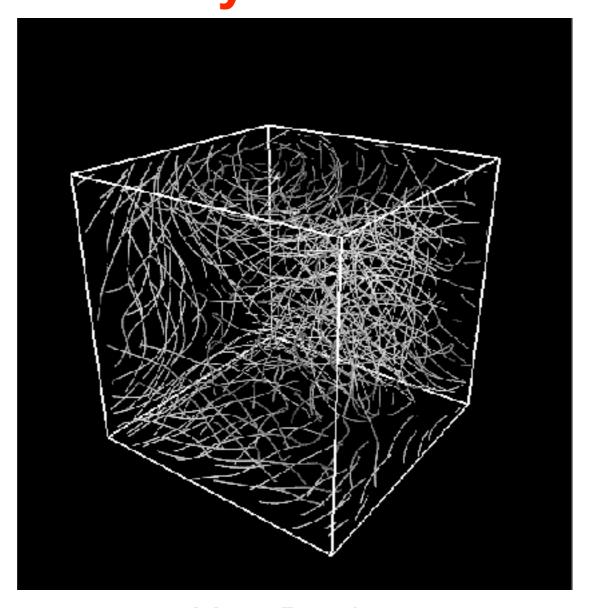# Thermalization in hydrodynamical systems

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LPS/ENS

Workshop « Geometrical and statistical fluid dynamics »
Simons Center for Geometry and Physics
Stony Brook University
Thursday October 12, 2017

Plan of talk

- Definitions. Hydrodynamical systems: Burgers; Euler (compressible and inc.); Gross-Pitaevskii Equation (GPE=Nonlinear Schrödinger) Madelung's transformation. Example: Quantum shocks in (linear) Schrödinger Equation.

- Definitions. Thermalization: Examples: shocks and tygers in Burgers Equation. Thermalization of incompressible Euler with helical Arnold–Beltrami–Childress (ABC) initial data.

- Equilibrium, phase transition and thermalization in the GPE equation

- How can we define helicity in the Gross-Pitaevskii equation? Is it conserved in simple knots? How close is helical turbulence in GPE ABC to Navier-Stokes ABC?

- Conclusions

Definition. Hydodynamical Systems

- Perfect fluids

- Superfluids

- Simple examples using Burgers equation

What is a perfect fluid?

- Real classical fluids are viscous and conduct heat

- Perfect fluids are idealized models in which these mechanisms are neglected

- Perfect fluids have zero shear stresses, viscosities, and heat conduction

- Good approximation in some physical cases

Euler Equations

- A perfect fluid can be completely characterized by its velocity and two independent thermodynamic variables.

- If only one thermodynamic variable exists (e.g. isentropic perfect fluid) the fluid is barotropic.

- The density of a barotropic fluid is a function of pressure only.

Barotropic Euler equations

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p$$

$$\partial_t \rho + \nabla(\rho \mathbf{v}) = 0$$

Barotropic: $\quad p(\mathbf{x}, t) = f(\rho(\mathbf{x}, t))$

Acoustic propagation: $\quad c = \sqrt{\dfrac{\partial p}{\partial \rho}}$

Note that the system is time-reversible:

$$t \to -t \; ; \mathbf{v} \to -\mathbf{v} \; ; \rho \to \rho \; ; p \to p$$

Two useful limits

1. incompressible:

$$\rho = cte$$

$$\nabla \mathbf{v} = 0$$

$$c \to \infty$$

There is no equation of state and p is determined by maintaining the incompressibility

2. irrotational:

$$\nabla \times \mathbf{v} = 0$$

$$\mathbf{v} = \nabla \phi$$

$$c = \sqrt{\frac{\partial p}{\partial \rho}}$$

Only compressible modes...

Variational approach

- For the general case see e.g. : R. L. Seliger and G. B. Whitham, Variational Principles in Continuum Mechanics, Proc. R. Soc. Lond. A. 1968 305 1-25.

- Here I'll show how to deal only with the compressible irrotational case..

Irrotational case

$$\mathcal{L} = \rho\phi_t + \frac{\rho(\nabla\phi)^2}{2} + g(\rho)$$

$$\frac{\delta\mathcal{L}}{\delta\phi} = 0 \rightarrow \rho_t + \nabla(\rho(\nabla\phi)) = 0$$

define: $\quad \mathbf{v} = \nabla\phi$

$$\rho g'' = p'$$

$$\frac{\delta\mathcal{L}}{\delta\rho} = 0 \rightarrow \phi_t + \frac{(\nabla\phi)^2}{2} + g' = 0$$

taking the gradient of the last equation:

$$\mathbf{v}_t + \mathbf{v} \cdot \nabla\mathbf{v} = -\nabla g' \quad = -\frac{\nabla p}{\rho}$$

What is a superfluid?
Is it just an Eulerian perfect fluid?
No! **Superfluids obey the Gross-Pitaevskii equation (GPE)**

The quantum nature of the GPE does disturb some classical traditions of fluid mechanics. This often makes it unpopular…

One should fight this attitude!

Say no to Superphobia!

superphobia
noun
unreasoning hostility, aversion, etc., toward superfluid flows.
Origin of superphobia
super(fluidity) + phobia

The Gross-Pitaeveski Equation (GPE)

$$i\hbar \partial_t \Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + g|\Psi|^2\Psi$$

$$\Psi = \sqrt{\rho/m}\,\exp i\frac{m}{\hbar}\Phi$$

- Describes a superfluid Bose-Einstein condensate at zero temperature

- Applies to a complex field

- Madelung's transformation gives hydrodynamical form

- Contains quantum vortices with quantized velocity circulation h/m

Variatitional formulation of the GPE

$$\mathcal{L} = -i\hbar\bar{\Psi}\partial_t\Psi + \frac{\hbar^2|\nabla\Psi|^2}{2m} + \frac{g|\Psi|^4}{2}$$

$$\Psi = \sqrt{\rho/m}\,\exp i\frac{m}{\hbar}\Phi$$

$$\mathcal{L} = \rho\partial_t\Phi + \frac{\rho\nabla\Phi^2}{2} + \frac{g\rho^2}{2m^2} + \frac{\hbar^2(\nabla\sqrt{\rho})^2}{2m^2}$$

Contrast and compare with Euler Equation Lagrangian:

$$\mathcal{L} = \rho\phi_t + \frac{\rho(\nabla\phi)^2}{2} + g(\rho)$$

GPE and Madelung

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + g|\Psi|^2\Psi$$

$$\psi(\mathbf{x},t) = \sqrt{\frac{\rho(\mathbf{x},t)}{m}}\exp\left[i\frac{m}{\hbar}\phi(\mathbf{x},t)\right], \quad \mathbf{V} = \boldsymbol{\nabla}\phi$$

Speed of sound $\qquad c = \sqrt{g|A_0|^2/m}$

Coherence length $\qquad \xi = \sqrt{\hbar^2/2m|A_0|^2 g}.$

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\,\boldsymbol{\nabla}\,\phi) = 0, \qquad\qquad \frac{\partial\phi}{\partial t} + \frac{1}{2}(\nabla\phi)^2 = c^2(1-\rho) + c^2\xi^2\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}.$$

Continuity and Bernoulli equations for a compressible fluid

Irrotational fluid, except near nodal lines of ψ = superfluid vortices, with quantum of circulation $\Gamma = 4\pi c\xi/\sqrt{2}$, which can naturally reconnect in this model.

Energies

The GPE conserves the total energy E, which can be decomposed as [24, 25]: $E = E_{\mathrm{kin}} + E_{\mathrm{int}} + E_{\mathrm{q}}$, with $E_{\mathrm{kin}} = \langle |\sqrt{\rho}\mathbf{v}|^2/2 \rangle$, $E_{\mathrm{int}} = \langle c^2(\rho - 1)^2/2 \rangle$ and $E_{\mathrm{q}} = \langle c^2\xi^2|\nabla\sqrt{\rho}|^2 \rangle$. The kinetic energy E_{kin} can be also decomposed into compressible $E_{\mathrm{kin}}^{\mathrm{c}}$ and incompressible $E_{\mathrm{kin}}^{\mathrm{i}}$ components, using $(\sqrt{\rho}\mathbf{v}) = (\sqrt{\rho}\mathbf{v})^{\mathrm{c}} + (\sqrt{\rho}\mathbf{v})^{\mathrm{i}}$ with $\nabla \cdot (\sqrt{\rho}\mathbf{v})^{\mathrm{i}} = 0$.
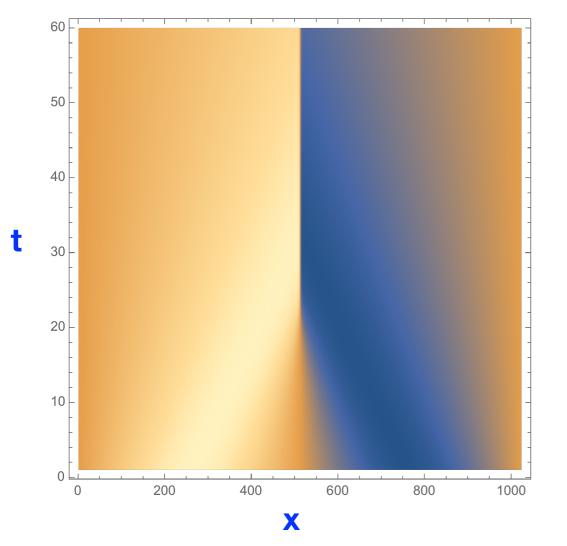
- See e.g. Nore, et al., Phys. Rev. Lett. 78, 3896, 1997
- Paresval's theorem yields definition of energy spectra

Burgers equation, GPE and Madelung's transformation

- Euler, irrotational case with zero pressure is called inviscid Burgers

- In this case, the GPE reduces to the (linear) Schrödinger equation

- Madelung transforms yields inviscid Burgers with an extra quantum pressure term

- In what immediately follows, we will compare the (slightly) viscous Burgers case with the quantum case
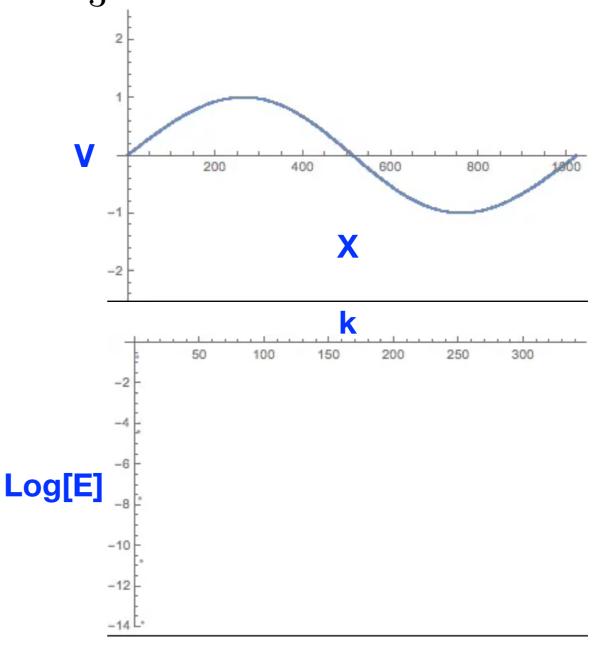
Viscous Burgers

$$\partial_t \phi + \frac{1}{2}(\partial_x \phi)^2 = \nu \partial_{xx} \phi$$

$$\phi(t=0) = -\cos x$$

$$v = \partial_x \phi$$

Pseudospectral calculation
$\nu = 0.006136$
$\frac{2}{3}$ dealiasing 1024 grid points

Quantum shocks in (linear) GPE

Schrödinger equation: $i\partial_t \psi = -\frac{\epsilon}{2}\partial_{xx}\psi$

Madelung's transformation: $\psi = \rho^{1/2}\exp i\frac{\phi}{\epsilon}$

Equations of motion:

$\partial_t \phi + \frac{1}{2}(\partial_x \phi)^2 = \frac{\epsilon^2 \partial_{xx}\sqrt{\rho}}{2\sqrt{\rho}}$

$\partial_t \rho + \partial_x(\rho\partial_x\phi) = 0$

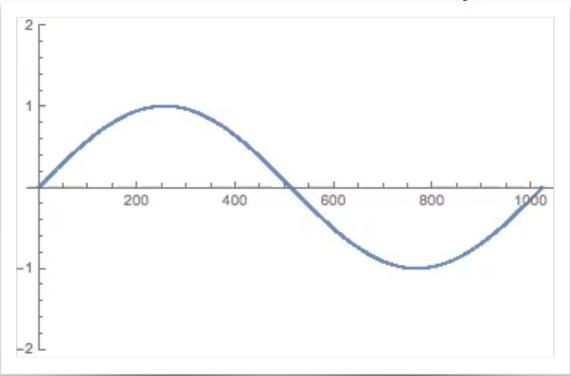Initial data

$\phi(t = 0) = -\cos x$
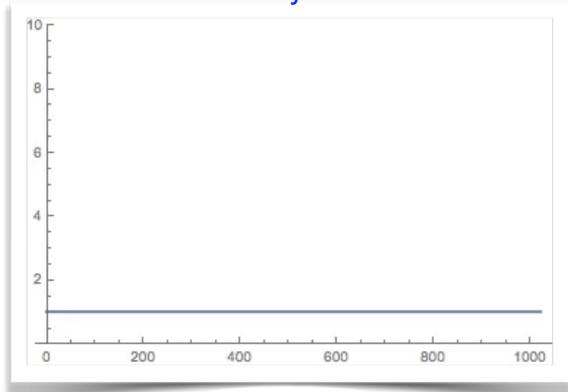
$\rho(t = 0) = 1$

$v = \partial_x \phi$

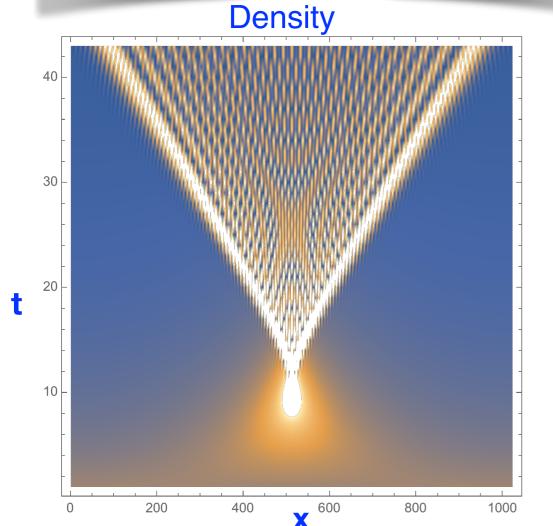$\epsilon = 0.0117188$

Single QFD shock

Density

Velocity
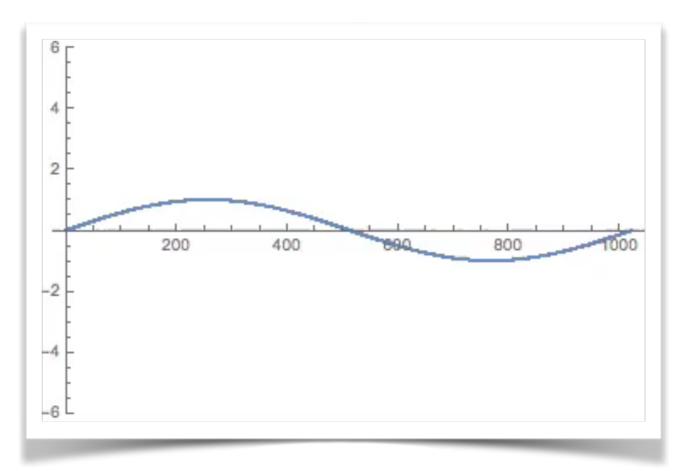

Density

t

x
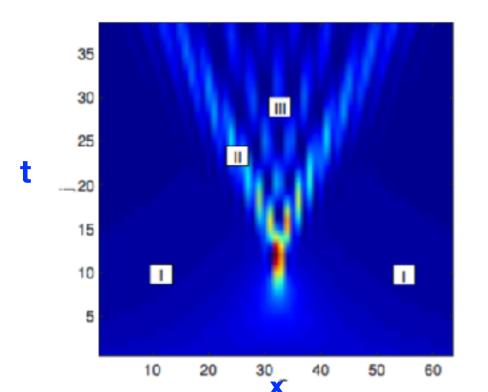
Momentum=Density * Velocity

Single QFD shock

The Green function for Schrödinger's equation $i\partial_t \psi = -\frac{\epsilon}{2}\partial_{xx}\psi$ reads

$$G_0(x,t|x_0,t_0) = \sqrt{\frac{1}{2i\pi m(t-t_0)}} e^{\frac{i(x-x_0)^2}{2\epsilon(t-t_0)}}$$

The shock solution thus reads

$$\psi(\mathbf{x},t) = \int_{-\infty}^{\infty} dy \sqrt{\frac{1}{2i\pi\epsilon t}} e^{\frac{i}{\epsilon}\left(\frac{(y-x)^2}{2t}+\cos(y)\right)} \tag{1}$$

In the $\epsilon \to 0$ limit, this integral can be computed by using Pearcey's integral defined by

$$I_{\mathcal{P}}(T,X) = \int_{-\infty}^{\infty} dy\, e^{i\left(Xy+Ty^2+y^4\right)}$$

Asymptotic expressions can be readily obtained

see refs. in https://arxiv.org/abs/1709.10417

Definition. Thermalization

- By spectral truncation, the fluid mechanical PDE devolves into a large number of conservative time reversible ODE's

- Thermalization is defined as the standard thermal equilibrium of statistical mechanics for these ODE's

- Ergodicity is assumed

- Microcanonical and canonical distributions should give comparable results for large number of ODE's

Classical truncated systems
where first introduced in 1952 by TD Lee in hydrodynamics

T.D. Lee, Quart. Appl. Math., 10(1):69 (1952).

—NOTES—

ON SOME STATISTICAL PROPERTIES OF HYDRODYNAMICAL AND
MAGNETO-HYDRODYNAMICAL FIELDS*

By T. D. LEE (*University of California, Berkeley*)

equilibrium distribution every mode of the Fourier components of magnetic field and velocity field must be in energy equipartition. Let $M(k)$ be the corresponding energy spectrum of magnetic field per unit volume, then we have

$$M(k) = F(k) \propto k^2. \tag{22}$$

3. Turbulence and magneto-turbulence. In the case of a real fluid, due to the energy

General definition of truncated systems

- The basic idea is to perform a truncation (in Fourier space) of the partial differential equation (PDE), as is always done whenever performing an actual numerical computation

- The truncated system is a large number of ordinary differential equations (ODE) with standard statistical mechanical properties

- It contains dissipative processes, thus furnishing a description finite temperature effects

Fourier-Galerkin truncation

Example: Let F be a non-linear function

$$\text{PDE:} \begin{cases} \dfrac{\partial \mathbf{u}}{\partial t}(\mathbf{x}, t) = \mathbf{F}[\mathbf{u}, \partial_i \mathbf{u}, \partial_{ij} \mathbf{u}, \dots] \\[2mm] \text{Periodic B.C. on } \quad \Omega = [0, 2\pi]^D \end{cases}$$

with a conserved quantity E

$$\mathbf{u}(\mathbf{x}, t) = \sum_{\mathbf{k}} \hat{\mathbf{u}}(\mathbf{k}, t) e^{i\mathbf{k} \cdot \mathbf{x}}$$

Non linear terms imply convolutions in Fourier space

$$\frac{\partial \hat{\mathbf{u}}}{\partial t}(\mathbf{k}, t) = \hat{\mathbf{F}}[\hat{\mathbf{u}}, \mathbf{k}]$$

$$\mathbf{k} \in \mathbb{Z}^D$$

Galerkin-truncated equation

$$\frac{\partial \hat{\mathbf{u}}}{\partial t}(\mathbf{k}, t) = \hat{\mathbf{F}}[\hat{\mathbf{u}}, \mathbf{k}]$$

$$\hat{\mathbf{u}}(\mathbf{k}, t) = \mathbf{0} \quad \text{if} \quad |\mathbf{k}| \geq k_{\max}$$

- Finite-dimensional system of ODE
- **PDE is approximated by the truncated system only as long as the spectral convergence is ensured** **(dynamics is not influenced by the cut-off)**
- Inherits some of the conservation laws of the original PDE
- The stationary solutions are given by the associated Liouville equation

$$\mathbb{P}[\hat{\mathbf{u}}(\mathbf{k})] = \mathcal{N} e^{-\eta E} \quad \text{absolute equilibria}$$

General properties of truncated system

- System relaxes toward the thermodynamical equilibrium

- Partial thermalization at small scales

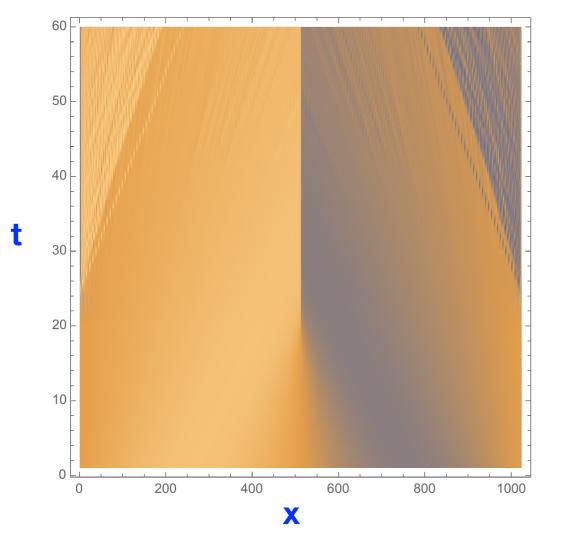- Thermalized modes generate an effective dissipation acting at large scales.

Truncated inviscid Burgers

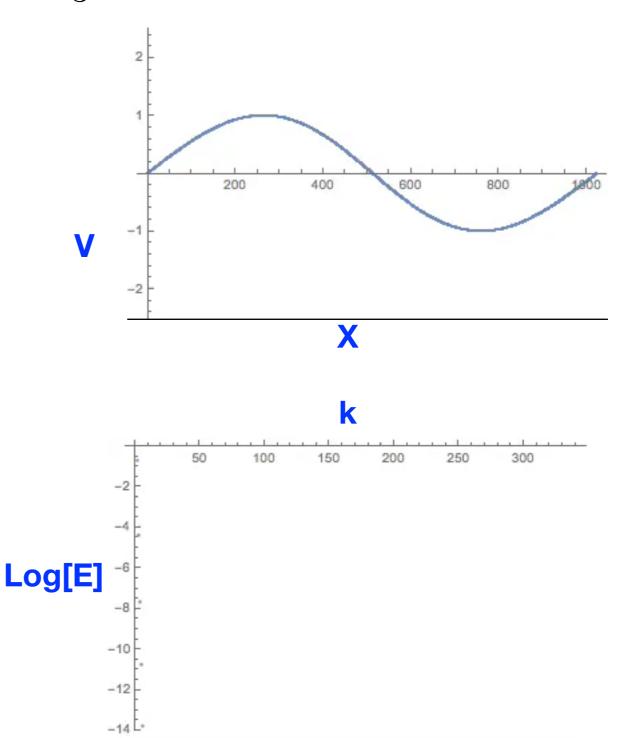$$\partial_t \phi + \frac{1}{2}(\partial_x \phi)^2 = 0$$

$$\phi(t=0) = -\cos x$$

$$v = \partial_x \phi$$

Tygers: See Frisch et al.

Pseudospectral calculation
$\frac{2}{3}$ dealiasing 1024 grid points

Truncated Euler equation

Euler PDE:

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\mathbf{u}(\mathbf{x}, t) = \sum_{\mathbf{k}} \hat{\mathbf{u}}(\mathbf{k}, t) e^{i\mathbf{k} \cdot \mathbf{x}}$$

$$\partial_t \hat{u}_\alpha(\mathbf{k}, t) = -\frac{i}{2} \mathcal{P}_{\alpha\beta\gamma}(\mathbf{k}) \sum_{\mathbf{p}} \hat{u}_\beta(\mathbf{p}, t) \hat{u}_\gamma(\mathbf{k} - \mathbf{p}, t)$$

where $\mathcal{P}_{\alpha\beta\gamma} = k_\beta P_{\alpha\gamma} + k_\gamma P_{\alpha\beta}$ with $P_{\alpha\beta} = \delta_{\alpha\beta} - k_\alpha k_\beta / k$

Truncated Euler equation
Conserved quantities

Energy $\longrightarrow$

$$E = \frac{1}{(2\pi)^3} \int \frac{|\mathbf{u}(\mathbf{x})|^2}{2} \, d^3x = \sum_k E(k)$$

Helicity $\longrightarrow$

$$H = \frac{1}{(2\pi)^3} \int \mathbf{u}(\mathbf{x}) \cdot \omega(\mathbf{x}) \, d^3x = \sum_k H(k) \quad , \quad \omega = \nabla \times \mathbf{u}$$

H. Moffatt, J. Moreau in the 60's. Discovered 200 years after Euler work

$$E(k) = \sum_{k-\Delta k/2 < |\mathbf{k}'| < k+\Delta k/2} \frac{1}{2}|\hat{\mathbf{u}}(\mathbf{k}',t)|^2$$

$$H(k) = \sum_{k-\Delta k/2 < |\mathbf{k}'| < k+\Delta k/2} \hat{\mathbf{u}}(\mathbf{k}',t) \cdot \hat{\omega}(-\mathbf{k}',t)$$

Both Energy and Helicity are exactly conserved by the truncated dynamics

Kraichnan's Helical

Absolute Equilibrium

(J. FLuids Mech. 73)

$$\hat{\mathbf{u}}(\mathbf{k}) \sim e^{-\beta E - \alpha H}$$

Gaussian distribution

$$E(k) = \frac{k^2}{\beta} \frac{4\pi}{1 - \alpha^2 k^2/\beta^2} \sim k^2 \qquad H(k) = \frac{k^4 \alpha}{\beta^2} \frac{8\pi}{1 - \alpha^2 k^2/\beta^2} \sim k^4$$

For the case presented here: $\alpha^2 k_{\max}^2/\beta^2 \ll 1$

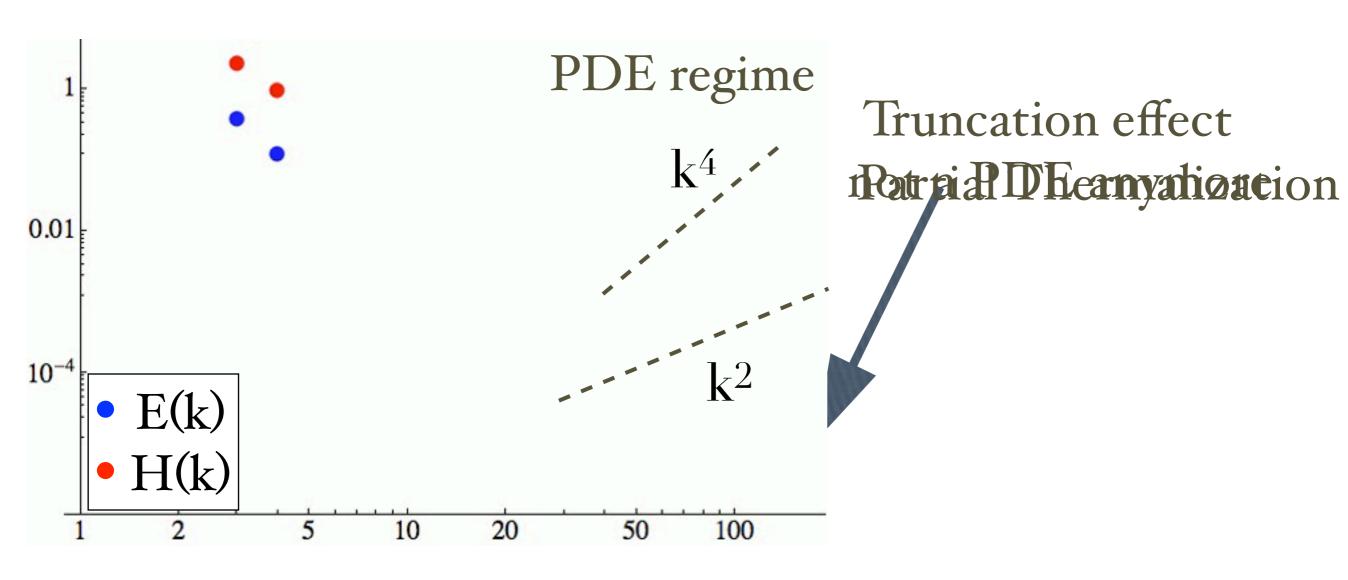# Numerical simulation ABC flow

Resolution of 512^3

$$\nabla \times \mathbf{u}_{\text{ABC}}^{(k)} = \lambda_k \mathbf{u}_{\text{ABC}}^{(k)}$$

$$E(k) = \frac{k^2}{\beta} \frac{4\pi}{1 - \alpha^2 k^2/\beta^2} \sim k^2 \qquad H(k) = \frac{k^4 \alpha}{\beta^2} \frac{8\pi}{1 - \alpha^2 k^2/\beta^2} \sim k^4$$

PDE regime

Truncation effect

Partial thermalization

k^4

k^2

E(k)

H(k)

Truncated Euler: basic facts

- Relaxation toward Kraichnan helical absolute equilibrium

- Transient mixed energy and helicity cascades

- Thermalized small-scales act as microworld providing an effective dissipation in the system

Truncation of GPE

$$i\hbar\frac{\partial \psi}{\partial t} = \mathcal{P}_{\mathrm{G}}[-\frac{\hbar^2}{2m}\nabla^2\psi + g\mathcal{P}_{\mathrm{G}}[|\psi|^2]\psi]$$

$$H = \int d^3x \left(\frac{\hbar^2}{2m}|\nabla\psi|^2 + \frac{g}{2}[\mathcal{P}_{\mathrm{G}}|\psi|^2]^2\right).$$

$$\mathcal{P}_{\mathrm{G}}[\hat{\psi}_k] = \theta(k_{\max} - k)\hat{\psi}_k$$

Heaviside function

Description of BEC at finite temperature: classical field model

Conserved quantities

Energy, number of particles and momentum

$$H = \int_V d^3x \left(\frac{\hbar^2}{2m} |\nabla\psi|^2 + \frac{g}{2} |\psi|^4 \right)$$

$$N = \int_V |\psi|^2 \, d^3x$$

$$\mathbf{P} = \int_V \frac{i\hbar}{2} \left(\psi\nabla\overline{\psi} - \overline{\psi}\nabla\psi \right) \, d^3x.$$

Conservation laws are valid in the truncated system, if dealiasing is done carefully enough

Thermalized microcanonical states
Condensation transition in TGPE

It was previously known that the k=0 mode of ψ vanishes at finite energy

MJ. Davis, SA. Morgan and K. Burnett
PRL **87,** (2001)

In fact: standard 2nd order phase transition with complex order parameter

For a full discussion of the subject, see:

Krstulovic and Brachet, Phys. Rev. E 83, 066311 (2011)

What is an 'absolute equilibrium' for GPE?

$$P_{\text{stat}} = \frac{1}{\mathcal{Z}} e^{-\beta F}$$

$$F = H - \mu N - \mathbf{W} \cdot \mathrm{P}$$

is non Gaussian
because H is quartic!

$$H = \int_V d^3x \left(\frac{\hbar^2}{2m} |\nabla \psi|^2 + \frac{g}{2} |\psi|^4 \right)$$
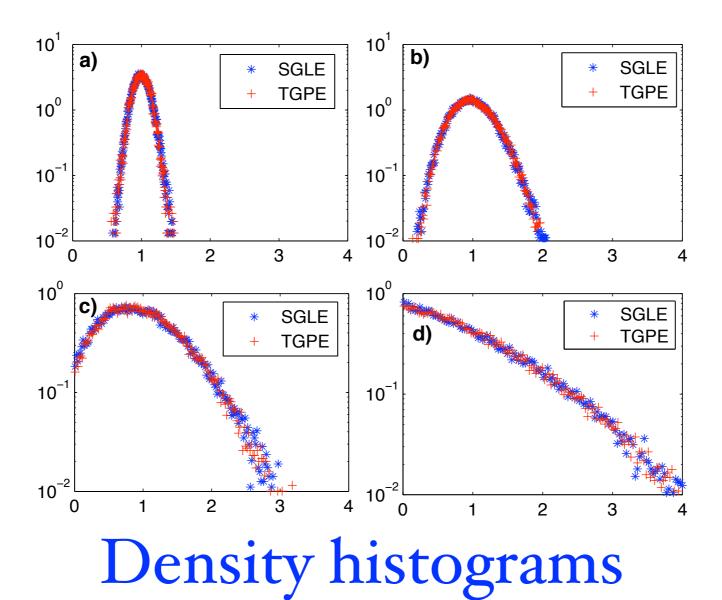
Stochastic pde used to generate absolute equilibrium

$$\hbar \frac{\partial A_{\mathbf{k}}}{\partial t} = -\frac{1}{V} \frac{\partial F}{\partial A_{\mathbf{k}}^*} + \sqrt{\frac{2\hbar}{V\beta}} \, \hat{\zeta}(\mathbf{k}, t)$$

$$\langle \zeta(\mathbf{x}, t) \zeta^*(\mathbf{x}', t') \rangle = \delta(t - t') \delta(\mathbf{x} - \mathbf{x}'),$$
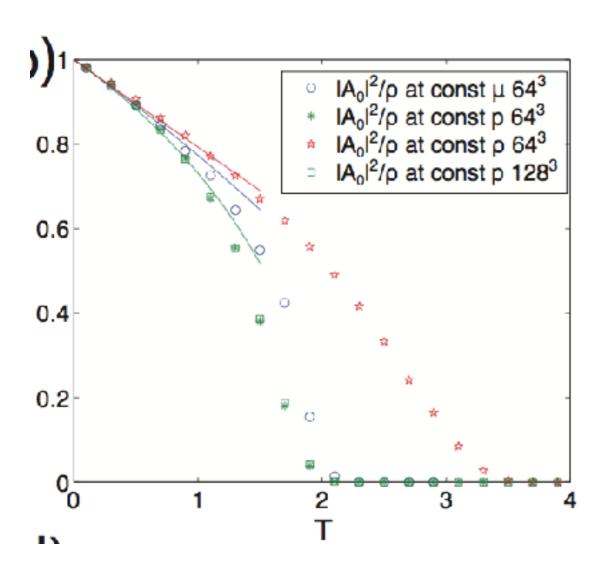
$$\hbar \frac{\partial \psi}{\partial t} = \mathcal{P}_{\mathrm{G}}[\frac{\hbar^2}{2m} \nabla^2 \psi + \mu \psi - g \mathcal{P}_{\mathrm{G}}[|\psi|^2]\psi - i\hbar \mathbf{W} \cdot \nabla \psi] + \sqrt{\frac{2\hbar}{V\beta}} \mathcal{P}_{\mathrm{G}}[\zeta(\mathbf{x}, t)]$$
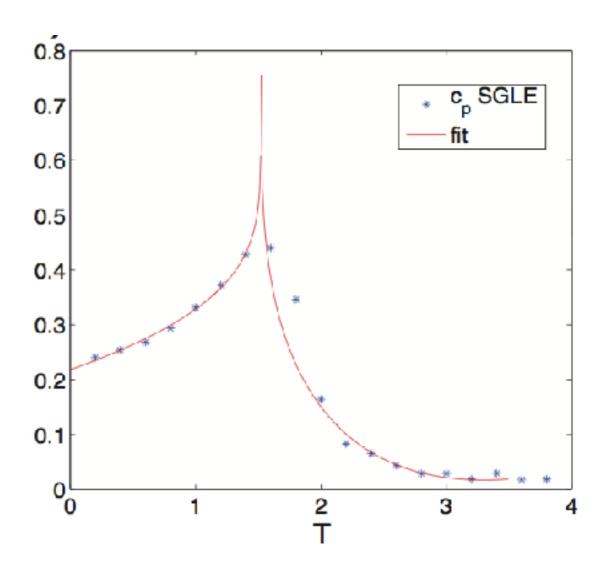
Micro canonical versus grand canonical

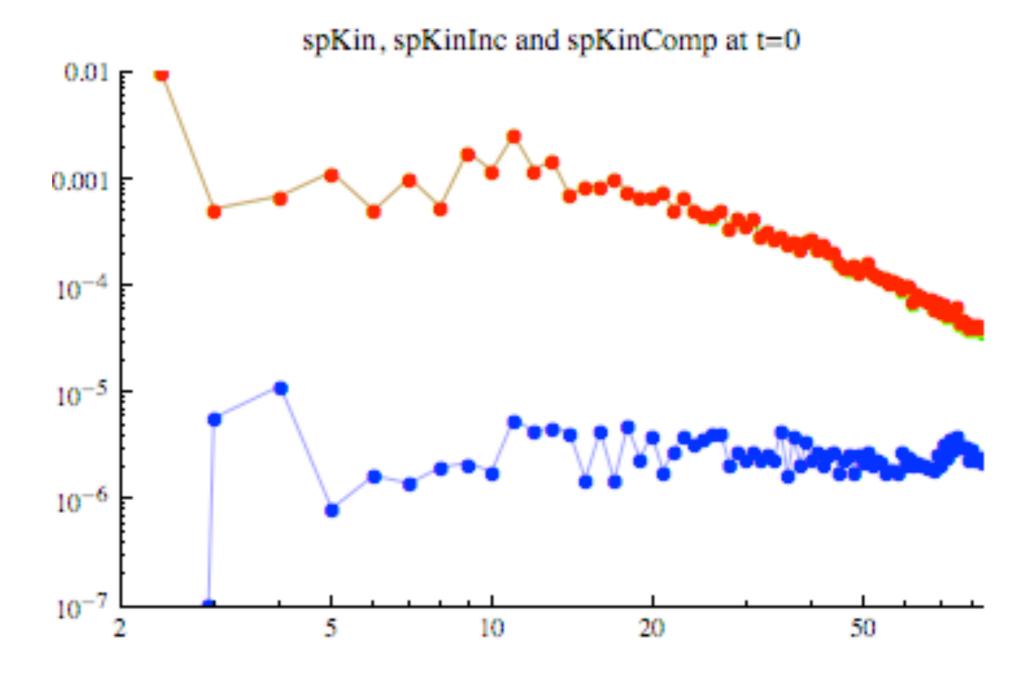| H	T	TGPE time steps	SGLE time steps
0.09	0.09	40000	9600
0.5	0.5	20000	9600
1.96	1.8	20000	9600
4.68	4	20000	5000

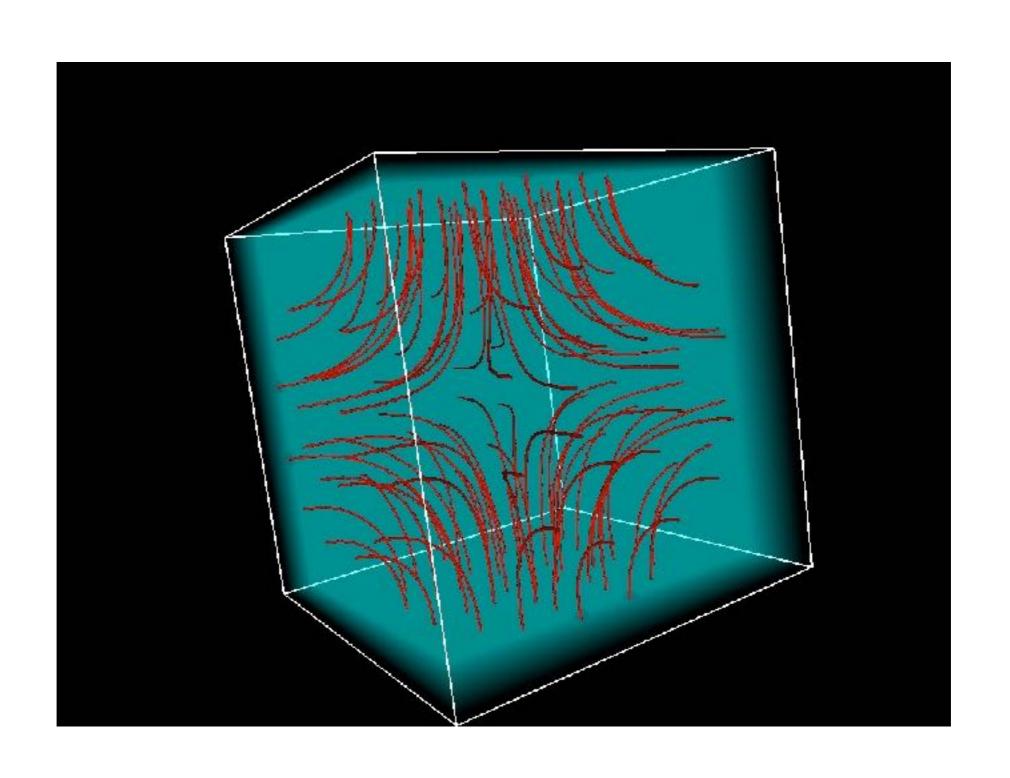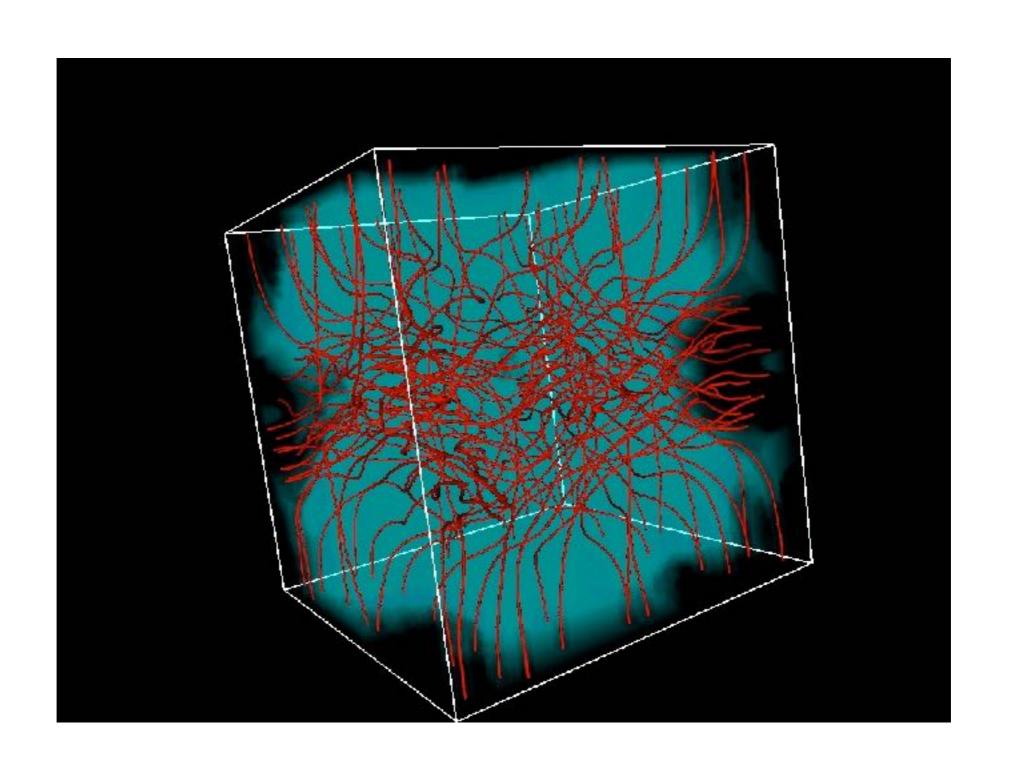Density histograms

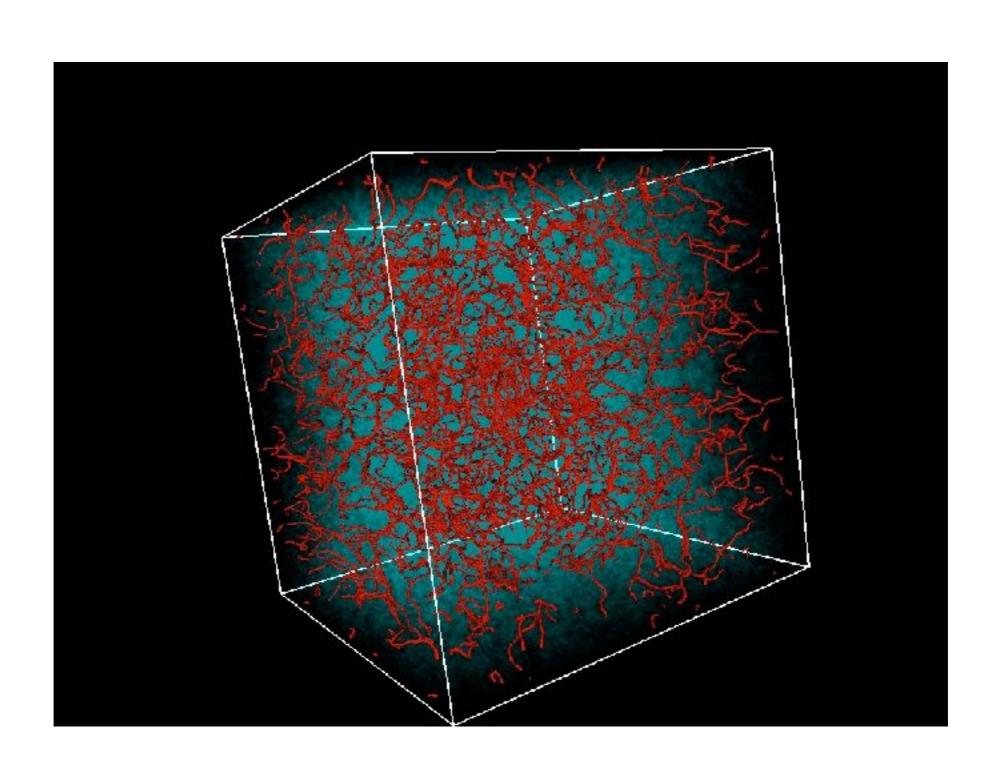# Condensation transition

$$\lambda - \phi^4 \quad (D = 3, n = 2)$$

Dynamics of thermalization in the GPE

Kinetic energy spectrum
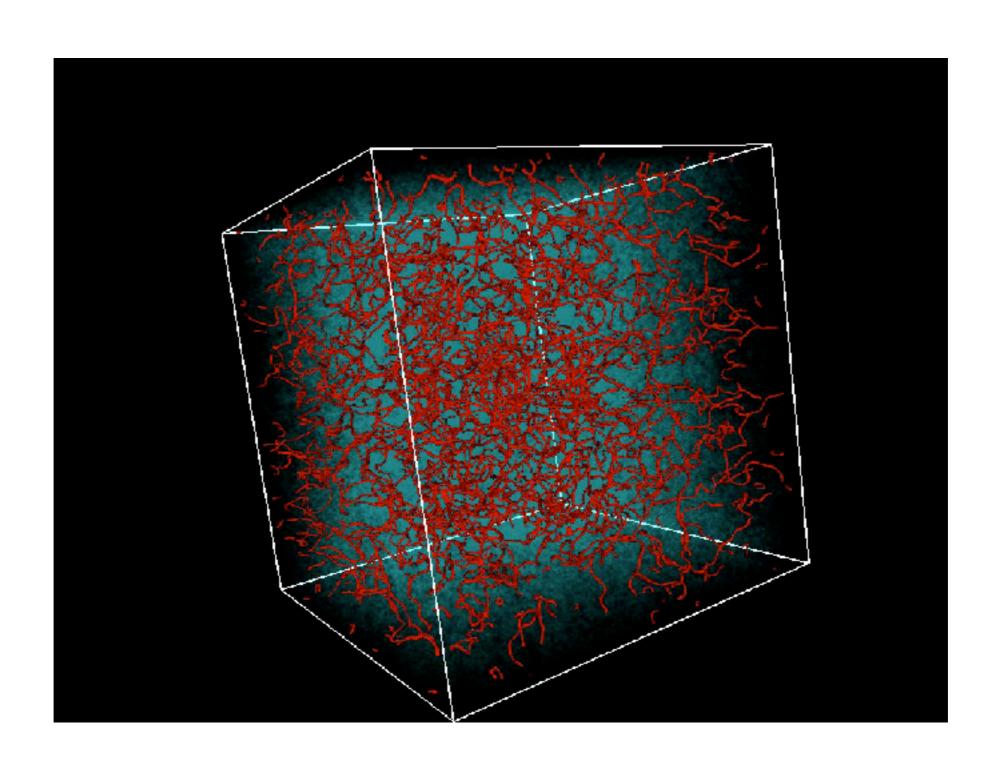
- $E_{kin\ tot}(k)$
- $E_{kin\ inc}(k)$
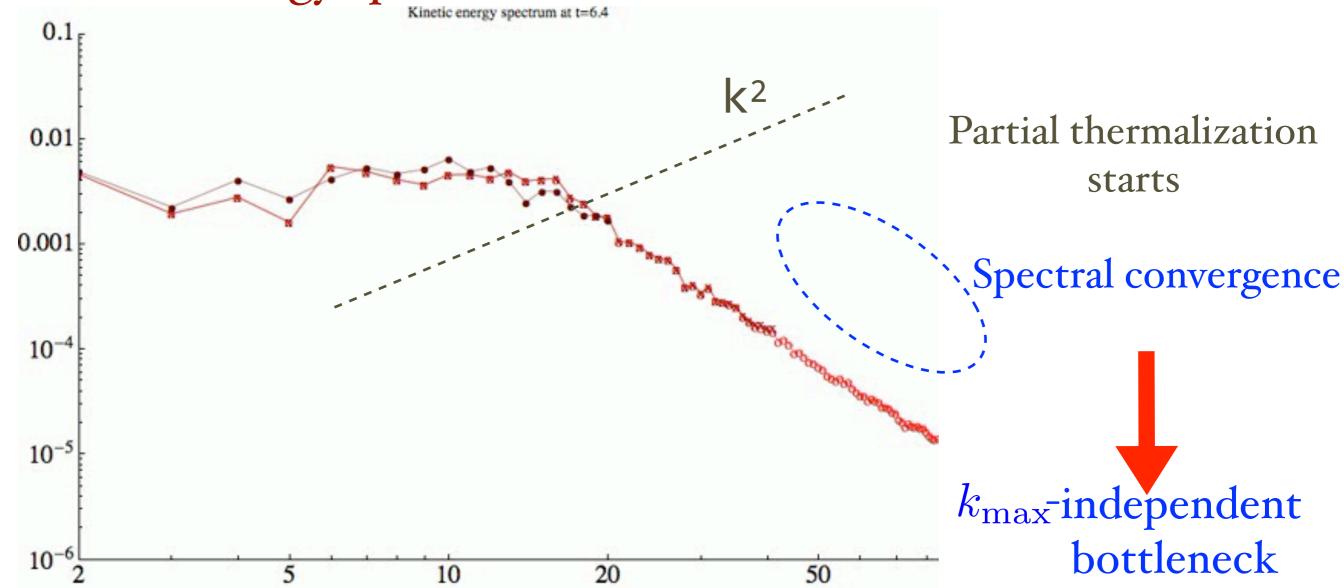- $E_{kin\ comp}(k)$

spKin, spKinInc and spKinComp at t=0

Taylor-Green vortex

Taylor-Green vortex

Taylor-Green vortex

Taylor-Green vortex

Dispersive "bottleneck" for thermalization of waves

Variable $\xi k_{\max}$ (ξ fixed, different resolutions)

Kinetic energy spectrum

Kinetic energy spectrum at t=6.4

k^2

Partial thermalization starts

Spectral convergence

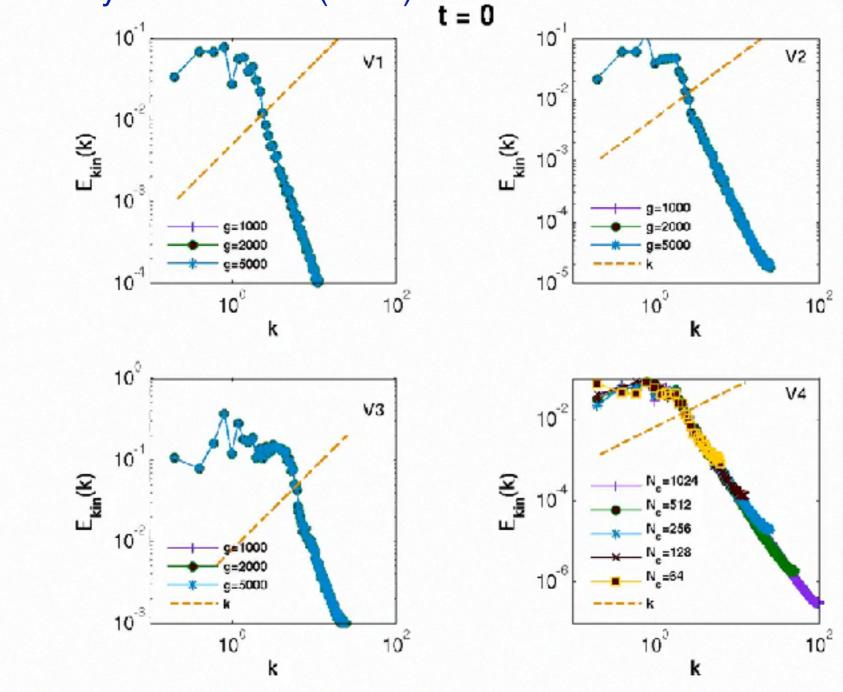$k_{\max}$-independent bottleneck

see: Krstulovic and Brachet, Phys. Rev. Lett. 106, 115303 (2011)

Self truncation in 2D

Vishwanath Shukla, Marc Brachet and Rahul Pandit
Turbulence in the two-dimensional Fourier-truncated Gross–Pitaevskii equation
New J. Phys. 15 113025 (2013)

[Top Left] $k_0 = 5\Delta k$ and $\sigma = 2\Delta k$, [Top Right] $k_0 = 15\Delta k$ and $\sigma = 2\Delta k$, [Bottom Left] $k_0 = 35\Delta k$ and $\sigma = 5\Delta k$, and [Bottom Right] different N_c.

Kelvin waves and helicity in the GPE

- 1. Detecting Kelvin Waves using spatiotemporal spectrum; 2. Helicity and Kelvin Waves in reconnecting quantum knots; 3. Dual cascade in helical quantum turbulence

- Work with P. Mininni et P. Clark Di Leoni

- PHYSICAL REVIEW A 92, 063632 (2015)

- PHYSICAL REVIEW A 94, 043605 (2016)

- PHYSICAL REVIEW A 95, 053636 (2017)

Detecting Kelvin Waves using spatiotemporal spectrum

- Main results:

- Space-time resolved spectra allow to find needles in haystacks : Kelvin waves in spatial spectrum

- A practical method to quantify their presence

GPE, Madelung and quantum vortices

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + g|\psi|^2\psi,$$

$$\psi(\mathbf{r},t) = \sqrt{\frac{\rho(\mathbf{r},t)}{m}}\,e^{im\phi(\mathbf{r},t)/\hbar},$$

$$\mathbf{v} = \nabla\phi,$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0,$$

$$\frac{\partial\mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} = -\frac{g}{m^2}\nabla\rho + \frac{\hbar^2}{2m^2}\nabla\left(\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}\right).$$

$$\Gamma = \oint_C \mathbf{v}(\ell)\,d\ell = 4\pi\alpha, \qquad \alpha = \hbar/(2m).$$

$$\omega(\mathbf{r}) = \Gamma\int ds\,\frac{d\mathbf{r}'}{ds}\delta^{(3)}(\mathbf{r}-\mathbf{r}'(s)),$$
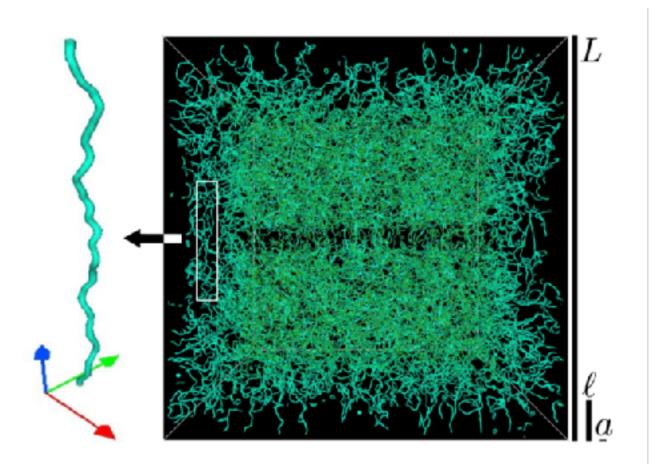
Spatiotemporal spectra

- Finding Kelvin waves in the energy spectra is like looking for needles in a haystack…

- Instantaneous flow visualization is insufficient to identify and extract all the waves in a turbulent flow.

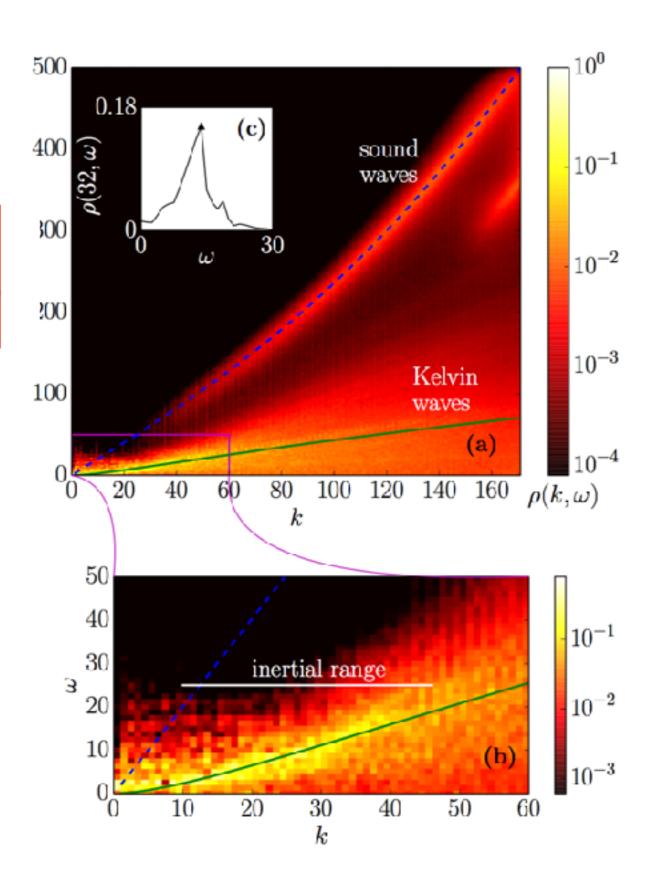- To quantify their amplitudes as a function of frequency and wave number : calculate space-time resolved spectra.

Space-time resolved Mass spectrum, Taylor Green

$$\omega_B(k) = k\sqrt{c^2 + \frac{c^2\xi^2}{2}k^2},$$

$$\xi = \sqrt{\hbar^2/(2m|\psi|^2 g)} \qquad c = \sqrt{g|\psi|^2/m}$$

$$\omega_K(k) = \frac{2c\xi}{\sqrt{2}a^2}\left(1 \pm \sqrt{1 + ka\frac{K_0(ka)}{K_1(ka)}}\right)$$

Incompressible Kinetic energy spectrum associated to Kelvin Waves

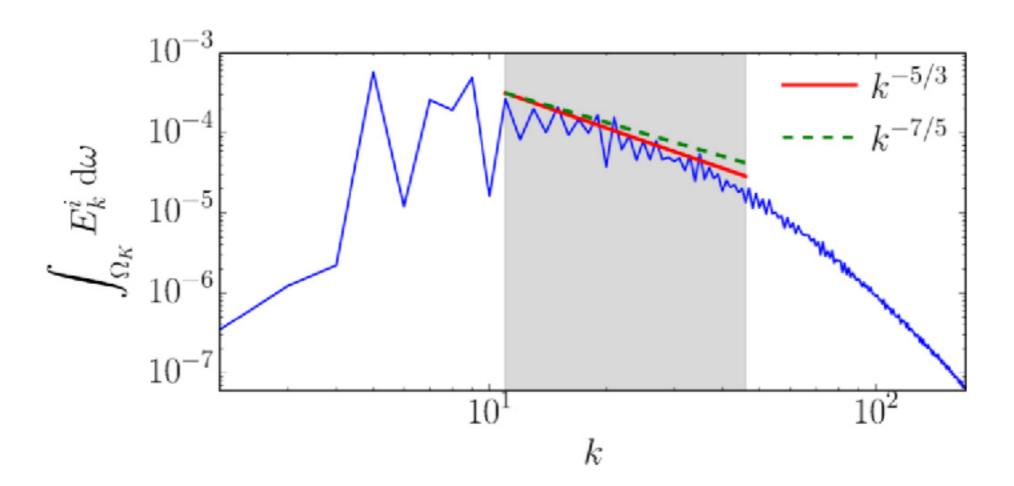

FIG. 5. (Color online) Spectrum of the incompressible kinetic energy associated with Kelvin wave modes, $\int_{\Omega_K} E_k^i(k,\omega)d\omega$, where Ω_K are the modes neighboring $\omega_K(k)$. The two predictions for the Kelvin wave spectrum are shown as references. The shaded area corresponds to the region with strong Kelvin excitations identified as "inertial range" in Fig. 3(b).

Helicity and Kelvin Waves in reconnecting quantum knots

- Main results

- Helicity can be directly computed from the GPE 3D complex wave function field using our new regularization method

- Conservation or non-conservation of quantum helicity is an open problem involving not only topological changes, but also excitation (and decay) of Kelvin waves

What is helicity in a classical flow?

For a localized vorticity distribution $\boldsymbol{\omega}(\mathbf{x}, t) = \nabla \times \mathbf{u}$ in a fluid of infinite extent, the helicity of the associated flow is defined by

$$\mathcal{H} = \int \mathbf{u} \cdot \boldsymbol{\omega} \, \mathrm{d}V, \qquad [2]$$

the integral being over all space. This integral is, like energy, an invariant of the Euler equations of ideal fluid flow, and its physical interpretation is that it provides a measure of the degree of knottedness and/or linkage of the vortex lines of the flow (1). It is also a measure of the lack of mirror symmetry of the flow (see below), which is why it is appropriate to denote it with the non–mirror-symmetric script character $\mathcal{H}$.

Helicity and singular structures in fluid dynamics

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Helicity in quantum flows

$$\Gamma = \oint_C \mathbf{v}(\ell)\, d\ell = 4\pi\alpha, \qquad\qquad \alpha = \hbar/(2m).$$

$$\boldsymbol{\omega}(\mathbf{r}) = \Gamma \int ds \frac{d\mathbf{r}'}{ds} \delta^{(3)}(\mathbf{r} - \mathbf{r}'(s)),$$

$$\mathbf{v} = \frac{\mathcal{P}}{n}, \qquad\qquad \mathcal{P}_j = 2\alpha \frac{\overline{\Psi}\partial_j\Psi - \Psi\partial_j\overline{\Psi}}{2i}$$

$$n = \Psi\Psi,$$

$$\mathbf{v} = \frac{\alpha}{i}\left(\frac{\nabla\Psi}{\Psi} - \frac{\nabla\overline{\Psi}}{\overline{\Psi}}\right)$$

Singularity of v

(notice that these definitions are analogous to those derived via the Madelung transformation $\Psi = \sqrt{n}e^{i\phi}$, where the velocity is given by $\mathbf{v} = 2\alpha\nabla\phi$). At a distance $r \to 0$ from a straight vortex line these quantities are known [27] to behave as $n \sim r^2$ and $\mathbf{v} = 2\alpha\mathbf{e}_\theta/r$ where $\mathbf{e}_\theta$ is the azimuthal unit vector and r the radial distance in a cylindrical coordinate system $(\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_z)$ having its origin on the straight vortex line. Thus, the velocity $\mathbf{v}$ has an r^{-1} singularity *perpendicular* to the vortex line.

Need to regularize v

Therefore, as the vorticity (see Eq.(2)) also has a singularity *parallel* to those lines, the standard definition of helicity

$$\mathcal{H} = \int d\mathbf{r}\, \boldsymbol{\omega}(\mathbf{r}) \cdot \mathbf{v}(\mathbf{r}), \tag{6}$$

is not well behaved, as it involves the product of two singular distributions. The idea of the *regularized* helicity is to replace in Eq. (6) the field $\mathbf{v}$ by a regularized smooth field $\mathbf{v}_{\text{reg}}$ having no divergences perpendicular to the line, and the same regular behavior as $\mathbf{v}$ parallel to the line.

$$\mathbf{v} = \frac{\alpha}{i}\left(\frac{\nabla\Psi}{\Psi} - \frac{\nabla\bar{\Psi}}{\bar{\Psi}}\right)$$

Along the line: 0/0

Idea: use L'Hôpital's rule

Singularities of v

Without loss of generality we can suppose that there is a vortex line going through $\mathbf{r} = 0$ (the radial cylindrical vector) in the direction of the z-axis. Let us define the unit vector basis $(\hat{\mathbf{e}}_x, \hat{\mathbf{e}}_y, \hat{\mathbf{e}}_z)$. The existence of a vortex line passing through $\mathbf{r} = \mathbf{0}$ and pointing in the z-direction implies that $\Psi(0) = 0$, $\bar{\Psi}(0) = 0$, $\hat{\mathbf{e}}_z \cdot \boldsymbol{\nabla}\Psi(0) = 0$, and $\hat{\mathbf{e}}_z \cdot \boldsymbol{\nabla}\bar{\Psi}(0) = 0$. Thus $\boldsymbol{\nabla}\Psi(0)$ and $\boldsymbol{\nabla}\bar{\Psi}(0)$ are linear combinations of $\hat{\mathbf{e}}_x$ and $\hat{\mathbf{e}}_y$. Taylor-expanding to first order the numerator and denominator of the above expression for $\mathbf{v}(\mathbf{r})$ around $\mathbf{r} = 0$ one finds

$$\Psi(x, y, z) = x\partial_x \Psi(0) + y\partial_y \Psi(0) + \mathcal{O}(\mathbf{r}^2), \quad (2)$$

$$\bar{\Psi}(x, y, z) = x\partial_x \bar{\Psi}(0) + y\partial_y \bar{\Psi}(0) + \mathcal{O}(\mathbf{r}^2), \quad (3)$$

$$\boldsymbol{\nabla}\Psi(x, y, z) = \boldsymbol{\nabla}\Psi(0) + \mathbf{r} \cdot \boldsymbol{\nabla}(\boldsymbol{\nabla}\Psi)(0) + \mathcal{O}(\mathbf{r}^2), \quad (4)$$

$$\boldsymbol{\nabla}\bar{\Psi}(x, y, z) = \boldsymbol{\nabla}\bar{\Psi}(0) + \mathbf{r} \cdot \boldsymbol{\nabla}(\boldsymbol{\nabla}\bar{\Psi})(0) + \mathcal{O}(\mathbf{r}^2). \quad (5)$$

$$\mathbf{v}_\perp(\mathbf{r}) = \frac{\hbar}{2im} \left(\frac{\boldsymbol{\nabla}\Psi(0)}{x\partial_x \Psi(0) + y\partial_y \Psi(0)} - c.c \right). \quad (6)$$

On the other hand, the velocity component parallel to the centerline vorticity $v_\parallel(\mathbf{r}) = \mathbf{v}(\mathbf{r}) \cdot \hat{\mathbf{e}}_z$ reads

$$v_\parallel(\mathbf{r}) = \frac{h}{2im} \left(\frac{x(\partial_{xz}\Psi)(0) + y(\partial_{yz}\Psi)(0) + z(\partial_{zz}\Psi)(0)}{x\partial_x \Psi(0) + y\partial_y \Psi(0)} \right.$$
$$\left. - c.c. \right), \quad (7)$$

In order to turn the above expression into a workable ansatz for $v_\parallel(0)$, we need to pick a reasonable direction along which Ψ will have a significant variation. The simplest vectors we have at point $\mathbf{r} = 0$, perpendicular to the vortex line and satisfying the condition, are $\boldsymbol{\nabla}\Psi(0)$ and $\boldsymbol{\nabla}\bar{\Psi}(0)$. Thus we can multiply the first term in the r.h.s. of Eq. (7) by $\boldsymbol{\nabla}\bar{\Psi}$, and its complex conjugate by $\boldsymbol{\nabla}\Psi$ in order to maintain the reality of the velocity field. In this way we arrive to the following expression

$$v_\parallel(0) = \frac{\hbar}{2m\,i} \left(\frac{\partial_x \bar{\Psi}\partial_{xz}\Psi + \partial_y \bar{\Psi}\partial_{yz}\Psi + \partial_z \bar{\Psi}\partial_{zz}\Psi}{\partial_x \bar{\Psi}\partial_x \Psi + \partial_y \bar{\Psi}\partial_y \Psi + \partial_z \bar{\Psi}\partial_z \Psi} - c.c. \right). \quad (8)$$

As a final remark, it is important to note that for arbitrarily aligned vortex lines, the direction parallel to the vortex line ($\hat{z}$ in the particular case considered above) can be easily obtained by doing the vector product between $\boldsymbol{\nabla}\Psi$ and $\boldsymbol{\nabla}\bar{\Psi}$.

Definition of regular v

$$v_{\parallel} = \frac{2\alpha}{2i} \frac{\mathcal{W}_j \left[(\partial_j \partial_l \Psi) \partial_l (\overline{\Psi})) - (\partial_j \partial_l \overline{\Psi}) \partial_l (\Psi)) \right]}{\sqrt{\mathcal{W}_l \mathcal{W}_l} (\partial_m \Psi)(\partial_m \overline{\Psi})},$$

where

$$\mathcal{W}_j = \epsilon_{jkl} \partial_k \mathcal{P}_l = \frac{2\alpha}{i} \epsilon_{jkl} \partial_k \overline{\Psi} \partial_l \Psi \qquad (7)$$

is a smooth field oriented along the vortex line. Then, we can define the regularized helicity

$$\mathcal{H} = \int d\mathbf{r}\, \boldsymbol{\omega}(\mathbf{r}) \cdot \mathbf{v}_{\text{reg}}(\mathbf{r}) \qquad (8)$$

with $\mathbf{v}_{\text{reg}} = v_{\parallel} \mathcal{W} / \sqrt{\mathcal{W}_j \mathcal{W}_j}$. We show next how this regularized helicity still holds the geometrical interpretations valid for the standard one.

Relation with writhe. For and isolated structure, helicity can be decomposed into twist (loosely speaking, the total number of helical turns a ribbon does), and writhe (the "coiling" of the structure). Let's start by analyzing the relation between the regularized helicity and the writhe. For a single curve, the writhe Wr is, by definition [28], given by the expression

$$Wr = \frac{1}{4\pi} \frac{\int \int (\mathrm{d}\mathbf{r} \times \mathrm{d}\mathbf{r}_1) \cdot (\mathbf{r} - \mathbf{r}_1)}{|(\mathbf{r} - \mathbf{r}_1)|^3}. \tag{9}$$

It is easy to see that if one uses a velocity field $\mathbf{V}(\mathbf{r})$ given by the Biot-Savart law

$$\mathbf{V}(\mathbf{r}) = \frac{\Gamma}{4\pi} \frac{\int \mathrm{d}\mathbf{r}_1 \times (\mathbf{r} - \mathbf{r}_1)}{|(\mathbf{r} - \mathbf{r}_1)|^3}, \tag{10}$$

where $\mathbf{r}_1$ corresponds to the position of the vortex lines, and the vorticity as defined in Eq. (2), then helicity $\mathcal{H}$ is given by

$$\mathcal{H} = \int \mathbf{V}(\mathbf{r}) \cdot \boldsymbol{\omega}(\mathbf{r}) \mathrm{d}V = \Gamma \int \mathbf{V}(\mathbf{r}) \cdot \mathrm{d}\mathbf{r},$$

$$= \frac{\Gamma^2}{4\pi} \frac{\int \int \mathrm{d}\mathbf{r} \cdot (\mathrm{d}\mathbf{r}_1 \times (\mathbf{r} - \mathbf{r}_1))}{|(\mathbf{r} - \mathbf{r}_1)|^3}.$$

From the identity $(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})$ one finds that in this simple case (for a *single* line)

$$\mathcal{H} = \Gamma^2 Wr.$$

Regularized helicity defined as the twist of constant phase ribbon. First we recall that the twist Tw of a ribbon (defined by *both* a curve $\mathbf{r(s)}$, and a vector $\mathbf{U}(s)$ perpendicular to the curve) is defined by the integral over the curve

$$Tw = \frac{1}{2\pi} \int \left(\frac{d\mathbf{U}}{ds} \times \mathbf{U} \right) \cdot \frac{d\mathbf{r}}{ds} ds. \qquad (11)$$
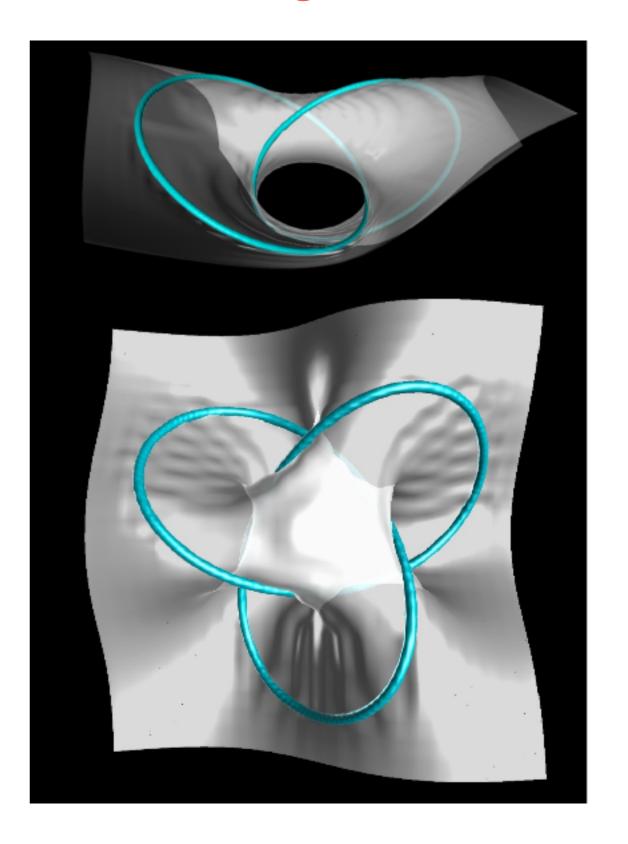
One can further show that [6]

$$Tw = N + \frac{1}{2\pi} \int \tau(s) ds, \qquad (12)$$
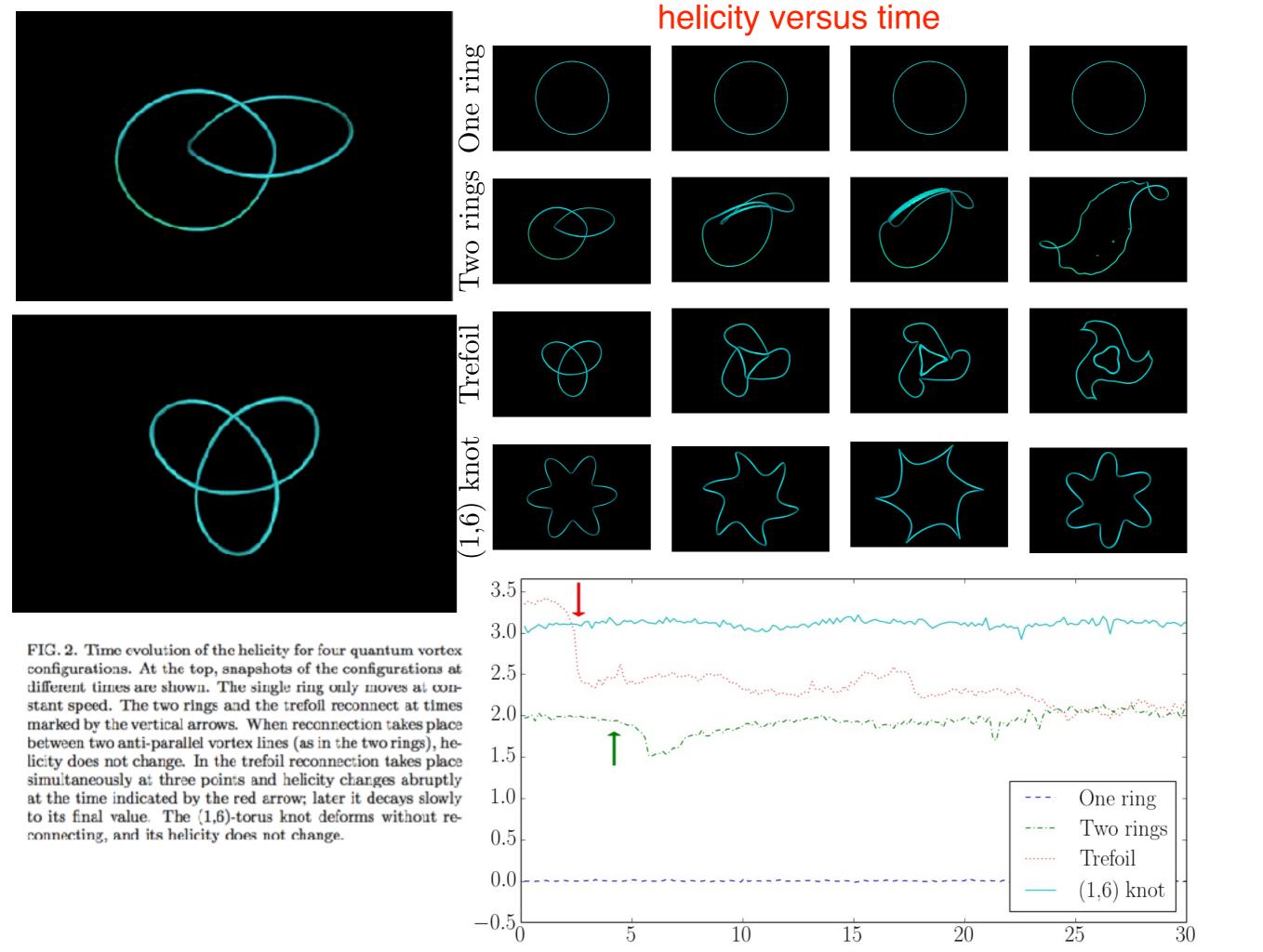
where τ is the torsion, and N the number of turns round the curve of $\mathbf{U}$ in the Frenet-Serret frame (see *Methods*). The regularized helicity can be presented in a purely geometrical way. Under the GPE, constant phase surfaces will intersect on the vortex lines. Now consider a line at a close distance of the vortex line and lying on a constant phase surface (note that we could construct an equivalent line in the classical Biot-Savart case by requiring the line to be perpendicular to the velocity field). The vortex line and the constant phase line defines a ribbon. Now, using Eqs. (2), (7) and (11) we can see that

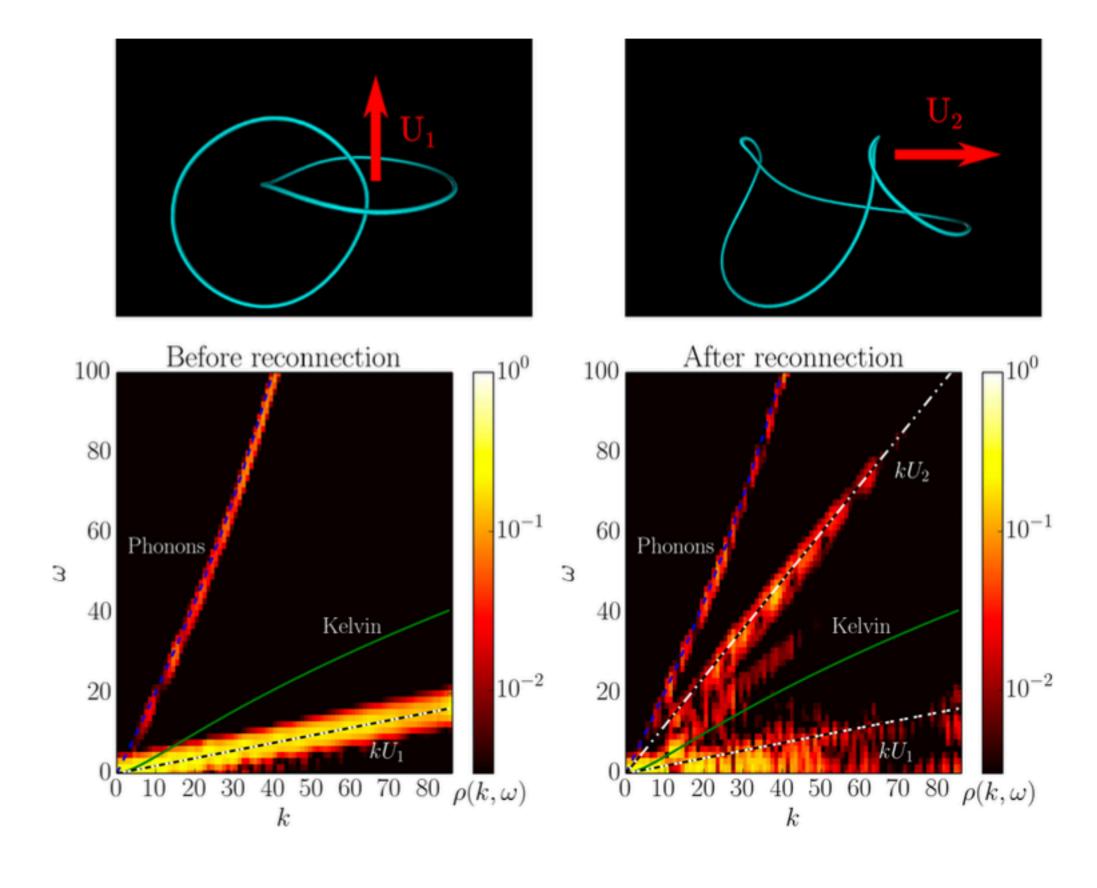$$\mathcal{H} = \Gamma^2 \, Tw.$$

Constant phase surfaces : 2 linked rings and trefoil knot

FIG. 1. Renderings of the surface of zero phase for two knots in a quantum fluid. Top: two linked rings, note the surface has one hole. Bottom: trefoil knot, with three holes. The number of holes is associated to the number of turns the vector that lies on the surface perpendicular to the vortex lines does as it moves along the curve.
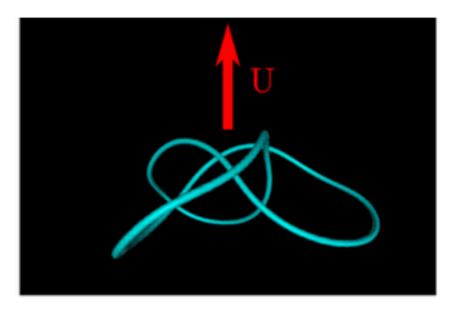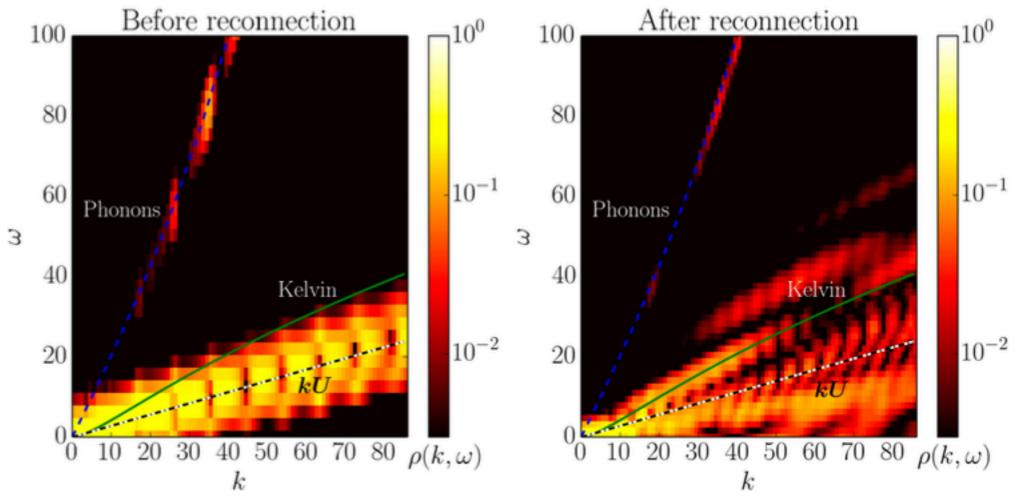
helicity versus time

One ring

Two rings

Trefoil

(1,6) knot

FIG. 2. Time evolution of the helicity for four quantum vortex configurations. At the top, snapshots of the configurations at different times are shown. The single ring only moves at constant speed. The two rings and the trefoil reconnect at times marked by the vertical arrows. When reconnection takes place between two anti-parallel vortex lines (as in the two rings), helicity does not change. In the trefoil reconnection takes place simultaneously at three points and helicity changes abruptly at the time indicated by the red arrow; later it decays slowly to its final value. The (1,6)-torus knot deforms without reconnecting, and its helicity does not change.

2 linked rings

Trefoil knot

Dual cascade

- Dual cascade in helical quantum turbulence

- Initial Data: ABC flow

- GPE turbulent decay

- Evolutions of energies and helicity

- Evolution of spectra

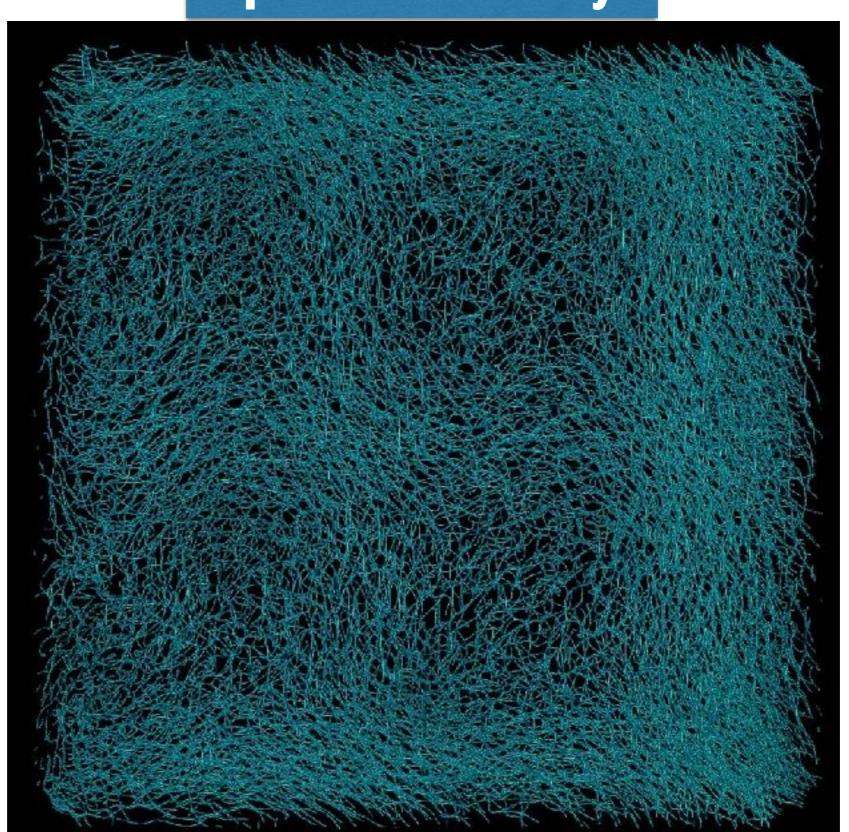- Kelvin waves and large scale structures

ABC initial data

As initial condition we use a superposition of $k = 1$ and $k = 2$ basic ABC flows: $\mathbf{v}_{\text{ABC}} = \mathbf{v}_{\text{ABC}}^{(1)} + \mathbf{v}_{\text{ABC}}^{(2)}$, with

$$\mathbf{v}_{\text{ABC}}^{(k)} = [B\cos(ky) + C\sin(kz)]\,\hat{x} + [C\cos(kz) + A\sin(kx)]\,\hat{y} + [A\cos(kx) + B\sin(ky)]\,\hat{z}, \quad (2)$$

and $(A, B, C) = (0.9, 1, 1.1)/\sqrt{3}$. The basic ABC flow is a 2π-periodic stationary solution of the Euler equation with maximal helicity. To build its quantum version we first take the flow with $B = C = 0$ and use Madelung transformation to obtain a wavefunction

$$\Psi_{A,k}^{x,y,z} = \exp\{i[A\sin(kx)\,m/\hbar]y + i[A\cos(kx)\,m/\hbar]z\},$$

where $[a]$ stands for the nearest integer to a to enforce periodicity. The wavefunction of the quantum ABC flow is then obtained as $\Psi_{\text{ABC}}^{(k)} = \Psi_{A,k}^{x,y,z} \times \Psi_{B,k}^{y,z,x} \times \Psi_{C,k}^{z,x,y}$. Finally, $\Psi_{\text{ABC}} = \Psi_{\text{ABC}}^{(1)} \times \Psi_{\text{ABC}}^{(2)}$ corresponds to the initial flow $\mathbf{v}_{\text{ABC}}$. In practice, to correctly set the initial density with defects along the vortex lines and to correct frustration errors arising from periodicity, following [24, 25] we first evolve Ψ_{ABC} using the advected real Guinzburg-Landau equation [31], whose stationary solutions are solutions of the GPE with minimal emission of acoustic energy.

2048³ ABC initial data with 45000 quanta of helicity
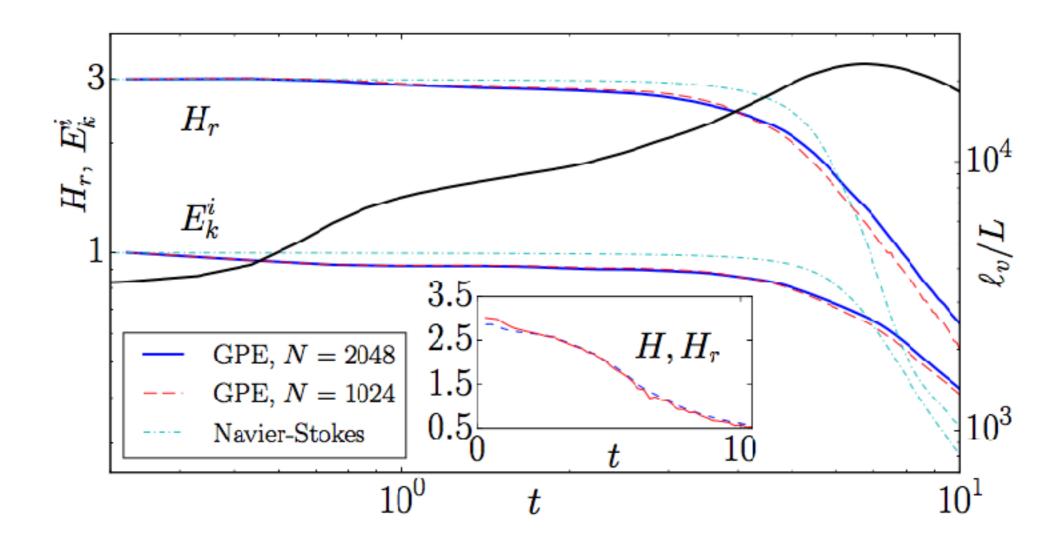
Time-evolution of energy and helicity

FIG. 1. Evolution of the incompressible energy E_k^i and of the regularized helicity H_r in the 1024^3 and 2048^3 GPE runs, and in Navier-Stokes. Note the early "inviscid" phase in which quantities are approximately constant. The solid black line shows the total vortex length in the 2048^3 GPE run. Inset: $H_r(t)$ (dashed blue line) and the nonregularized helicity $H(t)$ (solid red line) in the 2048^3 GPE run.

Dual energy-helicity cascade

$$E(k) \approx \epsilon^{2/3} k^{-5/3}, \qquad H(k) \approx \eta \epsilon^{-1/3} k^{-5/3}, \qquad (3)$$

and with ϵ and η calculated directly using

$$\epsilon = -dE_k^i/dt, \quad \eta = -dH/dt, \qquad (4)$$

A. Brissaud, U. Frisch, J. Leorat, M. Lesieur, and A. Mazure, Phys. Fluids **16**, 1366 (1973).

Dual cascade spectra
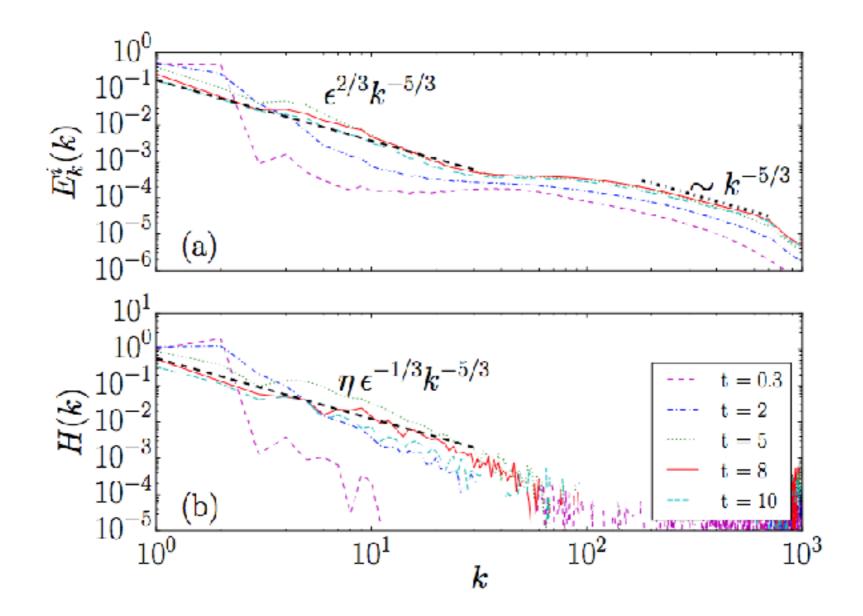
FIG. 2. Spectrum of the (a) incompressible kinetic energy, and (b) helicity in the 2048^3 GPE run. At large scales both follow a scaling compatible with a classical dual cascade (thick dashed lines). At scales smaller than the intervortex scale ($k_\ell \approx 80$) a second range compatible with a Kelvin wave cascade is observed in E_k^i (thick dash-dotted line). The helicity spectrum broadens in time indicating a direct transfer.

compensated helicity spectra
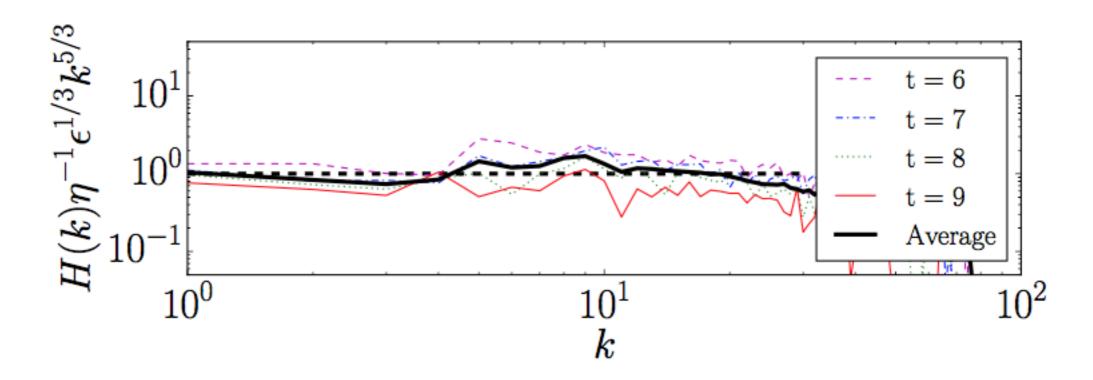
FIG. 3. Compensated helicity spectra in the 2048^3 GPE run. The spectrum is compatible with $\eta\epsilon^{-1/3}k^{-5/3}$ scaling. The time-averaged spectrum is also shown.
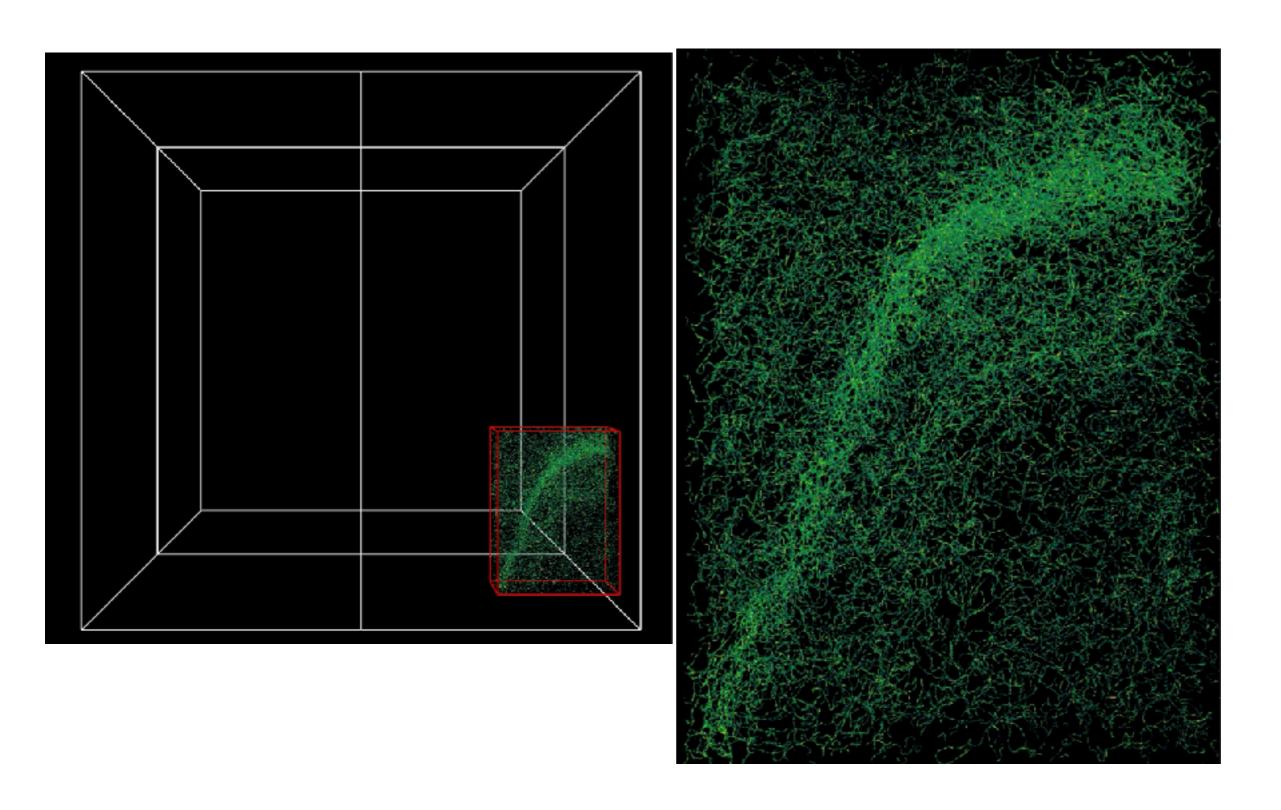
Kelvin waves
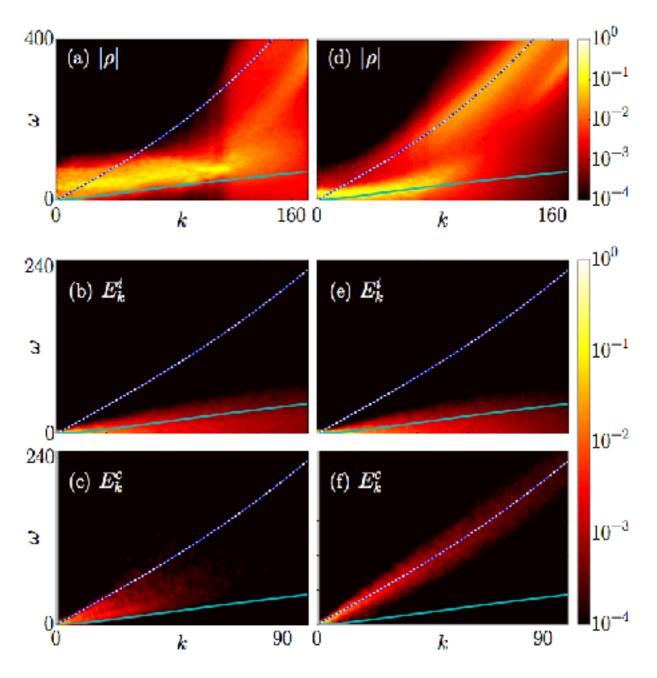
FIG. 4. Spatiotemporal power spectra for the 512^3 GPE run between $t = 0$ and 2 for (a) the mass density ρ, and zooms between $k = 0$ and 100 for (b) the incompressible and (c) compressible velocity. Same for late times ($t \in [8,10]$) are shown in (d), (e), and (f). The solid (green) curve is the dispersion relation of Kelvin waves, while the dotted (white) curve corresponds to sound waves.
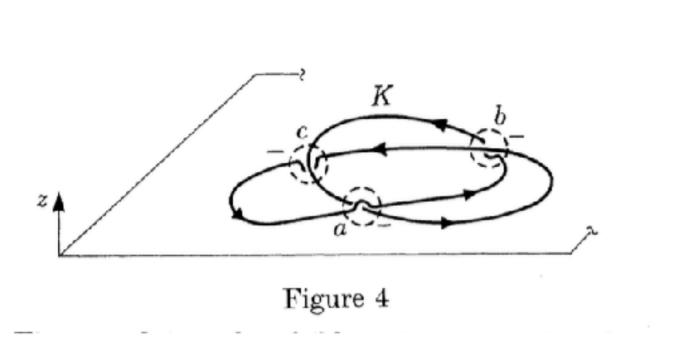
Quantum tornados?

Link with classical vortex tubes
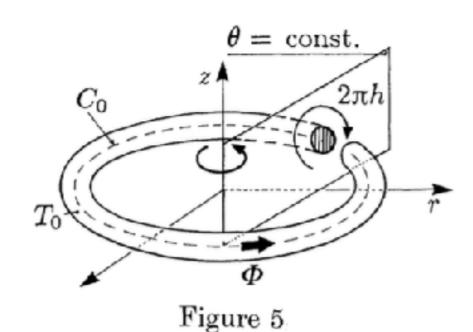
Helicity and the Călugăreanu invariant†

By H. K. Moffatt and Renzo L. Ricca‡

*Department of Applied Mathematics and Theoretical Physics, Silver Street,
Cambridge CB3 9EW, U.K.*

Figure 4

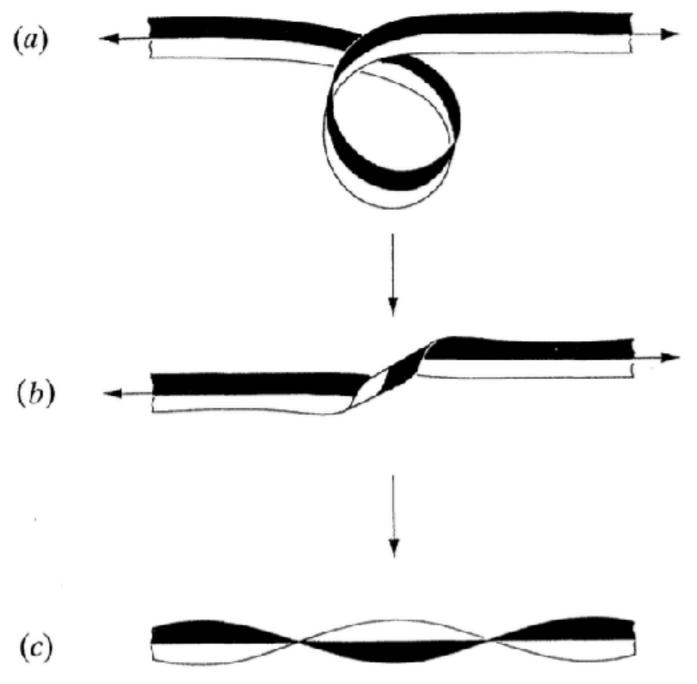Figure 5

Link with classical vortex tubes

Figure 12. (a) Writhe, (b) torsion and (c) twist contributions of a ribbon to the Călugăreanu invariant. If a coiled ribbon is stretched so that its centre-line becomes straight, then the initial torsion of the centre-line is converted to the final twist of the ribbon about its centre-line.
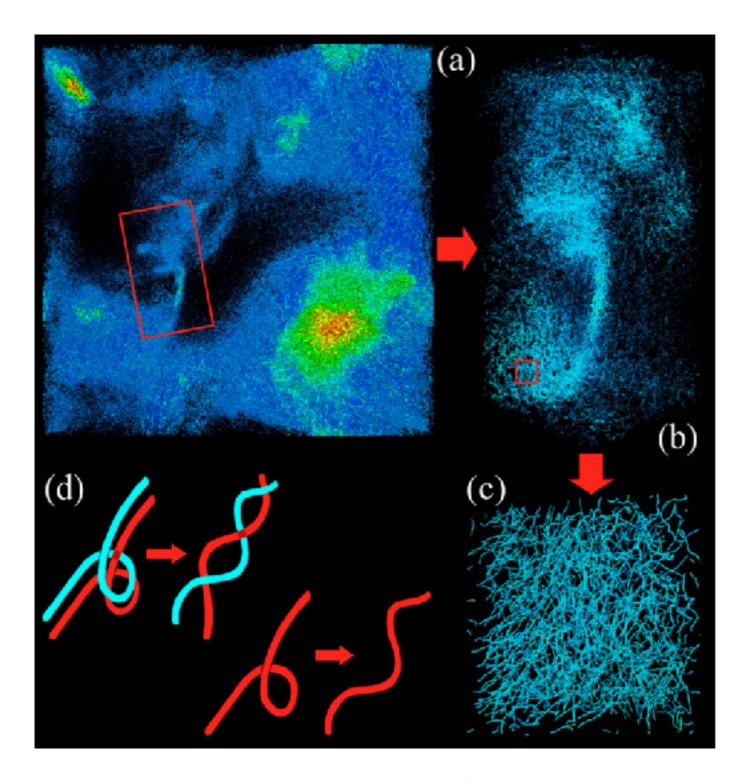
Quantum tornados?

FIG. 5. Three-dimensional rendering of vortex lines at the onset of the decay in the 2048^4 GPE run of (a) a slice of the full box, and successive zooms in (b) and (c) into the regions indicated by the (red) rectangles. (d) Sketch of the transfer of helicity from writhe to twist in a bundle of vortices, and for an individual vortex.

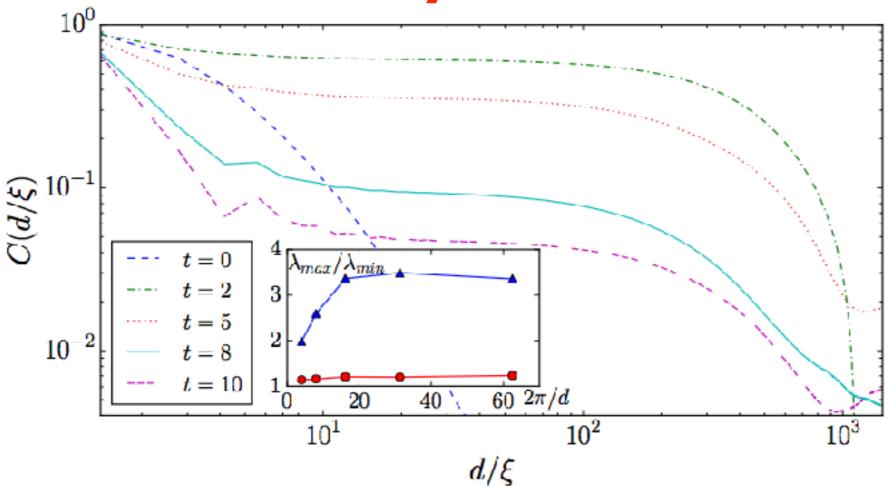# Polarization of vortex bundles and density correlations

FIG. 6. Correlation function of ρ in the 2048^3 GPE run. At $t = 0$ it decays rapidly in units of the healing length ξ, but then quickly develops long-range correlations. Inset: Ratio of eigenvalues $\lambda_{max}/\lambda_{min}$ as a function of $2\pi/d$, with d the size of the box used for the average (blue triangles: regions with structures; red triangles: regions of quiescence).
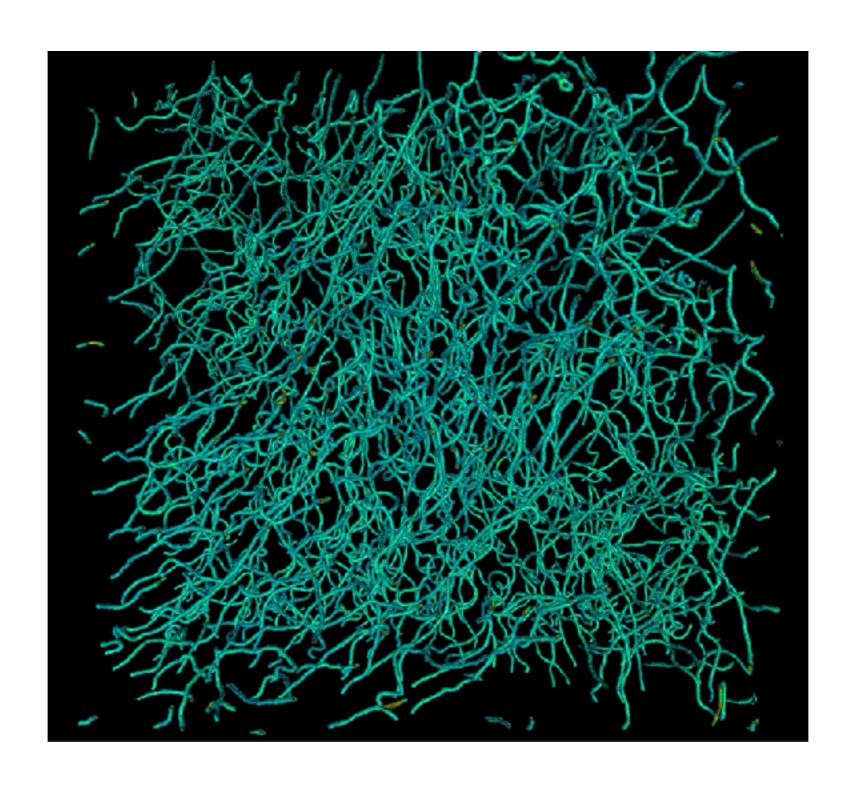
Conclusion

- Turbulence is still an open problem [physically and mathematically]

- It is, perhaps, the most important unsolved problem of nonlinear science

- Spectral truncation allows for (pseudo)dissipative effects

- Self truncation: a new direct statistical approach to PDE's?

Conclusion

- Perhaps turbulence is simpler to resolve starting from GPE rather than Navier-Stokes? The existence of GPE solutions is well established mathematically, see e.g. The Cauchy problem for the Gross–Pitaevskii equation, P. Gérard Ann. I. H. Poincaré – AN 23 (2006) 765–779.

- Statistical mechanics of interacting and reconnecting vortex lines?

- Truncated GPE computations can be used to study finite Temperature effects

Conclusion

- Space-time resolved spectra allow to detect and quantify Kelvin Waves

- Regularized helicity is directly computable from 3D complex wave function field

- Conservation or non-conservation of quantum helicity is an open problem involving not only topological changes but also excitation (and decay) of Kelvin waves

- Dual cascade in helical quantum turbulence

- Polarization and large scale correlations

Thank you!