Wave Turbulence for the Gross-Pitaevskii Equation of a Superfluid

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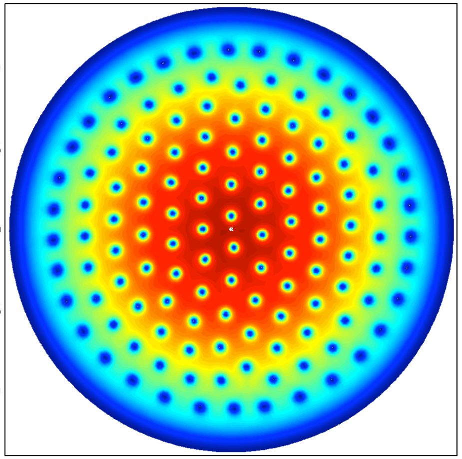
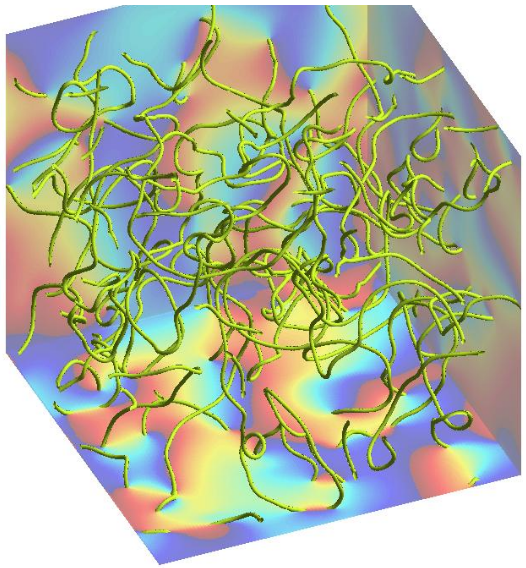
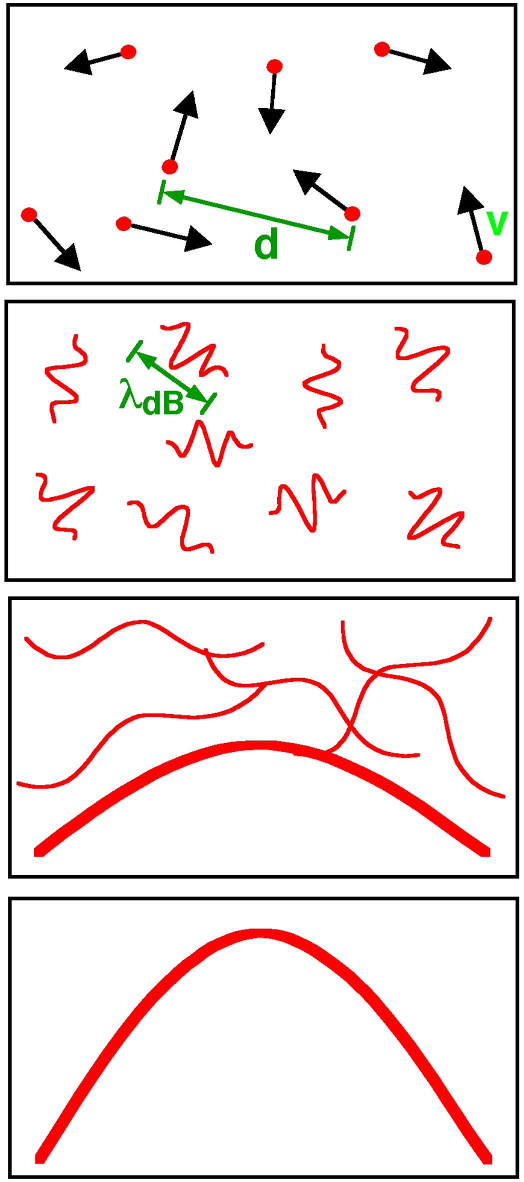




The Leverhulme Trust

Bose-Einstein Condensation?:



High Temperature T:

thermal velocity v

density d^{-3}

"Billiard balls"

Low Temperature T:

De Broglie wavelength

$\lambda_{dB}=h/mv \propto T^{-1/2}$

"Wave packets"

$T=T_{crit}$:

Bose-Einstein Condensation

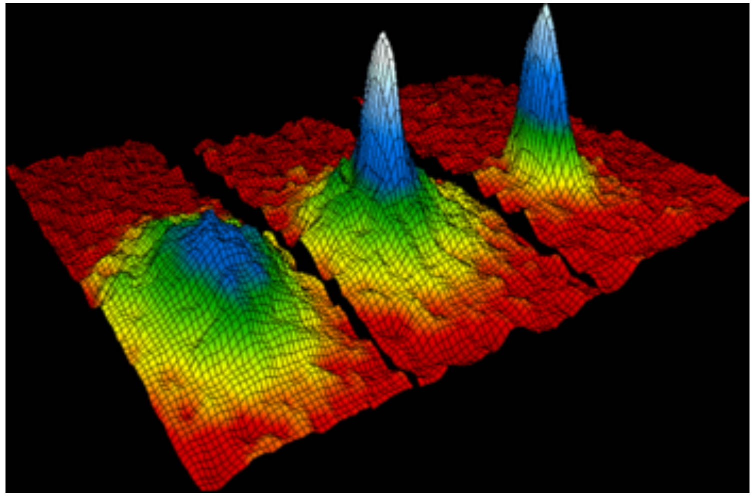
$\lambda_{dB} \approx d$

"Matter wave overlap"

T=0:

Pure Bose condensate

"Giant matter wave"



Velocity distribution of particles in ultracold atomic gas taken from experimental measurements

- Finite-temperature effects always present in atomic BECs
- Need methods to model thermal cloud in condensates

Microscopic Description of the Quantum Gas:

- Our quantum gas is described by many-body wave function $\Psi(\mathbf{x}_1,\cdots,\mathbf{x}_N)$
  - weakly interacting dilute Bose gas
  - s-wave scattering length (a) at low energies

$$i\Psi_t = \hat{H}\Psi, \qquad \hat{H} = \frac{-\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + 2\pi\hbar^2 a \sum_{\substack{i,j=1 \\ i\neq j}}^{N,N}\delta(\mathbf{x}_i - \mathbf{x}_j)$$

- In fully condensed state, bosons are in single particle state
  - we write $\Psi(\mathbf{x}_1,\cdots,\mathbf{x}_N) = \prod_{i=1}^{N}\phi(\mathbf{x}_i),$ where $\int|\phi(\mathbf{x})|^2\,d\mathbf{x} = 1.$

$$H = \int\left(\frac{N\hbar^2}{2m}|\nabla\phi|^2 + \frac{gN(N-1)}{2}|\phi|^4\right)d\mathbf{x} \approx \int\left(\frac{N\hbar^2}{2m}|\nabla\phi|^2 + \frac{gN^2}{2}|\phi|^4\right)d\mathbf{x}, \quad g = 4\pi\hbar^2 a$$

- Introducing the macroscopic wave-function $\psi(\mathbf{x}) = N^{1/2}\phi(\mathbf{x})$ we have

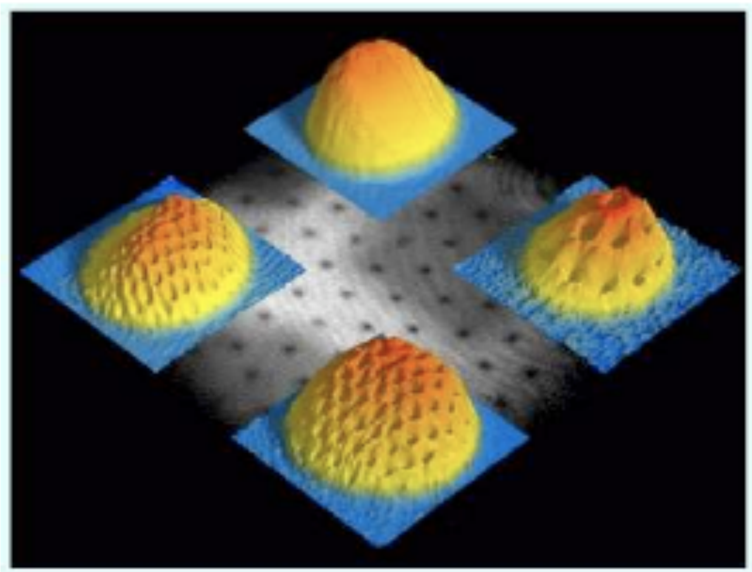
$$H = \int\left(\frac{\hbar^2}{2m}|\nabla\psi|^2 + \frac{g}{2}|\psi|^4\right)d\mathbf{x}$$

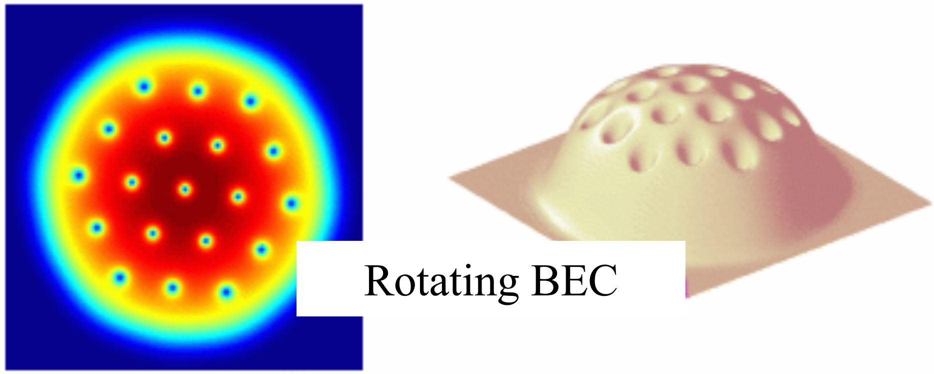
The Gross Pitaevskii Equation:

- The resulting evolution equation is an NLS equation (defocussing type)
- Gross-Pitaevskii equation includes an external trapping potential

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + g\,|\psi|^2\,\psi + V_{ext}\psi\,,$$

- Successfully predicts many experimental observations
  - (e.g. quantized vortex lattice, grey/dark solitons, etc.)





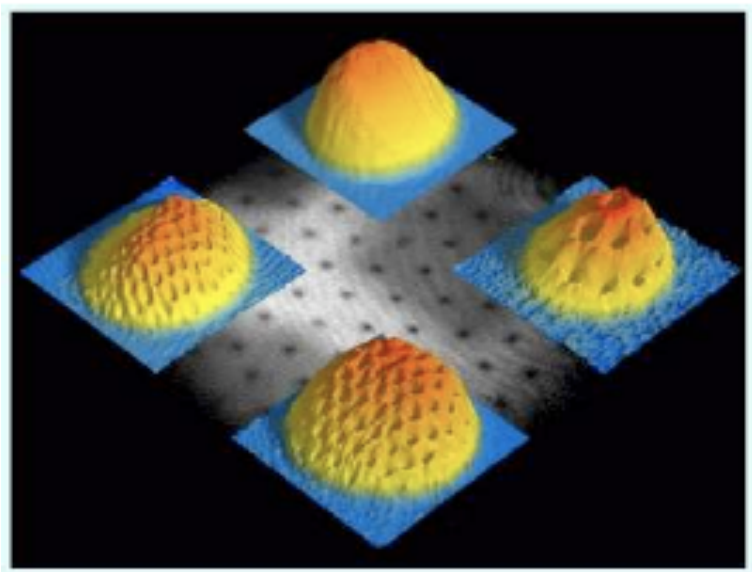
Rotating BEC

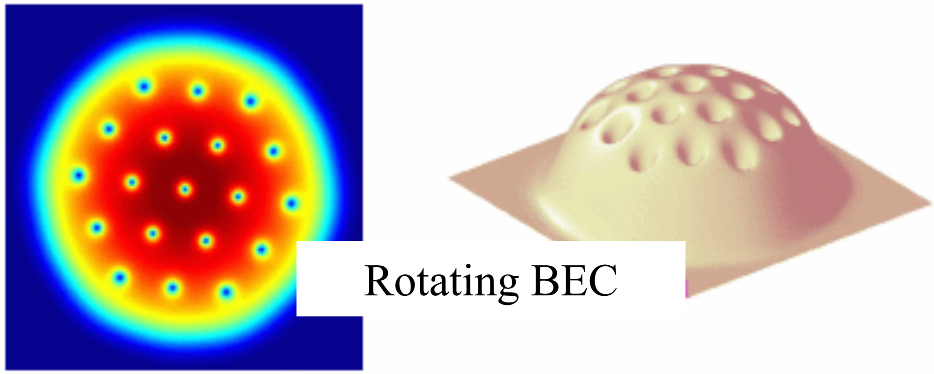
The Gross Pitaevskii Equation:

- The resulting evolution equation is an NLS equation (defocussing type)
- Gross-Pitaevskii equation includes an external trapping potential

$$i\partial_t \psi = -\nabla^2 \psi + \gamma \mid \psi \mid^2 \psi + V_{\mathrm{ext}} \psi \, ,$$

- Successfully predicts many experimental observations
  - (e.g. quantized vortex lattice, grey/dark solitons, etc.)





Rotating BEC

Classical Field Approximation:

- GP equation accurately describes dynamics of condensate at zero temperature
  - close to ground state energy
- Alternative derivation is to start with second quantized form of Hamiltonian

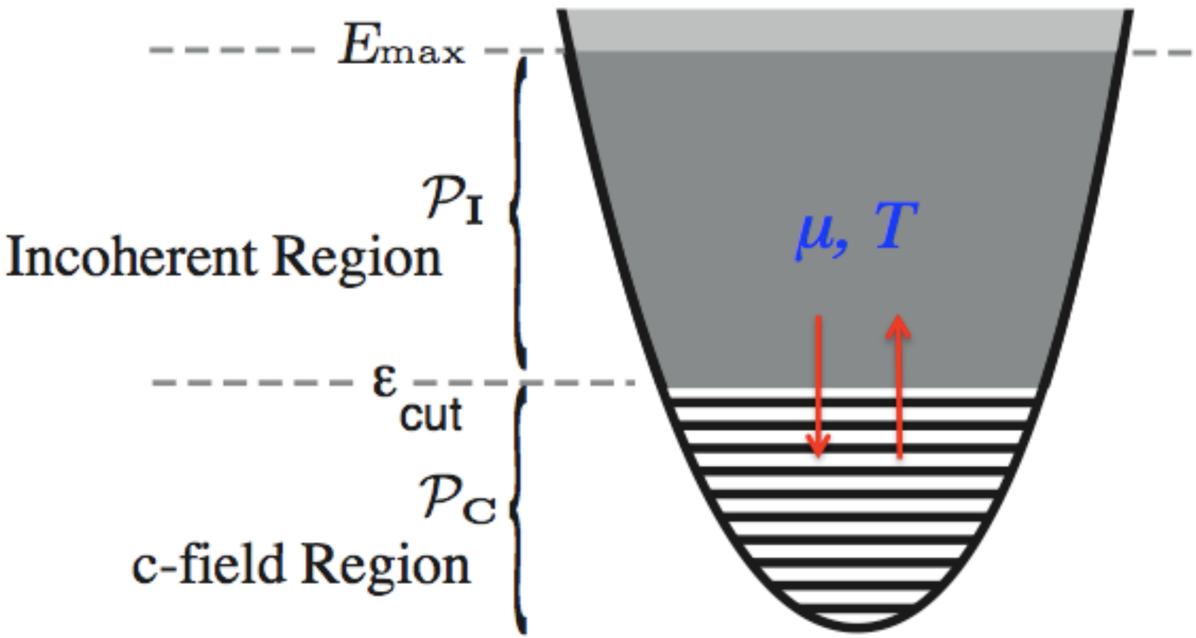
$$\hat{H} = \int \hat{\psi}^{\dagger}(\mathbf{x}) \left\{ \frac{-\hbar^2 \nabla^2}{2m} + V_{ext}(\mathbf{x}) \right\} \hat{\psi}(\mathbf{x}) d\mathbf{x} + \frac{g}{2} \int d\mathbf{x} \int d\mathbf{x}' \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}^{\dagger}(\mathbf{x}') \delta(\mathbf{x} - \mathbf{x}') \hat{\psi}(\mathbf{x}) \hat{\psi}(\mathbf{x}'),$$

- Decompose into basis of coherent states such that

$$\widehat{\Psi}(\mathbf{x},t) = \sum \hat{a}_k(t) \varphi_k(\mathbf{x}) \rightarrow \psi(\mathbf{x},t) \approx \sum \alpha_k(t) \varphi_k(\mathbf{x}), \quad \hat{a}_k^{\dagger} \hat{a}_k \left| n_k \right\rangle = n_k \left| n_k \right\rangle, \quad n_k \gg 1$$

- Retain *only* modes that are macroscopically occupied (*no quantum fluctuations*)
- At leading order, we obtain GP equation for the classical field ψ
  - so GP equation includes finite temperature effects (at least qualitatively)

- BEC + low energy excitations are treated as a classical field
- High energy atoms are treated as a thermal bath
  - in simplest approximation, we neglect coupling to thermal bath



- The GP equation for classical fields has two integrals of motion
  - number of particles and total energy

$$N = \int |\psi|^2 \, d\mathbf{x} \qquad H = \int \left(|\nabla \psi|^2 + \frac{\gamma}{2} |\psi|^4 + V_{ext} |\psi|^2 \right) d\mathbf{x}$$

Derivation of Kinetic Description:

- First regime (*assume no condensate*)
- If N/V<1, then $|\psi|^4 \sim \epsilon^2 |\psi|^2, \quad \epsilon \ll 1$
- Fourier transforming GP equation ($A_{\mathbf{k}}$ are Fourier coefficients)

$$\partial_t A_{\mathbf{k}} + ik^2 A_{\mathbf{k}} = \epsilon^2 \frac{-i}{(2\pi)^3} \int A_{\mathbf{k}_1}{}^* A_{\mathbf{k}_2} A_{\mathbf{k}_3} \delta(\mathbf{k}+\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3) d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3$$

- Rewrite in interaction picture $\quad a_{\mathbf{k}}(t) = A_{\mathbf{k}}(t)\exp^{ik^2 t}$
- Combine with equation for complex conjugate and average $\quad M_2(\mathbf{p}_1;\mathbf{p}_2) = \left\langle a_{\mathbf{p}_1} a^*_{\mathbf{p}_2} \right\rangle$

$$M_2(\mathbf{p}_1;\mathbf{p}_2)(t) = \frac{i\epsilon^2}{(2\pi)^6} \int \left[\int_0^t \mathrm{e}^{i(k_2^2+k_3^2-p_2^2-k_1^2)} M_4(\mathbf{p}_1,\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)(\tau) d\tau \right] \delta(\mathbf{p}_2+\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3) d\mathbf{k}_{123}$$
$$- \frac{i\epsilon^2}{(2\pi)^6} \int \left[\int_0^t \mathrm{e}^{i(p_1^2+k_1^2-k_2^2-k_3^2)} M_4(\mathbf{k}_2,\mathbf{k}_3,\mathbf{p}_2,\mathbf{k}_1)(\tau) d\tau \right] \delta(\mathbf{p}_1+\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3) d\mathbf{k}_{123}$$

Kinetic Equation for Four-wave Resonances:

- After closing equations for moments using Wick's decomposition

$$\frac{\partial n_{\mathbf{p}_1}}{\partial t} = \epsilon^4 \frac{4\pi}{(2\pi)^6} \int \left[n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_3} + n_{\mathbf{p}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_3} - n_{\mathbf{p}_1} n_{\mathbf{k}1} n_{\mathbf{k}_3} - n_{\mathbf{p}_1} n_{\mathbf{k}1} n_{\mathbf{k}_2} \right]$$
$$\times \delta(p_1^2 + k_1^2 - k_2^2 - k_3^2) \delta(\mathbf{p}_1 + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) d\mathbf{k}_{123}$$

- Equation admits equilibrium solutions given by
  - equi-partition of particle number $n_{\mathbf{k}} = constant$
  - equipartition of energy $n_{\mathbf{k}} = \dfrac{T}{k^2 - \mu}$

- Solution realized in practice is one that maximises entropy

$$S = \int \ln(n_{\mathbf{k}})\, d\mathbf{k}$$

- Rayleigh Jeans distribution is most relevant
  - two free parameters: T – 'temperature' and μ – 'chemical potential'

- Note that this is the classical limit of the *quantum* kinetic equation when $n_{\mathbf{k}} >> 1$

$$\frac{\partial n_{\mathbf{p}_1}}{\partial t} = \epsilon^4 \frac{4\pi}{(2\pi)^6} \int \Big[(n_{\mathbf{p}_1} + 1)(n_{\mathbf{k}1} + 1) n_{\mathbf{k}2} n_{\mathbf{k}3} - n_{\mathbf{p}_1} n_{\mathbf{k}1} (n_{\mathbf{k}2} + 1)(n_{\mathbf{k}_3} + 1) \Big]$$
$$\times \delta(p_1^2 + k_1^2 - k_2^2 - k_3^2)\delta(\mathbf{p}_1 + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) d\mathbf{k}_{123}$$

- First derived by Nordheim (1928)

- Solution in this case given by Bose-Einstein distribution
  - Rayleigh-Jeans is corresponding classical limit

$$n_{\mathbf{k}} = \frac{1}{e^{(k^2 - \mu)/T} - 1}$$

Three-Wave Kinetic Equation:

- Second regime (*with strong condensate*)
- Begin by linearising about condensate solution
  - write wavefunction as $\psi = \psi_o + \psi'$ $\quad A_k = \left[\sqrt{n_o}\delta(\mathbf{k}) + \tilde{A}_{\mathbf{k}}(t)\right]e^{-in_o t}$
- Substituting into GP and Fourier transforming we find

$$\partial_t \tilde{A}_{\mathbf{k}} + i(k^2 + 2n_o)\tilde{A}_{\mathbf{k}} + in_o\tilde{A}^*_{\mathbf{k}} = \epsilon^2 \frac{-i}{(2\pi)^3}\int \tilde{A}_{\mathbf{k}_1}{}^* \tilde{A}_{\mathbf{k}_2}\tilde{A}_{\mathbf{k}_3}\delta(\mathbf{k}+\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3)d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3$$

- Resulting equation has non-diagonal leading order term.
- Diagonalise using (Bogoliubov transformation)
- Leading order behaviour of resulting equation

$$\partial_t \tilde{a}_{\mathbf{k}} = -i\Omega(k)\tilde{a}(t) + \cdots, \qquad \Omega(k) = k\sqrt{k^2 + 2\gamma(n_o / V)}$$

- Using weak turbulence theory we can then derive a closed kinetic equation for the thermal excitations

$$\frac{\partial \tilde{n}_{\mathbf{k}}}{\partial t} = \pi \int \left| V_{\mathbf{k},\mathbf{k}_1,\mathbf{k}_2} \right|^2 \left(\tilde{n}_{\mathbf{k}_1} \tilde{n}_{\mathbf{k}_2} - \tilde{n}_{\mathbf{k}} \tilde{n}_{\mathbf{k}_1} - \tilde{n}_{\mathbf{k}} \tilde{n}_{\mathbf{k}_2} \right) \delta(\Omega_{\mathbf{k}} - \Omega_{\mathbf{k}_1} - \Omega_{\mathbf{k}_2}) \delta(\mathbf{k} - \mathbf{k}_1 - \mathbf{k}_2) d\mathbf{k}_{12}$$
$$- \pi \int \left| V_{\mathbf{k}_1,\mathbf{k},\mathbf{k}_2} \right|^2 \left(\tilde{n}_{\mathbf{k}_1} \tilde{n}_{\mathbf{k}_2} + \tilde{n}_{\mathbf{k}} \tilde{n}_{\mathbf{k}_1} - \tilde{n}_{\mathbf{k}} \tilde{n}_{\mathbf{k}_2} \right) \delta(\Omega_{\mathbf{k}_1} - \Omega_{\mathbf{k}} - \Omega_{\mathbf{k}_2}) \delta(\mathbf{k}_1 - \mathbf{k} - \mathbf{k}_2) d\mathbf{k}_{12}$$
$$- \pi \int \left| V_{\mathbf{k}_2,\mathbf{k},\mathbf{k}_1} \right|^2 \left(\tilde{n}_{\mathbf{k}_1} \tilde{n}_{\mathbf{k}_2} + \tilde{n}_{\mathbf{k}} \tilde{n}_{\mathbf{k}_2} - \tilde{n}_{\mathbf{k}} \tilde{n}_{\mathbf{k}_1} \right) \delta(\Omega_{\mathbf{k}_2} - \Omega_{\mathbf{k}} - \Omega_{\mathbf{k}_1}) \delta(\mathbf{k}_2 - \mathbf{k} - \mathbf{k}_1) d\mathbf{k}_{12}$$

  - where $|V_{k_1,k_2,k_3}|$ denote coefficients of the integral

- Collision integral describes *three-wave interactions*

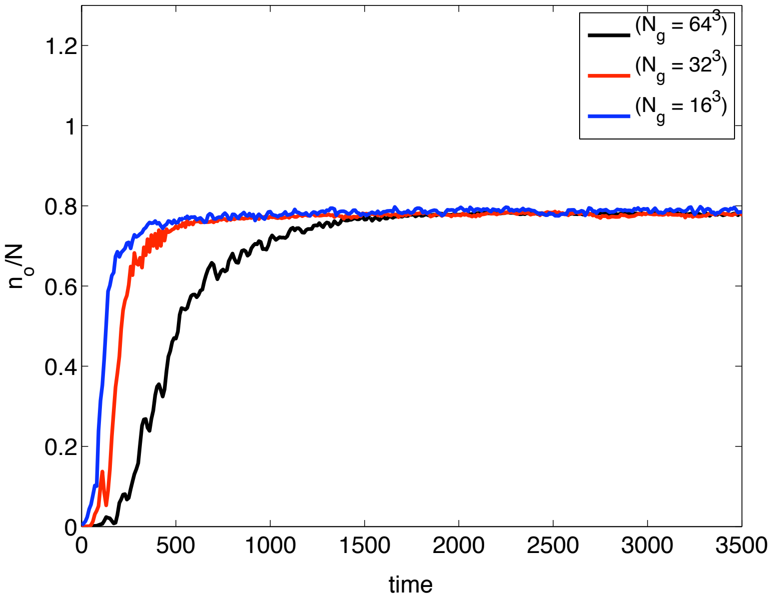
- This equation admits a one parameter family of solutions

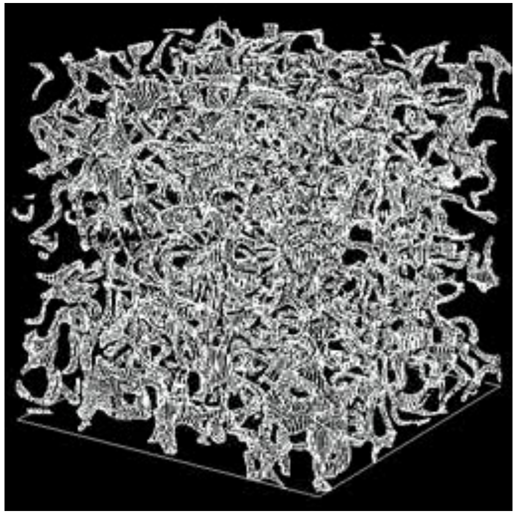
$$n_{\mathbf{k}} = \frac{T}{k\sqrt{k^2 + 2\gamma(n_o / V)}}$$

Numerical solution of NLS Equation at High Energies:

- Can model condensate formation from strongly non-equilibrium initial state
  - simulates evolution of system following rapid quench below phase transition temperature

- For homogenous system in periodic domain
  - particles initially distributed uniformly in momentum space

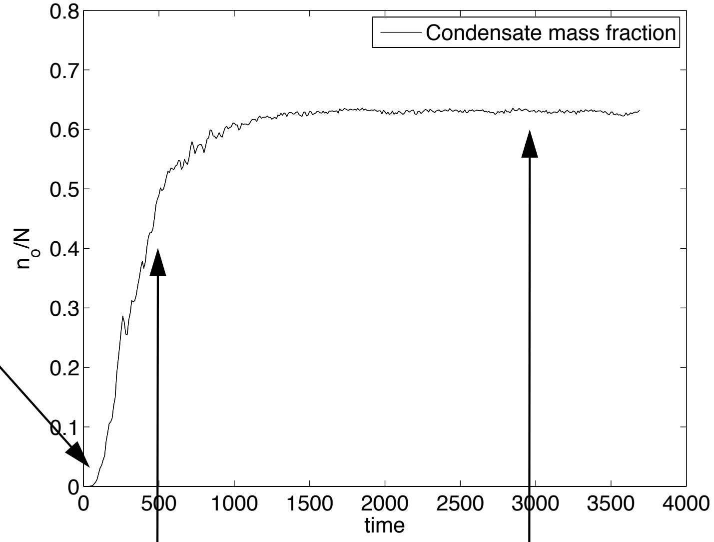




Berloff and Svistunov (2002)

- Accumulation of particles in zero momentum ground state observed
  - formation of a condensate

Relation to Kinetic Equations:



- Before condensate formation, 4 wave scattering dominates

- Low energies → breakdown of random phase approximation
  - phase coherence at low wavenumbers

- Leads to condensate growth
  - kinetics described by combination of 3/ 4 wave processes
  - intermediate regime → strong turbulence

- Final stage
  - 3 wave processes dominate
  - weak thermal excitations on strong condensate

Properties at Thermal Equilibrium:

- System thermalises at long times
  - what is equilibrium state as function of T?

- Use integrals of motion with equilibrium distributions
  - simulations in finite domain
  - consider discrete spectrum for consistency

$$N = n_o + \sum_k{}' \langle a_k a_k^* \rangle = n_o + \sum_k{}' \frac{(k^2 + \gamma n_o / V)}{k\sqrt{k^2 + 2\gamma n_o / V}} \tilde{n}_k$$

$$= n_o + \sum_k{}' \frac{T(k^2 + \gamma n_o / V)}{\Omega^2(k)}$$

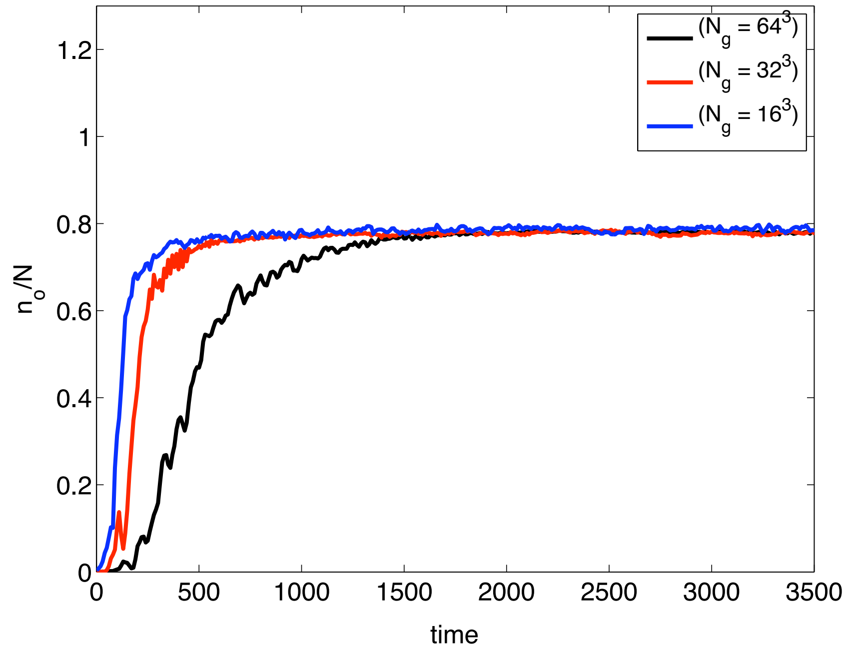
$$H = \frac{1}{2V}\left[N^2 + (N - n_o)^2\right] + T\sum_k{}' 1$$

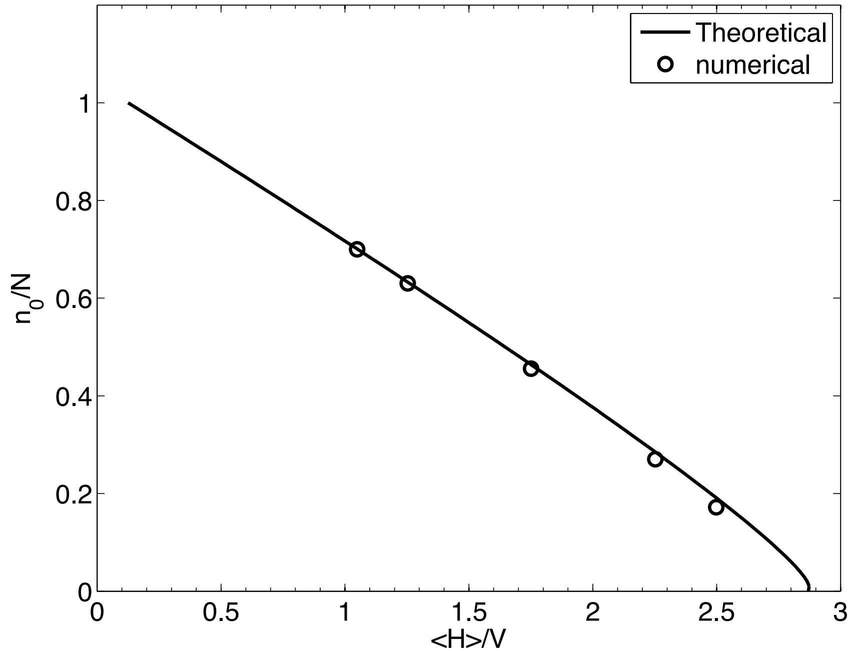
- We have two equations for n_o and T
  - determine $n_o(T)$

- Numerical simulations performed with different system size but constant number density
  - relaxation depends on size of system
  - but final state function of number density

- Simulation parameter
  - N/V=0.5

- Theory shows excellent agreement with numerical results





Extension to Two-Component Nonlinear Schrödinger Equation:

- We have extended results to two component system
  - governed by coupled NLS equations

- In non-dimensional form, equations given by

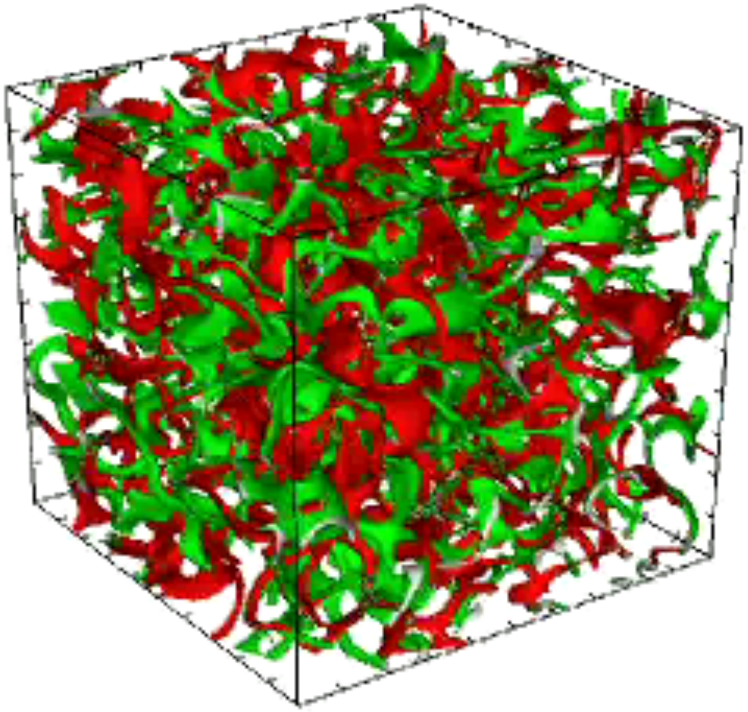
$$i\partial_t \psi_1 = -\nabla^2 \psi_1 + |\psi_1|^2 \psi_1 + \alpha |\psi_2|^2 \psi_1,$$
$$i\partial_t \psi_2 = -\nabla^2 \psi_2 + |\psi_2|^2 \psi_2 + \alpha |\psi_1|^2 \psi_2$$

- Components are in phase mixing regime for $0<\alpha<1$
  - occupy same region in space

- Kinetic description can be used in this case
  - ground states correspond to k=0 modes

Numerical Results for Two-Component System:

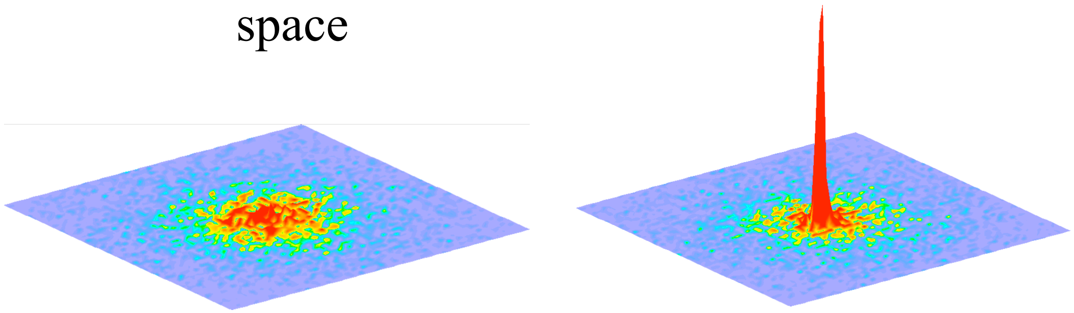
$$i\partial_t \psi_1 = -\nabla^2 \psi_1 + |\psi_1|^2 \psi_1 + \alpha |\psi_2|^2 \psi_1,$$
$$i\partial_t \psi_2 = -\nabla^2 \psi_2 + |\psi_2|^2 \psi_2 + \alpha |\psi_1|^2 \psi_2$$



- For intermediate energies, only one component condenses

(HS & Berloff, Physica D, 2009)

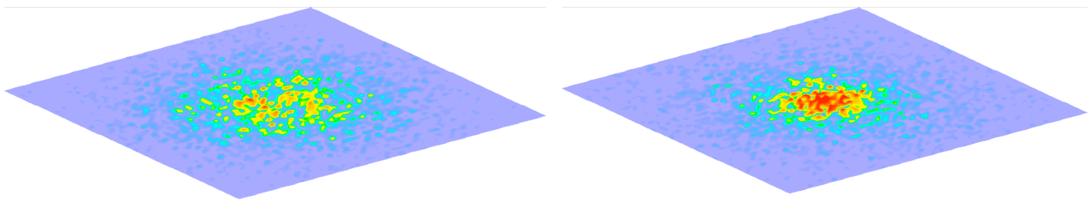
Particle distribution in momentum space



(a) t =100

(b) t =600

First component



(a) t =100

(b) t =600

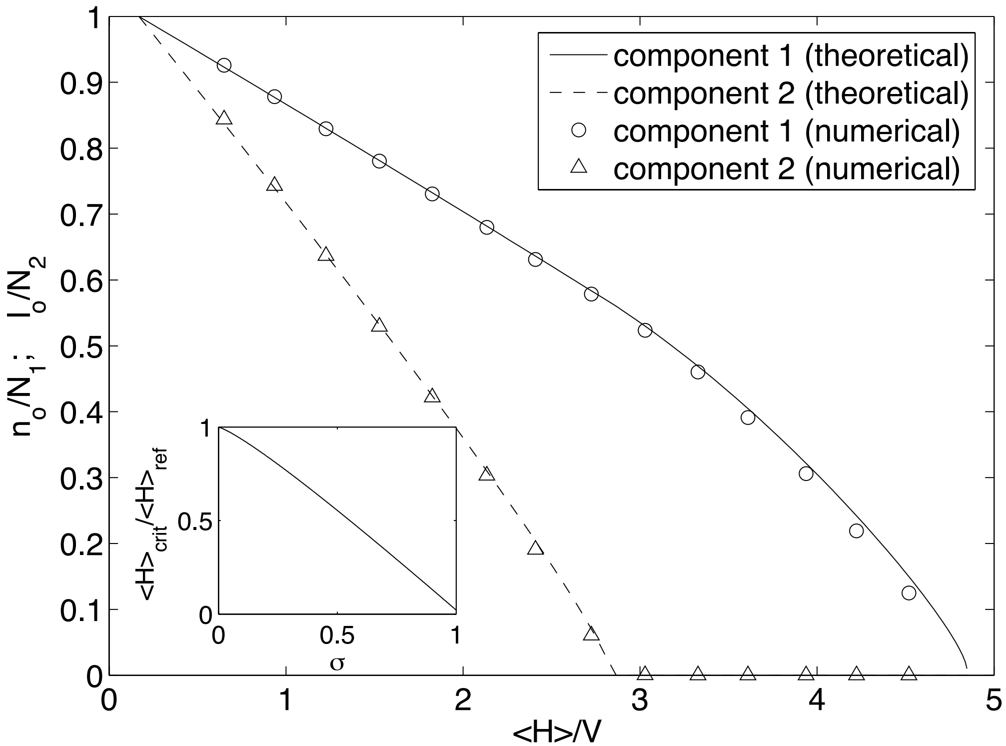
Second component

Determination of Equilibrium State:

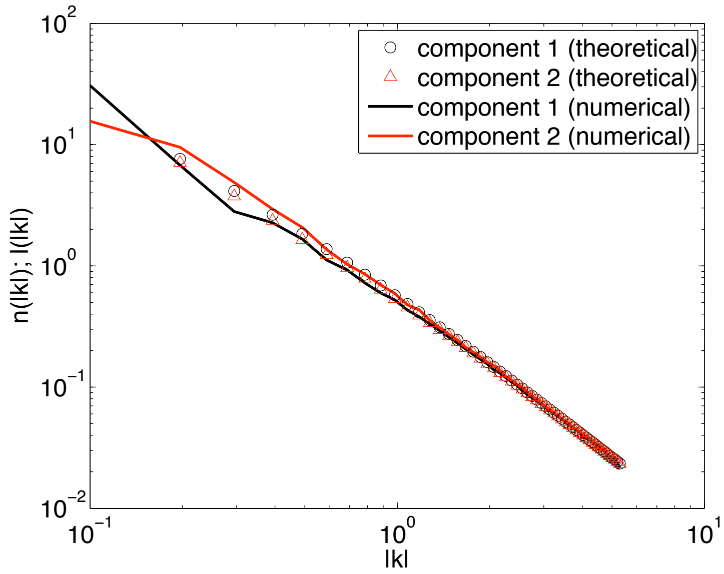
- We can compute equilibrium properties of system from constants of motion

$$N_1 = \int |\psi_1|^2 \, d\mathbf{x}, \quad N_2 = \int |\psi_2|^2 \, d\mathbf{x}$$

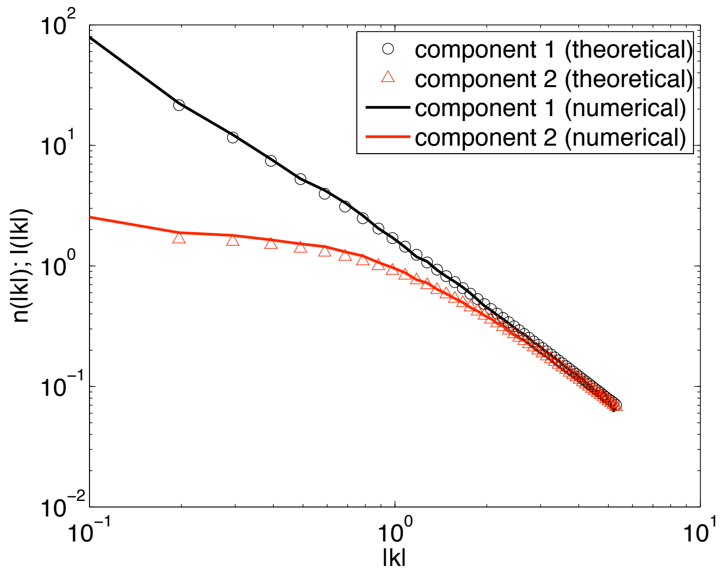
$$H = \int \left(\sum_{i=1}^{2} \left[|\nabla \psi_i|^2 + \frac{1}{2} |\psi_i|^4 \right] + \alpha |\psi_1|^2 |\psi_2|^2 \right) d\mathbf{x}$$



Distribution of spectral number densities



Both components condensed



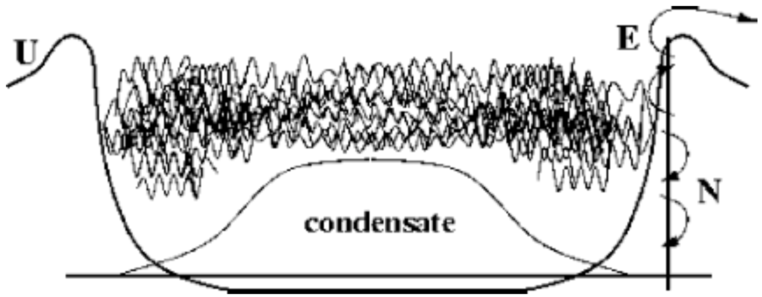
One component condensed

Condensates in a Trap:

- Homogenous Bose gas oversimplified
- How can we extend to an inhomogeneous system?
  - relevant to a BEC in a trap

$$i\partial_t \psi = -\nabla^2 \psi + \gamma |\psi|^2 \psi + V_{ext}\psi ,$$

- Global Fourier transform inapplicable
- Many experiments are in Thomas-Fermi regime
  - Laplacian term (kinetic energy) small
  - smooth potential
- Scale separation between excitations/ condensate
  - excitations (~ l) on top of condensate (~ L)
  - small parameter ε ~ l/L <<1
- Generalize equations to wave-packets



Lvov et al. 2001

Wavepacket Dynamics:

- Linear dynamics governed by wavepacket trajectories

$$D_t = \partial_t + \dot{\mathbf{x}}\cdot\nabla + \dot{\mathbf{k}}\cdot\partial_{\mathbf{k}}, \qquad \dot{\mathbf{x}} = \partial_{\mathbf{k}}\omega, \qquad \dot{\mathbf{k}} = -\nabla\omega$$

- Outside condensate
  - n corresponds to local atomic modes

$$D_t n(\mathbf{x},\mathbf{k},t) = 0, \qquad \omega = k^2 + V_{ext}(\mathbf{x},t)$$

(Ehrenfest theorem in quantum mechanics)

- Inside condensate
  - $\tilde{n}$ corresponds to local Bogoliubov modes

$$D_t \tilde{n}(\mathbf{x},\mathbf{k},t) = 0, \qquad \omega = k\sqrt{k^2 + 2\gamma(n_o/V)}$$

(Local Bogoliubov dispersion relation)

- Matching region is more subtle
  - will not consider here!

Kinetic Equations in Inhomogeneous BECs:

- Outside condensate

$$D_t n_k = C\int n_k n_1 n_2 n_3 \left(\frac{1}{n_k}+\frac{1}{n_1}-\frac{1}{n_2}-\frac{1}{n_3}\right)\delta(\mathbf{k}+\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3)$$
$$\times\,\delta(\omega_k(\mathbf{x})+\omega_1(\mathbf{x})-\omega_2(\mathbf{x})-\omega_3(\mathbf{x}))d\mathbf{k}_{123}$$

  - equilibrium solution $$n(\mathbf{k},\mathbf{x}) = \frac{T}{k^2+V_{ext}(\mathbf{x})-\mu}$$

- Inside condensate

$$D_t \tilde{n}_k = \pi\int \left|V_{\mathbf{k},\mathbf{k}_1,\mathbf{k}_2}\right|^2 \left(\tilde{n}_{\mathbf{k}_1}\tilde{n}_{\mathbf{k}_2}-\tilde{n}_{\mathbf{k}}\tilde{n}_{\mathbf{k}_1}-\tilde{n}_{\mathbf{k}}\tilde{n}_{\mathbf{k}_2}\right)\delta(\Omega_{\mathbf{k}}-\Omega_{\mathbf{k}_1}-\Omega_{\mathbf{k}_2})\delta(\mathbf{k}-\mathbf{k}_1-\mathbf{k}_2)d\mathbf{k}_{12}$$
$$-\pi\int \left|V_{\mathbf{k}_1,\mathbf{k},\mathbf{k}_2}\right|^2 \left(\tilde{n}_{\mathbf{k}_1}\tilde{n}_{\mathbf{k}_2}+\tilde{n}_{\mathbf{k}}\tilde{n}_{\mathbf{k}_1}-\tilde{n}_{\mathbf{k}}\tilde{n}_{\mathbf{k}_2}\right)\delta(\Omega_{\mathbf{k}_1}-\Omega_{\mathbf{k}}-\Omega_{\mathbf{k}_2})\delta(\mathbf{k}_1-\mathbf{k}-\mathbf{k}_2)d\mathbf{k}_{12}$$
$$-\pi\int \left|V_{\mathbf{k}_2,\mathbf{k},\mathbf{k}_1}\right|^2 \left(\tilde{n}_{\mathbf{k}_1}\tilde{n}_{\mathbf{k}_2}+\tilde{n}_{\mathbf{k}}\tilde{n}_{\mathbf{k}_2}-\tilde{n}_{\mathbf{k}}\tilde{n}_{\mathbf{k}_1}\right)\delta(\Omega_{\mathbf{k}_2}-\Omega_{\mathbf{k}}-\Omega_{\mathbf{k}_1})\delta(\mathbf{k}_2-\mathbf{k}-\mathbf{k}_1)d\mathbf{k}_{12}$$

  - equilibrium solution $$\tilde{n}(\mathbf{k},\mathbf{x}) = \frac{T}{\Omega(\mathbf{k},\mathbf{x})} = \frac{T}{k\sqrt{k^2+2\gamma(n_o/V)}}$$

- Thermal cloud maximum at edge of condensate

Numerical Modelling of Trapped BEC:

- A key feature of any classical field model of a finite temperature BEC is that it suffers from an ultraviolet catastrophe

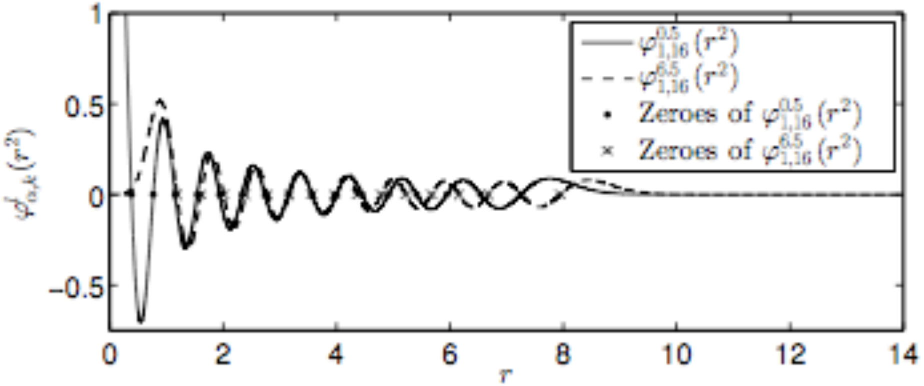
- In numerical simulations this is regularised by numerical discretisation
  - e.g. grid spacing in finite difference schemes
  - mode truncation in spectral methods

- In order to faithfully represent the macroscopically occupied modes, need to truncate the basis
  - retain modes up to energies where Bose-Einstein and Rayleigh-Jeans distributions diverge
  - this criterion is based on obtaining the correct equilibrium properties
  - BUT details of non-equilibrium relaxation can depend on this

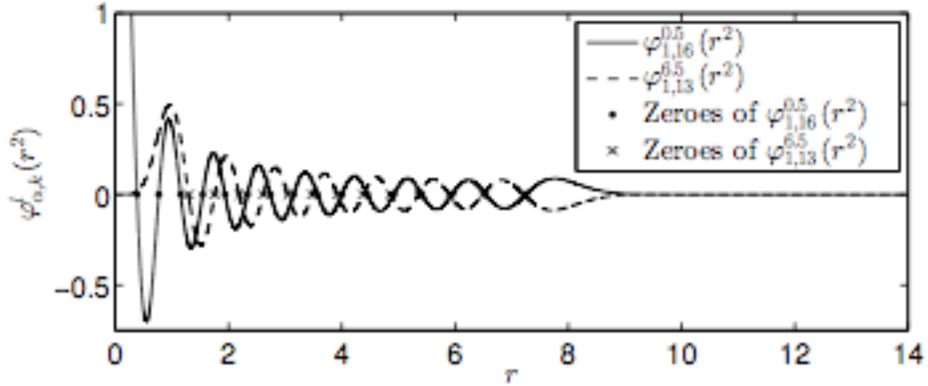
- Motivates a spectral numerical scheme for direct control over energy cut-off

Generalized Laguerre Basis:

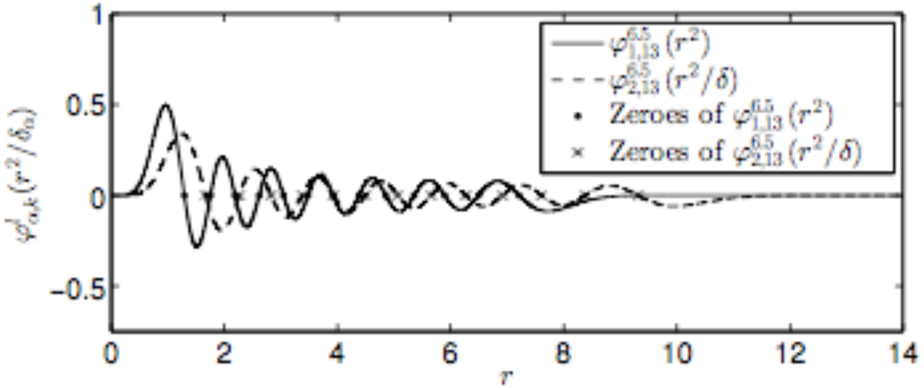
(HS, J. Comp. Phys, **258**, 185, 2014)



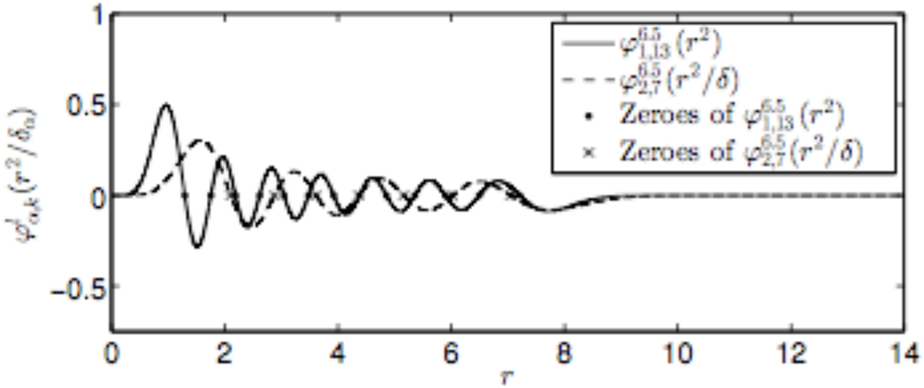
(a) Profiles and zeroes of polynomials for component 1 ($\delta_1 = 1$) corresponding to $\varphi^{0.5}_{1,16}(r^2)$ and $\varphi^{6.5}_{1,16}(r^2)$.



(b) Profiles and zeroes of polynomials for component 1 ($\delta_1 = 1$) corresponding to $\varphi^{0.5}_{1,16}(r^2)$ and $\varphi^{6.5}_{1,13}(r^2)$.



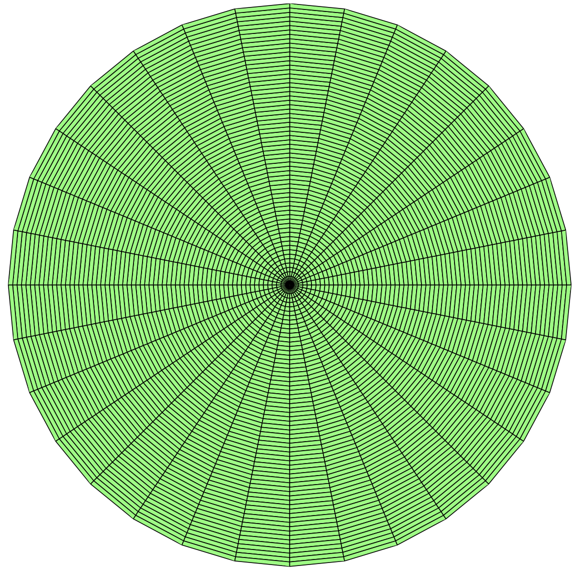
(c) Profiles and zeroes of polynomials for components 1 ($\delta_1 = 1$) and 2 ($\delta_2 = \delta = 1.667$) for $\varphi^{6.5}_{1,13}(r^2)$ and $\varphi^{6.5}_{2,13}(r^2/\delta)$.



(d) Profiles and zeroes of polynomials for components 1 ($\delta_1 = 1$) and 2 ($\delta_2 = \delta = 1.667$) for $\varphi^{6.5}_{1,13}(r^2)$ and $\varphi^{6.5}_{2,7}(r^2/\delta)$.

Figure 2: Comparison of different generalised-Laguerre polynomials $\varphi^{l+0.5}_{\alpha,k}(r^2/\delta_\alpha)$ of degree k and order l for component α in 3D.

Numerical Simulations of Trapped BEC:

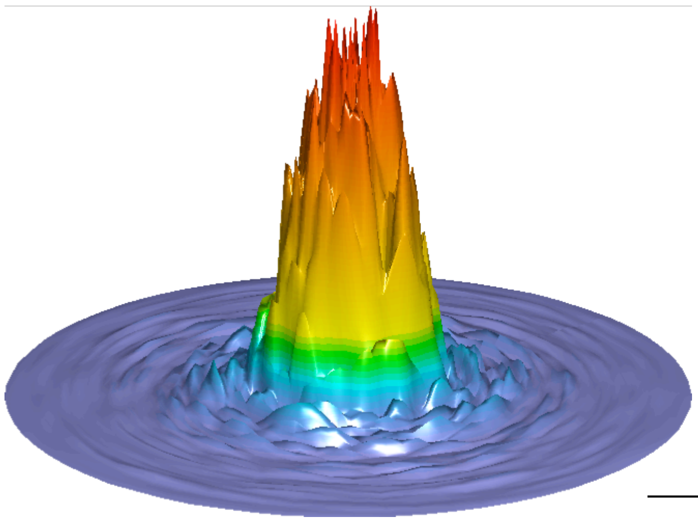


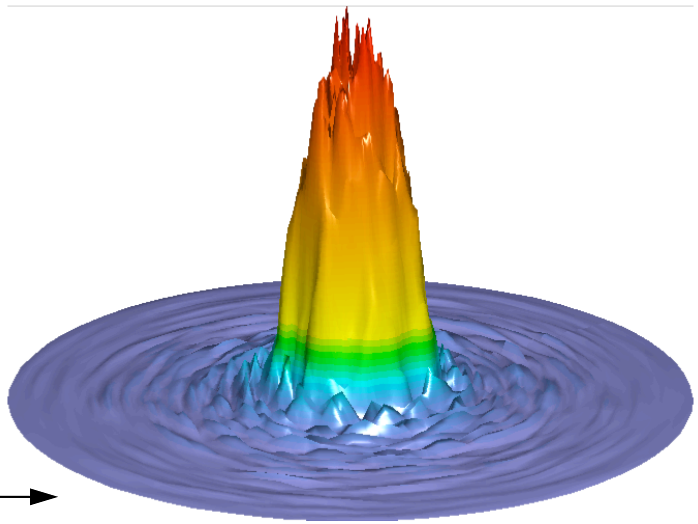
- We consider spherically symmetric harmonic trap

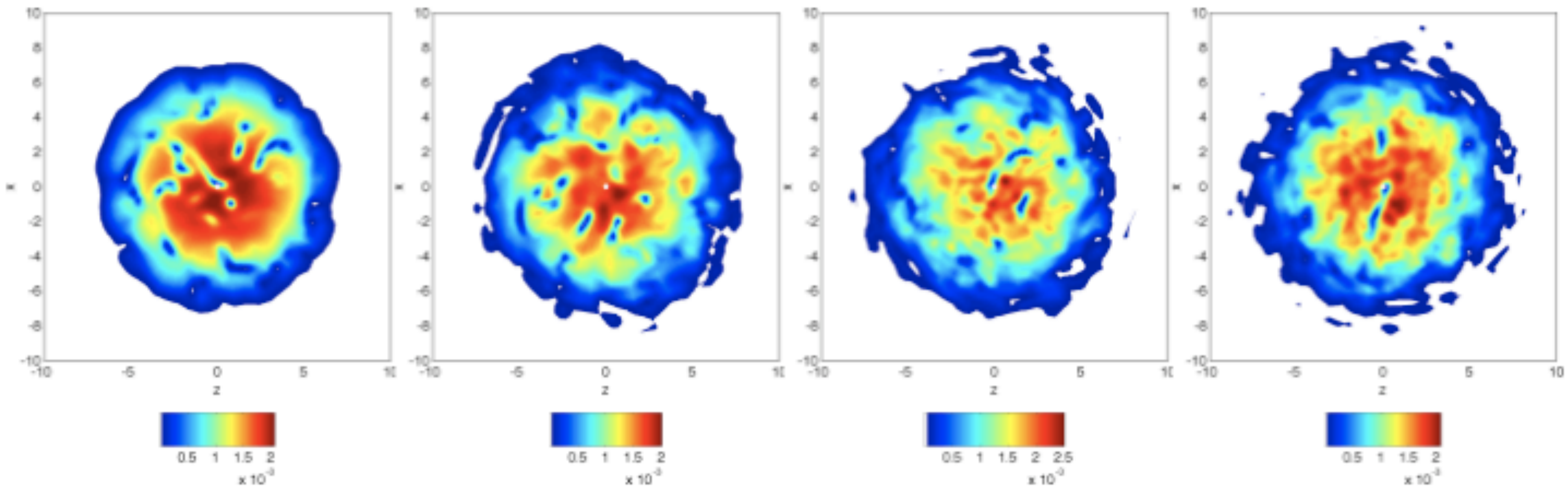
$$V_{ext}(\mathbf{x}) = \frac{1}{2}\omega^2(x^2 + y^2 + z^2)$$

- Strang operator splitting used for time integration
  - second order accurate in time
  - respects Hamiltonian structure of system (stable)

- We used spherical harmonics with Laguerre polynomials in radial direction

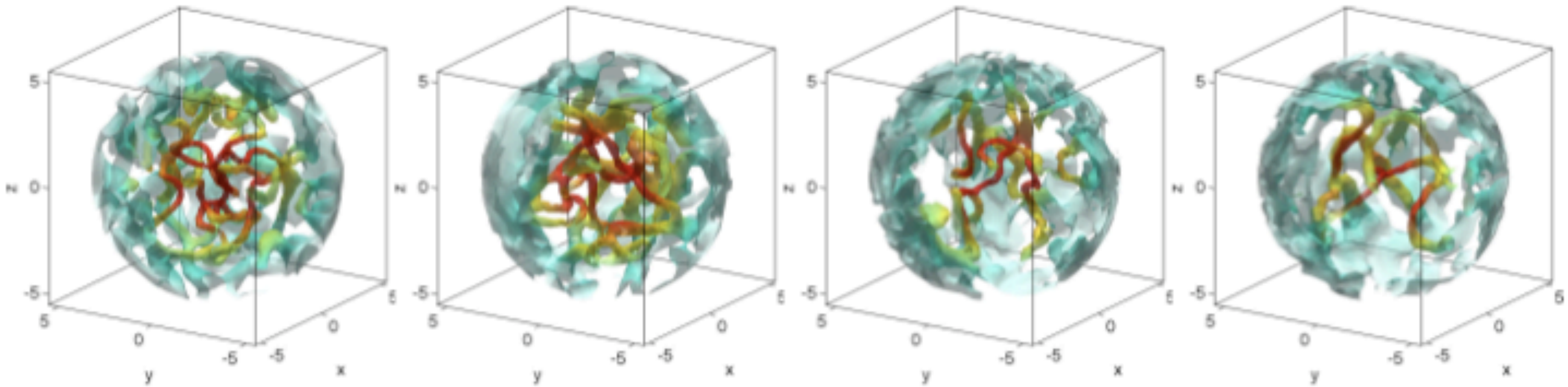






(a) t=0. (b) t=1.6 (c) t=3.2 (d) t=4.8

Figure 13: Cross-sectional denisty profiles of turbulent condensate state for case with $\{\gamma^{(3D)} = 12000, \lambda_{tr} = 0., \Omega_z = 0\}$.



(a) t=0. (b) t=1.6 (c) t=3.2 (d) t=4.8

Figure 14: Condensate isosurface corresponding to $|\psi| = 0.025$ showing relaxation of turbulent vortex tangle with time for $\{\gamma^{(3D)} = 12000, \lambda_{tr} = 0., \Omega_z = 0\}$. The isosurface contouring is given by the function $\sqrt{r}$ where r is the radius measured from the centre of the condensate and therefore reflects the distance that different isurfaces are located from the centre of the trap.

Computing the Condensate Fraction:

- How can we extract condensate?
  - does not coincide with a mode from our basis as in homogeneous system
- Use Penrose-Onsager definition of BEC (1956)
  - applicable even at non-equilibrium
  - compute the density matrix
  - replace ensemble average with time average (ergodicity hypothesis)
- Define the density matrix as

$$\overline{\rho(\mathbf{x},\mathbf{x}')} = \frac{1}{T}\int_{t-T/2}^{t+T/2} \psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau)\,d\tau$$

- Can decompose into eigenmodes $\psi_i(\mathbf{x},t)$

- Profiles of condensate and non-condensate fraction

– Wavepacket formalism gives the following distribution for the excitations

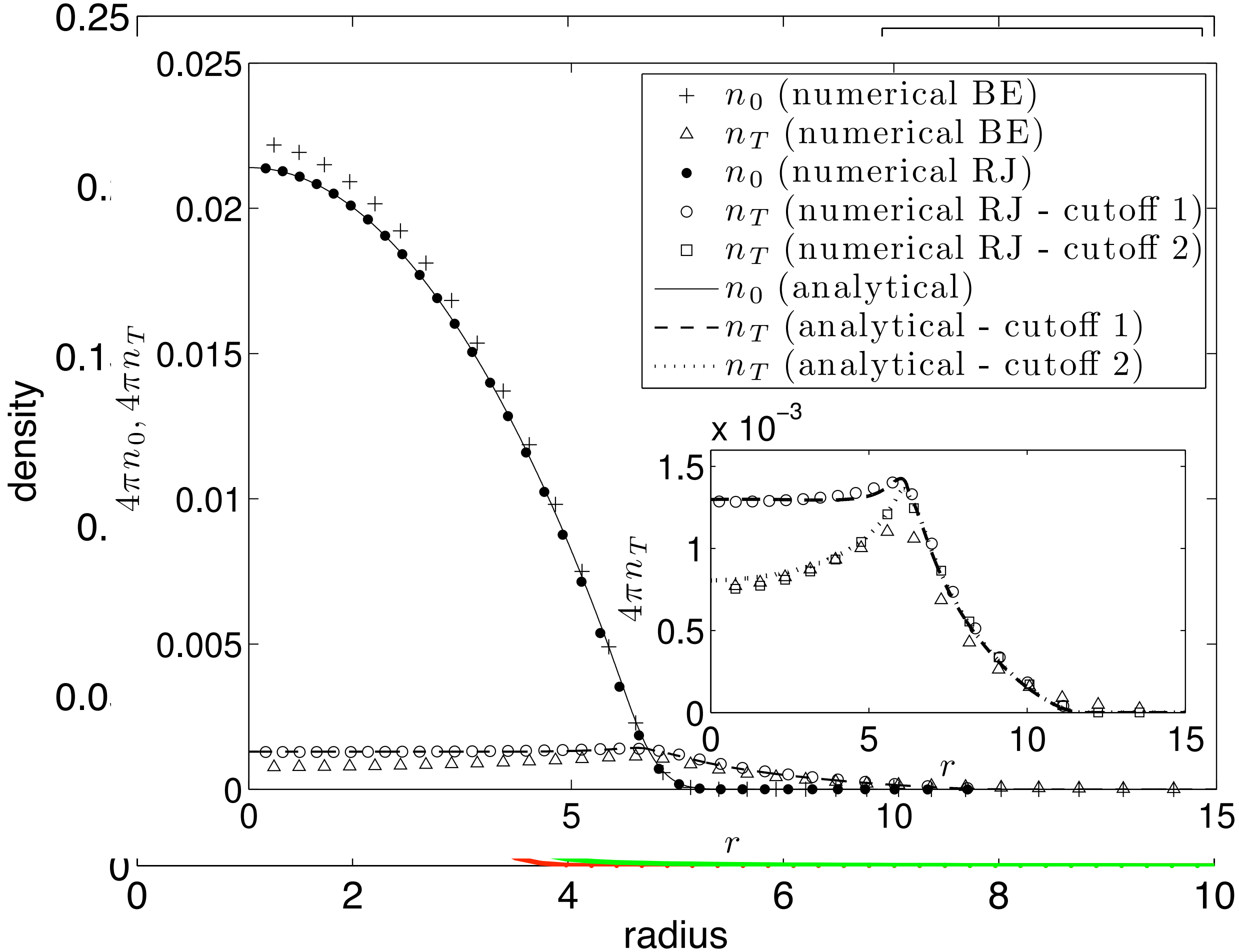
  – outside condensate

$$n(\mathbf{k},\mathbf{x}) = \frac{T}{k^2 + V_{ext}(\mathbf{x}) - \mu}$$

  – inside condensate

$$\tilde{n}(\mathbf{k},\mathbf{x}) = \frac{T}{k\sqrt{k^2 + 2\gamma\,(n_o / V)}}$$

- Thermal cloud shows expected asymptotic behaviour from theory



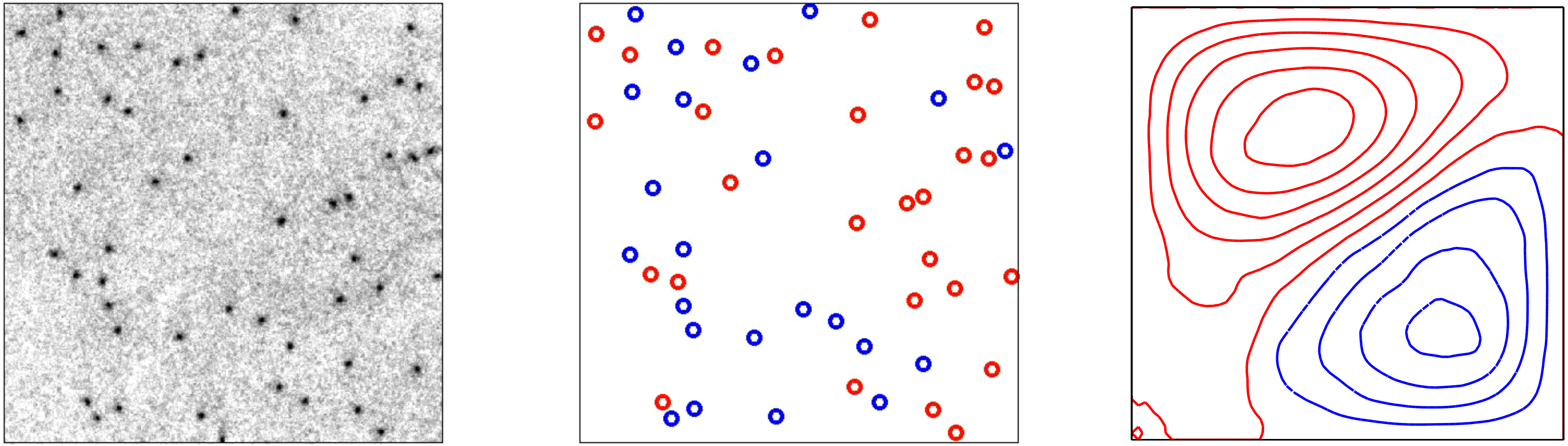
(HS, Phys. Rev. A, **85**, 063622, 2012)

Results from the 2D Gross-Pitaevskii Model (Reflective Boundaries):

- We simulate system in square domain with no-normal flow boundary conditions with 2D Gross-Pitaevskii equation

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2 \psi + g|\psi|^2 \psi \qquad g = \frac{\sqrt{8\pi}\hbar^2 a_s}{m a_z}, a_z = \sqrt{\frac{\hbar}{m\omega_z}}$$

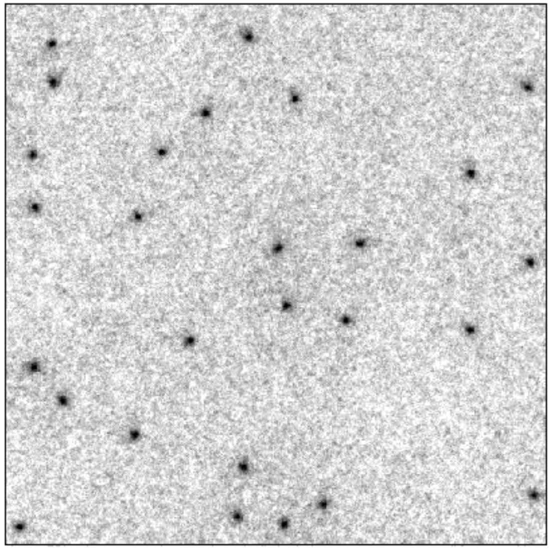
$$N^+ = 28,\ N^- = 23,\ \mathrm{frame}{=}800$$

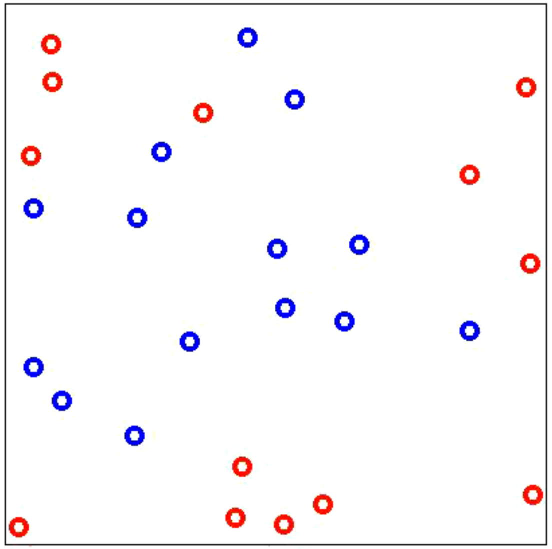


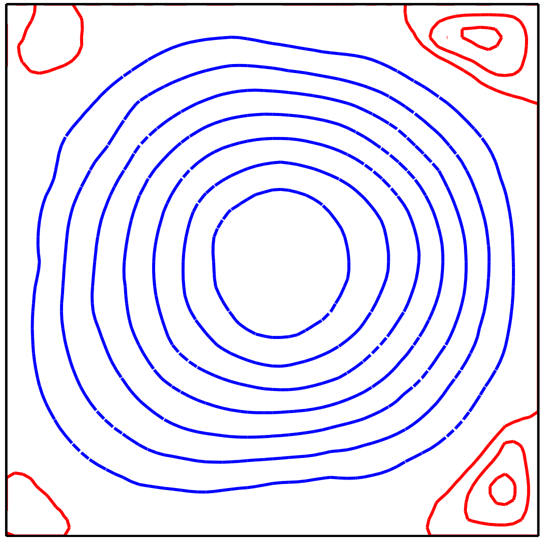
time averaged streamfunction

- At intermediate times, time-averaged stream-function recovers dipole state

$N^+ = 13,\ N^- = 14,$ frame=3200







time averaged streamfunction

(HS & Maestrini, Phys. Rev. A, **94**, 043642, 2016)

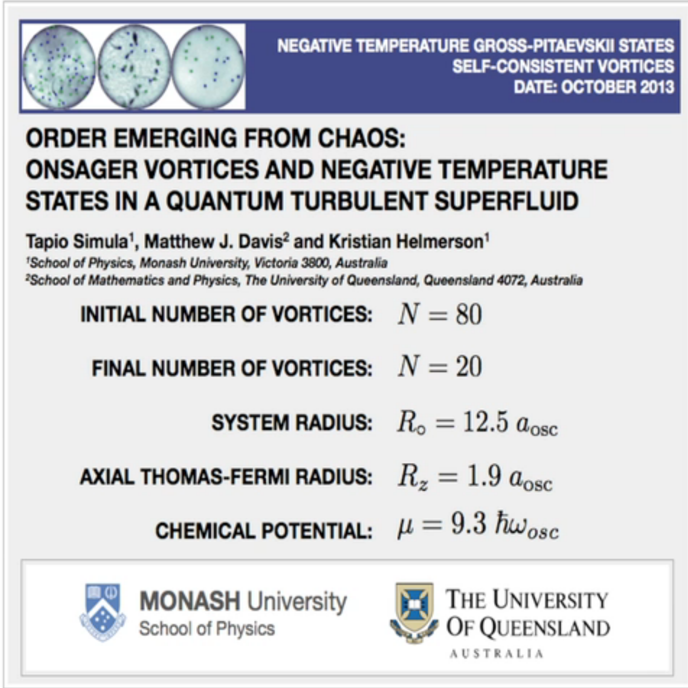
- Long time-averaged streamfunction now reveals monopole state
  - we observe strong symmetry breaking in the circulation with monopole
  - positive vortices near the boundaries screen negative vortices from annihilating with the boundaries

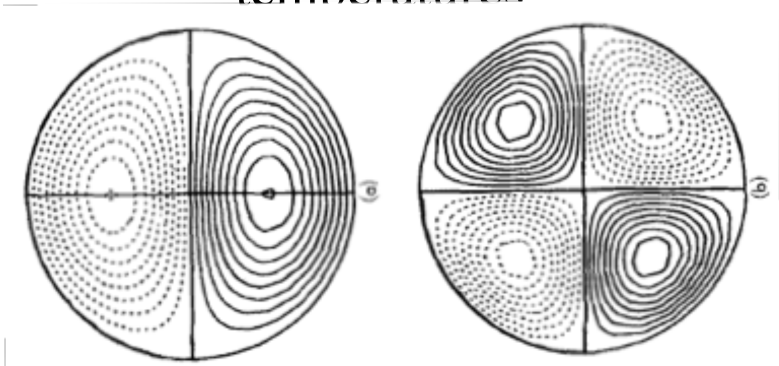
Boltzmann-Poisson Equation:

- Introducing a streamfunction $\nabla^2\psi = -\omega$ (order parameter for large scale flow)

$$\nabla^2\Psi + \frac{\lambda^2}{2}\left[\frac{\exp(\Psi)}{\langle\exp(\Psi)\rangle} - \frac{\exp(-\Psi)}{\langle\exp(-\Psi)\rangle}\right] = 0,$$

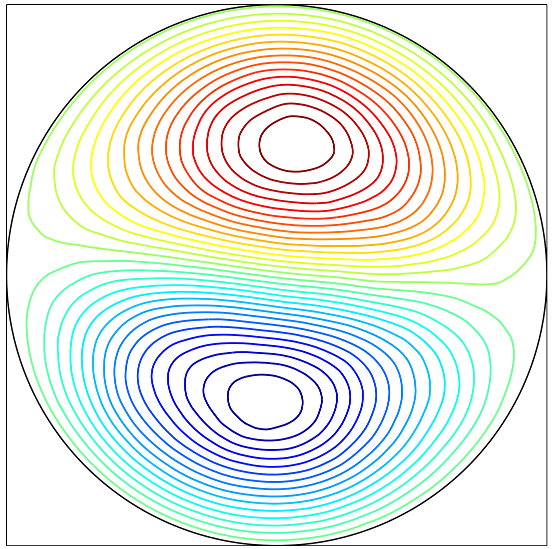
  - where $\gamma\beta\psi = \Psi,$ is the scaled streamfunction,
  - $\lambda^2/2 = -N\gamma^2\beta/\mathcal{D},$ is the scaled inverse temperature
  - nontrivial solutions only for negative temperatures



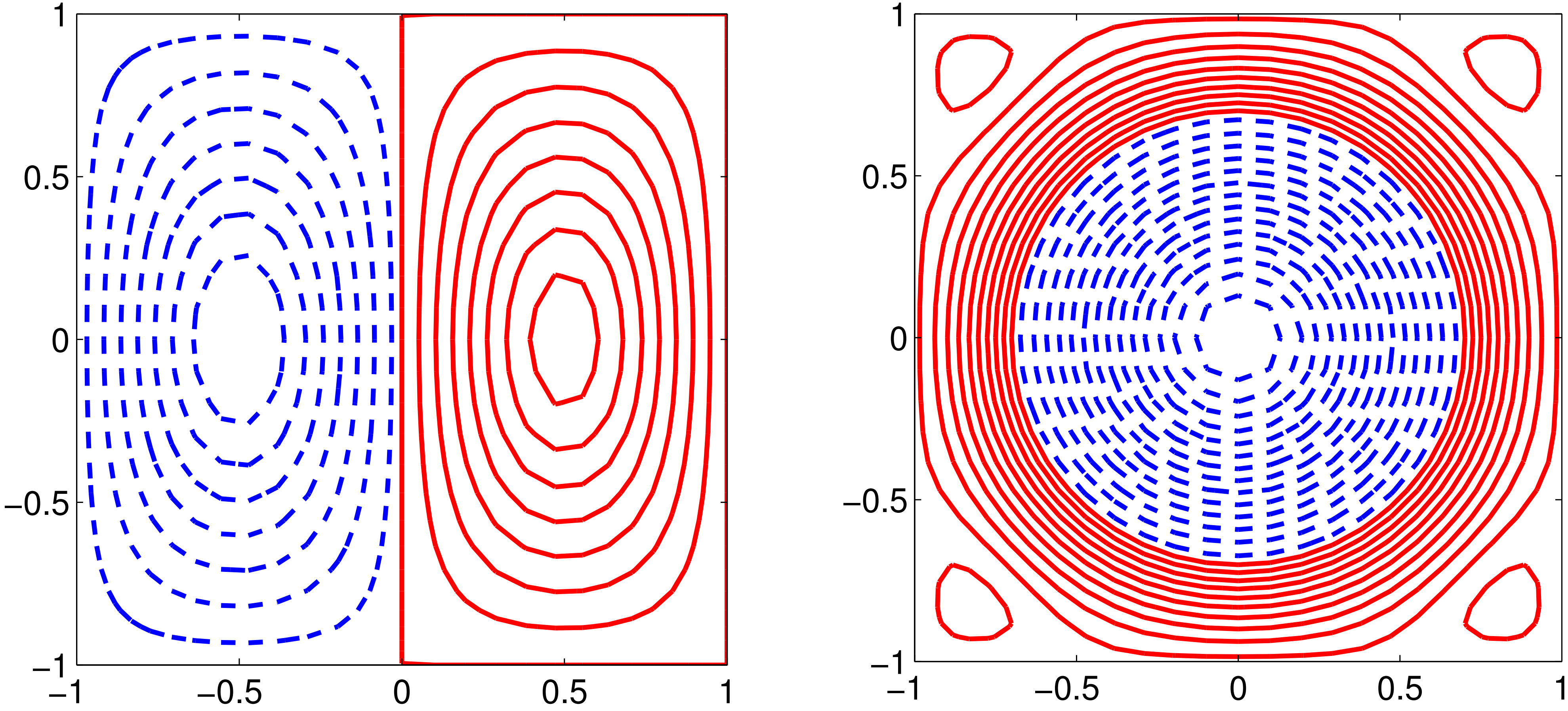


Streamfunction contours for circular domain

Averaged streamfunction from our numerical simulations →

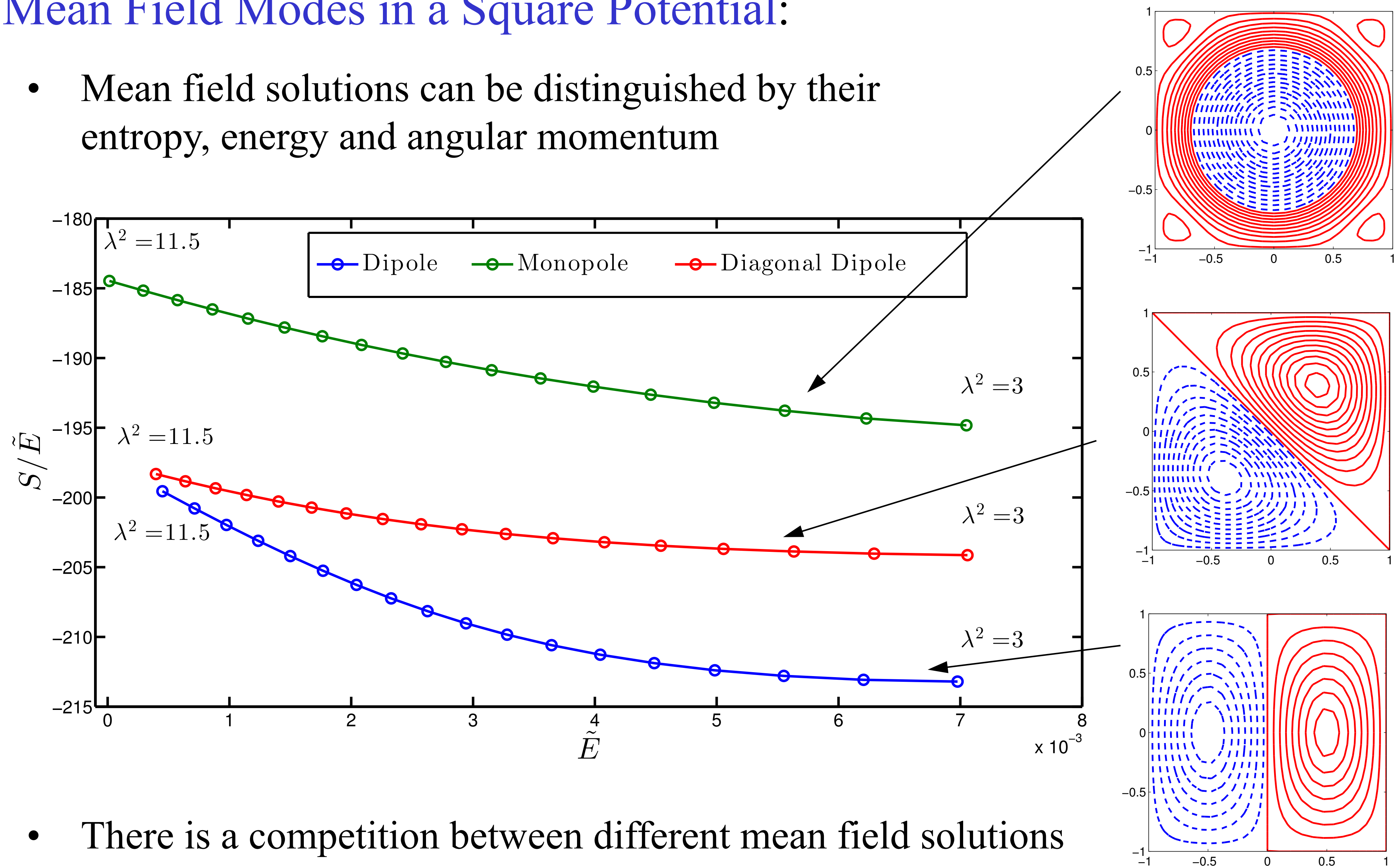


Mean Field Modes in a Square Potential:



Mean Field Modes in a Square Potential:

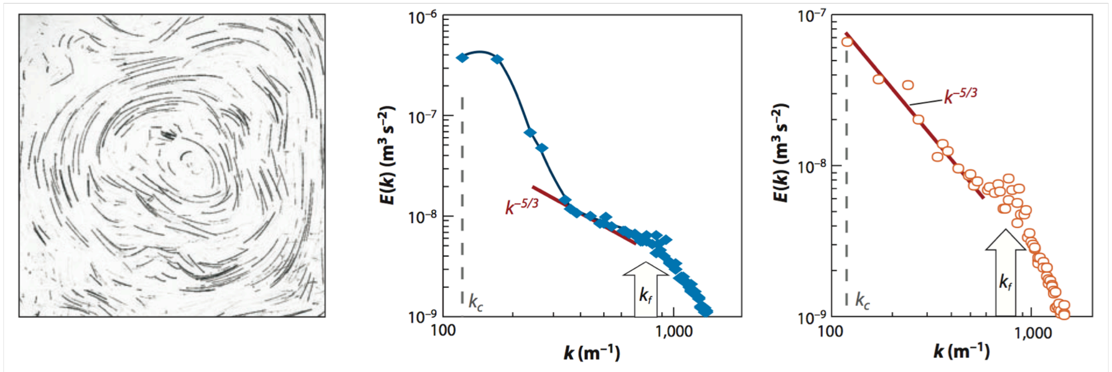
- Mean field solutions can be distinguished by their entropy, energy and angular momentum



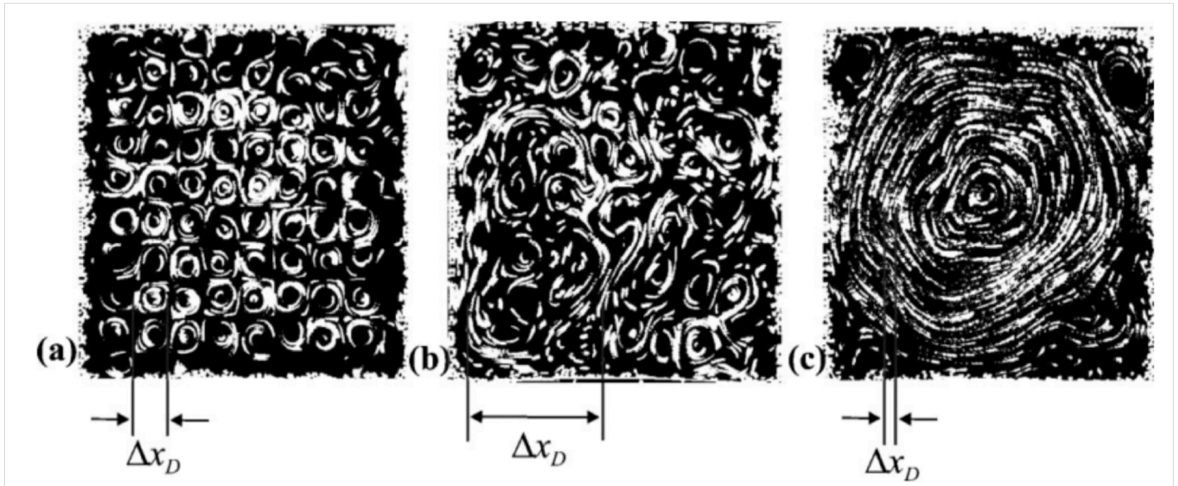
- There is a competition between different mean field solutions

Comparison with Classical Experiments:

- Emergent monopole flows also agree with observations made on 2D turbulence in classical experiments



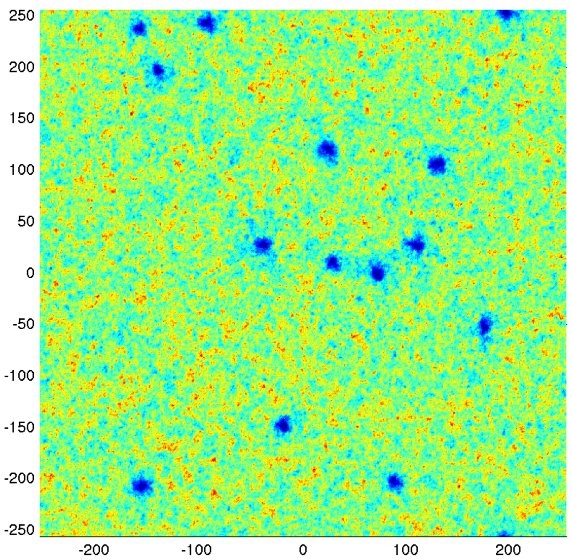
Shats, Xia, Punzmann (2005)

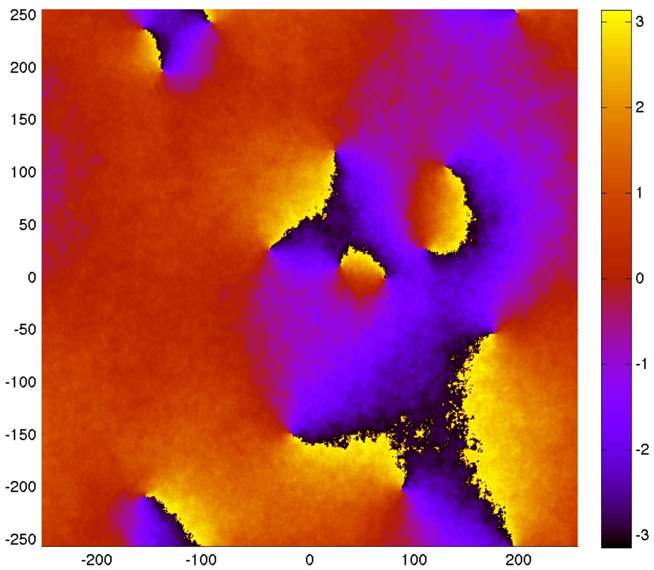


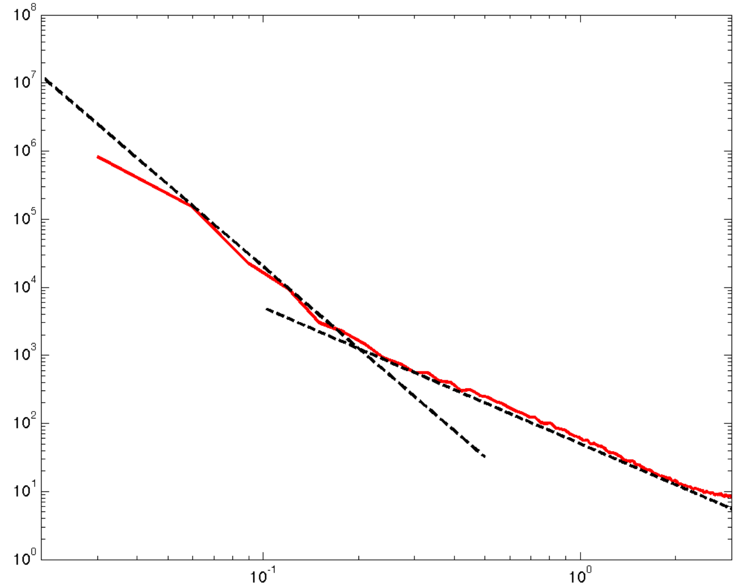
- Confirms emergence of quasiclassical regime and Onsager condensation in quantum turbulence

Non-equilibrium Phenomena:

- Spectra of relaxation dynamics in 2D periodic system reveals two co-existing regimes
  - shallow spectrum corresponds to weak wave turbulence prediction
  - steeper spectrum is a strong wave turbulence regime
  - steeper spectrum owes its existence to vortices







Computing Occupation Number Spectra in Square Domain:

- We recover the spectrum for a random distribution of vortices
  - modified at low k due to vortex clusters

$$E = \int \langle |\nabla\phi|^2 \rangle dx dy$$

$$= \int k^2 \langle |\tilde{a}(\mathbf{k})|^2 \rangle d^2\mathbf{k} = 2\pi \int_0^\infty k^3 n(k) dk,$$

where $n(k) = 1/(2\pi) \int_0^{2\pi} \langle |\tilde{a}(\mathbf{k})|^2 \rangle d\theta_k$ and

$$\tilde{a}(\mathbf{k}) \equiv \mathcal{F}[\psi(\mathbf{r})] = \frac{1}{2\pi} \int e^{-i\mathbf{k}\cdot\mathbf{r}} \psi(\mathbf{r}) d^2\mathbf{r}.$$

- Spectral contributions to kinetic energy can be decomposed into components

$$E_{\mathrm{IH}}^{Q} = \int \langle |\mathcal{F}[\mathbf{u}^i(\mathbf{r}) e^{i\varphi(\mathbf{r})}]|^2 \rangle \mathrm{d}^2\mathbf{k} = \int_0^\infty \mathcal{E}_{\mathrm{QIKE}} \mathrm{d}k.$$

$$E_{\mathrm{QP}}^{\mathrm{Q}} = \int \langle |\mathcal{F}[\nabla \sqrt{\rho(\mathbf{r})} e^{i\varphi(\mathbf{r})}]|^2 \rangle \mathrm{d}^2\mathbf{k}$$

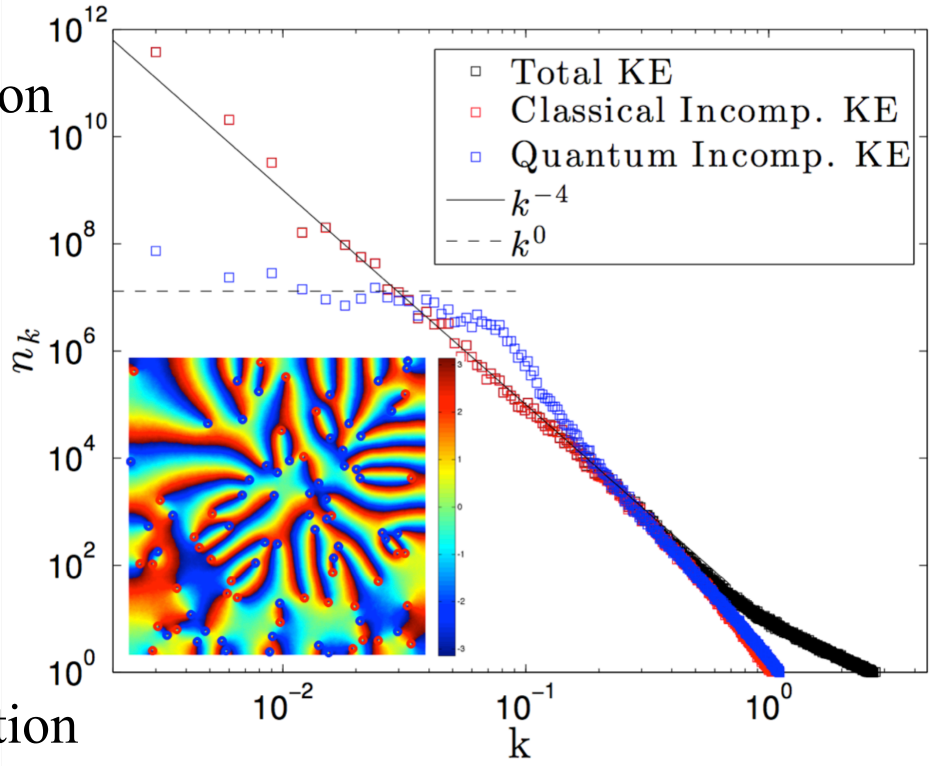
Numerical Evaluation of Spectra:

- Alternatively, we can define a classical analogue of kinetic energy spectrum
  - can not be measured in practice
  - is not related to momentum distribution

$$E_{\mathrm{H}}^{\mathrm{C}} = \int \langle \rho(\mathbf{r})|\mathbf{v}(\mathbf{r})|^2 \rangle \mathrm{d}^2\mathbf{r} = \int_0^\infty \mathrm{d}k \int_0^{2\pi} \langle |\tilde{\mathbf{u}}(\mathbf{k})|^2 \rangle k \mathrm{d}\theta_k$$

$$E_{\mathrm{QP}}^{\mathrm{C}} = \int \langle |\nabla \sqrt{\rho(\mathbf{r})}|^2 \rangle \mathrm{d}^2\mathbf{r}$$

$$E_{\mathrm{IH}}^{\mathrm{C}} = \int_0^\infty \mathrm{d}k \int_0^{2\pi} \langle |\tilde{\mathbf{u}}^i(\mathbf{k})|^2 \rangle k \mathrm{d}\theta_k = \int_0^\infty \mathcal{E}_{\mathrm{CIKE}} \mathrm{d}k.$$



(a) Occupation Number Spectra

- We recover spectrum for random distribution of vortices
  - modified at low k due to vortex clusters

- Signature of condensate clearer in "quantum definition" of kinetic energy

Summary:

- Nonequilibrium phenomena in BECs important for finite temperature models

- Statistical interpretation of NLS leads to kinetic equations (two regimes identified)
  - weak nonlinearity (low number densities)
  - strong condensate $(N-n_o)/N<<1$
  - changes kinetics from four wave to three wave interactions

- In wide range of parameter regimes non-equilibrium relaxation tends to lead to two spectra coexisting at same time
  - can be attributed to weak wave turbulence of compressible modes
  - strong turbulence related to presence of vortices

- How can we extend wave turbulence to model this important generic scenario that arise in Bose gases?