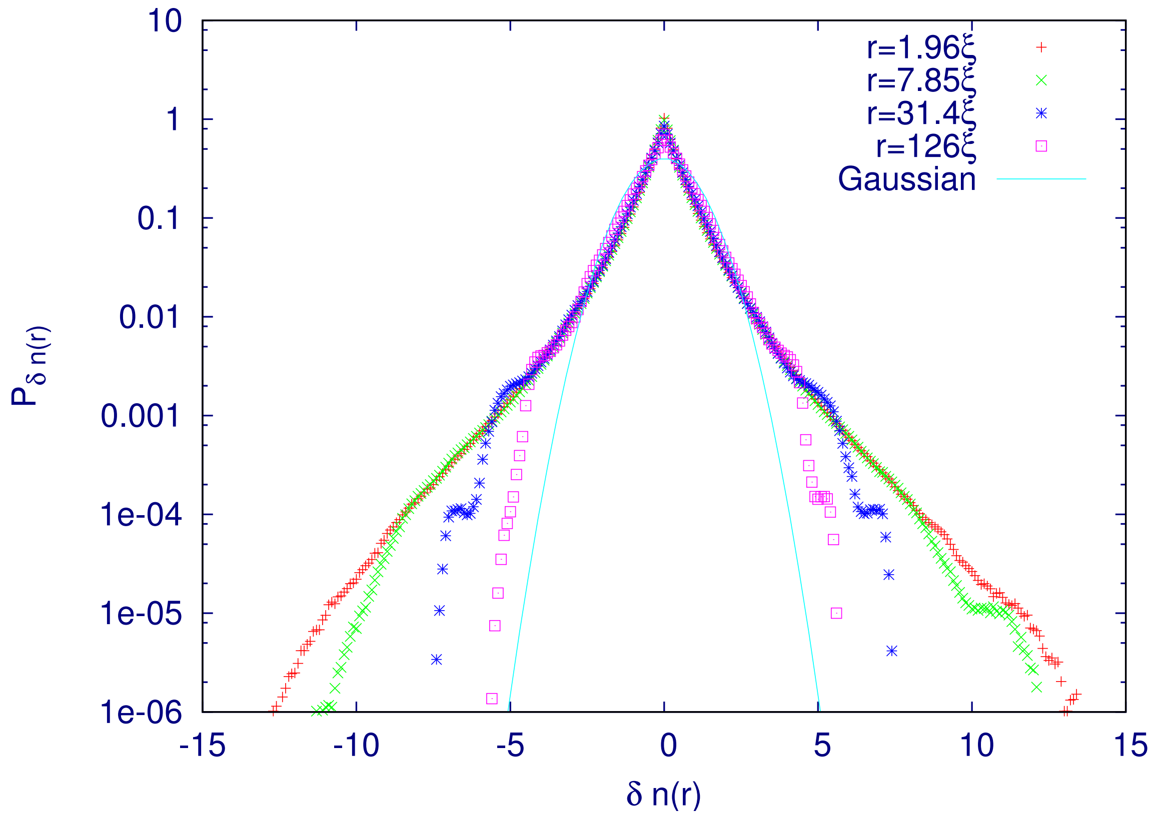
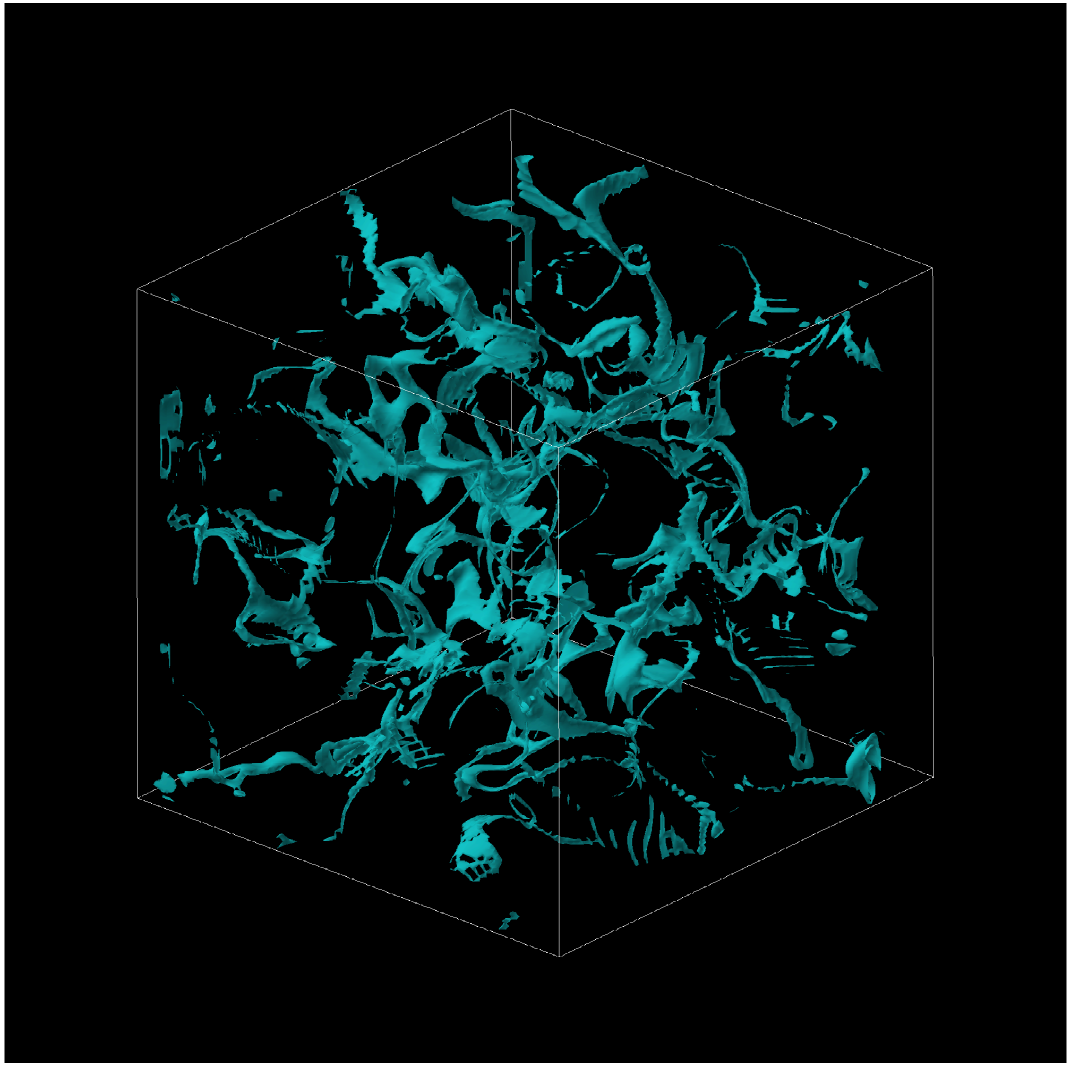
$$\delta\rho(\mathbf{r}) = \rho(\mathbf{x}+\mathbf{r}) - \rho(\mathbf{x})$$

PDF of $\delta\rho(r)$.



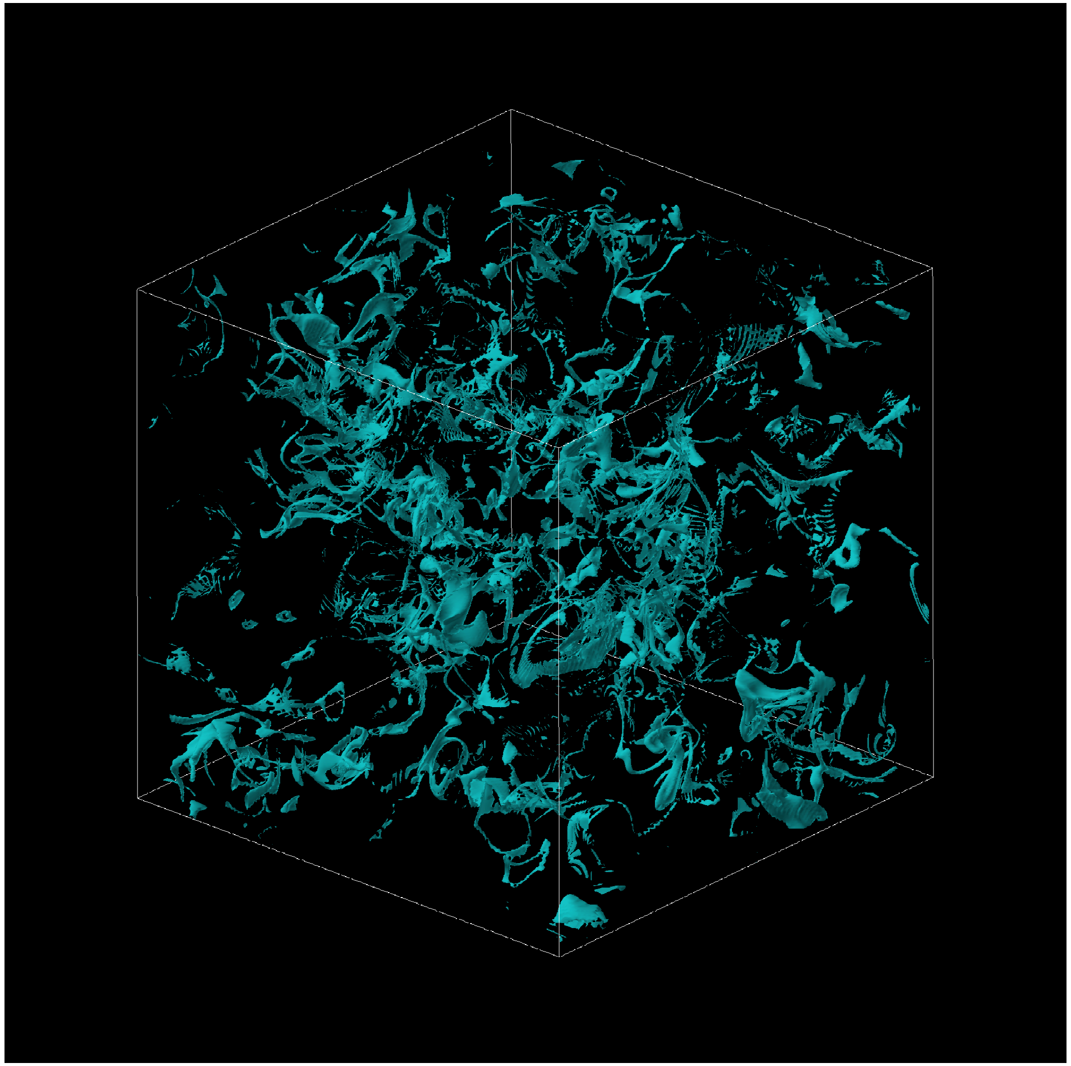
3.9 Low density region



$N = 128$

$\xi = 0.05$

$\rho < 0.01$



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$N = 256$

$\xi = 0.025$

$\rho < 0.005$

4 Summary

Numerical simulations of Gross-Pitaevskii equation with forcing and dissipation are performed up to 512^3 grid points.

- $E^{\mathrm{int}}(k) \sim k^{-5/3}$, $E^{\mathrm{kin}}(k) \sim k^{4/3}$.
- $E^{\mathrm{wi}} < E^{\mathrm{wc}}$.
- $E^{\mathrm{wi}}(k) \sim k^{-5/3}$ is not so clearly observed as in Kobayashi and Tsubota (2005).
- PDF of $\delta\psi(r)$ deviates from Gaussian as r decrease.
- Deviation from Gaussian of PDF of $\delta\rho(r)$ is larger than that of $\delta\psi(r)$.

5 Future Studies

- Closure analysis based on ψ, $\rho = |\psi|^2$.
  - Can $E^{\mathrm{int}}(k) \sim k^{-5/3}$ and $E^{\mathrm{kin}}(k) \sim k^{4/3}$ be derived?
- Investigation of singularities in the physical space.
  - Relation between the spatial and temporal structures of quantized vortex lines (reconnection etc.) and intermittency.
  - Singularity spectrum $f(\alpha)$.