Bose-Einstain Condensation and Superfluidity

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Introduction

Classical fluid mechanics
macroscopic
continuum approximation \( d \ll L \)

Quantum mechanics
microscopic
\( \lambda_{dB} \sim T^{-1/2} \)

Quantum fluid mechanics – macroscopic dynamics & quantum effects

\( \lambda_{dB} \sim d \)

There is no universal dynamical model of quantum fluids
derived from first principles
Superfluidity and BEC

Superfluidity - the ability to flow through narrow channels without friction; the existence of quantised vortices with the quantum of circulation $\hbar/m$.

Bose-Einstein Condensation (BEC) - macroscopic occupation of the single-particle state.

Relationship between BEC and superfluidity:
existence of the classical field $\psi$ (order parameter, wave function) associated with the macroscopic component of the field operator

$$\psi = \sqrt{\rho} \exp[iS], \quad \mathbf{v}_s = \frac{\hbar}{m} \nabla S$$

$\psi = 0$ represents quantised vortex line.
History

“The Golden Age” of the science of superfluids is characterised by four discoveries:
Discovery of superfluidity in $^4$He (Kapitza 1938, Nobel Prize 1978);
Mathematical model of superfluid (Landau 1941, Nobel Prize 1962);
Discovery of superfluidity in $^3$He (Lee, Osheroff, Richardson 1972, Nobel Prize 1996);

We are entering ”The Second Golden Age” characterised by explosion in number of new superfluid systems (Cornell, Ketterle, Wieman 1995, Nobel Prize 2001).
Superfluidity as frictionless flow

Frictionless flow – property of the excitation spectrum $\epsilon(p)$.
Consider a heavy obstacle moving at a constant velocity $v$ in a uniform fluid in its ground state.

**Question:** At what velocity does it become possible for excitations to be created?

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<th>Frame moving with obstacle</th>
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<td>$E_0$, $p = 0$</td>
<td>$E(v) = E_0 + \frac{1}{2}Nm v^2$</td>
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<tr>
<td>GS + Single excitation</td>
<td>$E = E_0 + \epsilon(p)$, $p$</td>
<td>$E(v) = E_0 + \epsilon(p) - p \cdot v + \frac{1}{2}Nm v^2$</td>
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No excitation can spontaneously grow in the fluid if

$$v < \min_p \frac{\epsilon(p)}{p}, \quad \text{Landau criterion}$$
Mathematical approaches

• Phenomenological Landau two-fluid model: mixture of superfluid and normal fluid;
  Superfluid – ideal inviscid Euler fluid at $T = 0$K; Normal fluid – Navier-Stokes fluid;
  Superfluid – adiabatic motion of a macroscopic ground state;
  Normal fluid – drift of excitations (quasi-particles).
  Validity: No vortices !!!

• Phenomenological Hall-Vinen-Bekharevich-Khalatnikov (HVBK) model:
  Landau + vortices. Extra forces: tension and friction with normal fluid.
  Validity: mean spacing between the vortex lines $\ll$ length scales of interest.

• Classical inviscid model of vortex motion
  Validity: Length scales $\gg$ vortex core, ad hoc vortex reconnections, no vortex formation

• Gross-Pitaevskii semi-classical model
  Validity: weakly interacting Bose gas

\[ i\hbar \psi_t(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_0 |\psi|^2 \psi \]

$V_0$ is the effective interaction potential.
Applicability of GP equation

Heisenberg representation of the field operator $\hat{\Psi}(r, t)$:

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi}(r, t) = \left[ -\frac{\hbar^2 \nabla^2}{2m} + \int \hat{\Psi}^\dagger(r, t)V(r - r')\hat{\Psi}(r', t) \, dr' \right] \hat{\Psi}(r, t).$$

$$\hat{\Psi}(r, t) \sim \psi(r, t)$$

- BEC (macroscopic occupation, large $N$)
- dilute gas at low temperature
  (range of interatomic forces $\ll$ average interparticle distance)

$$V \rightarrow V_{\text{eff}}, \quad V_0 = \int V_{\text{eff}}(r) \, dr, \quad V_0 = \frac{4\pi \hbar^2 a}{m}$$

- interested in phenomena taking place over distances $\gg a$ scattering length

Trapped BEC: $i\hbar \psi_t(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_0|\psi|^2 \psi + V_{\text{ext}}(r)\psi$

$$i\hbar \psi_t(r, t) = \delta E/\delta \psi^*, \quad \text{Energy} \quad E = \int \frac{\hbar^2}{2m}|\psi|^2 + V_{\text{ext}}(r)|\psi|^2 + \frac{V_0}{2}|\psi|^4 \, dr.$$
Challenge in superfluid modelling

1. New mathematical models of superfluidity
2. Rigorously derived models replacing phenomenological models

Outline

- Hydrodynamical equations, Madelung transformation;
- Stationary solutions (ground state, vortex);
- Harmonic modes; velocity of sound;
- Trapped BECs; rotating BECs;
- Vortex motion homogeneous and inhomogeneous backgrounds;
- GP for superfluid helium; nonlocal models.
- Solitary waves in condensates and mechanisms of their formation;
- Superfluid turbulence, normal fluid, mutual friction coefficient.
Hydrodynamical equations

\[ i\hbar \psi_t(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_0 |\psi|^2 \psi \]

Density \( n(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2 \); Velocity \( \mathbf{v}(\mathbf{r}, t) = \frac{\hbar}{m} \nabla S(\mathbf{r}, t) \).

Madelung transformation:

\[ \psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)} \exp[iS(\mathbf{r}, t)] \]

Continuity equation:

\[ \frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0, \]

Integrated momentum equation

\[ \hbar \frac{\partial S}{\partial t} + \left( \frac{1}{2} \mathbf{v}^2 + V_0 n - \frac{\hbar^2}{2m\sqrt{n}} \nabla^2 \sqrt{n} \right) = 0 \]

The quantum pressure term scales as \( \nabla^2 \sqrt{n}/\sqrt{n} \sim L^{-2} \), where \( L \) is the typical distance of the density variations. The quantum pressure term becomes negligible if \( L \gg \xi \), where \( \xi = \hbar/\sqrt{2mV_0n} \) is the healing length.
Stationary GP equation

How to find stationary solutions of the GP equation?

\[ \min E \text{ subject to } \int |\psi|^2 \, dr = N \]
or \[ \min(E - \mu N) \], where \( \mu \) is Lagrange multiplier (chemical potential).

\[ \frac{\delta (E - \mu N)}{\delta \psi^*} = 0 \]

Stationary GP equation

\[ \mu \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_0 |\psi|^2 \psi. \]

Uniform gas: \( n_0 = |\psi_0|^2 = \mu/V_0 \) – ground state (state of minimum energy for given \( N \))

Note: we can always include \( \mu \) into time-dependent GP equation by \( \psi \rightarrow \psi \exp[-i\mu t/\hbar] \):

\[ i\hbar \psi_t = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_0 |\psi|^2 \psi - \mu \psi. \]
Vortices in the GP equation

In cylindrical coordinates \((r, \theta, z)\) the wave function of a straight-line vortex takes form

\[
\psi = |\psi(r)| \exp[is\theta]
\]

where \(s\) is an integer ("winding number", "topological charge").

Fluid rotating around the z-axis with tangential velocity

\[
v = \frac{\hbar}{m} \nabla \theta = \frac{\hbar}{m} s
\]

\[
-\frac{\hbar^2}{2mr} \frac{1}{dr} \left( r \frac{d|\psi|}{dr} \right) + \frac{\hbar^2 s^2}{2mr^2} |\psi| + V_0 |\psi|^3 - \mu |\psi| = 0.
\]

At large distances the density is unperturbed, so \(|\psi| \to \sqrt{n_0}\).

Introduce the dimensionless function \(|\psi| = \sqrt{n_0} f(\eta)\),
where \(\eta = r/\xi\) and \(\xi = \hbar/\sqrt{2mV_0n_0}\) is the healing length.
A useful analytical form of \( f \) can be founds as a Padé approximant. A simplest form \( f(\eta)^2 = \eta^2 / (\eta^2 + 2) \) \cite{Fetter 1969}, so

\[
\psi = f(\eta)e^{i\theta} = (x + iy) / \sqrt{x^2 + y^2 + 2}, \quad x = \eta \cos \theta, \quad y = \eta \sin \theta. \tag{1}
\]
Harmonic modes

Elementary excitations (small amplitude harmonic modes) above the ground state

\[ \psi_0 = \sqrt{n_0} = \sqrt{\mu/V_0} : \psi = \psi_0(r) + \epsilon \psi_1(r, t) \]

Linearising time-dependent GP equation gives

\[ i\hbar \psi_{1t} = -\frac{\hbar^2}{2m} \nabla^2 \psi_1 + n_0 V_0 (\psi_1 + \psi_1^*). \]

Look for plane wave modes: \( \psi_1 = A \exp\left[i(k \cdot r - \omega t)\right] + B^* \exp\left[-i(k \cdot r - \omega t)\right] \)

Dispersion relation (Bogolyubov law)

\[ \omega^2 = \frac{n_0 V_0}{m} k^2 + \left(\frac{\hbar k^2}{2m}\right)^2. \]

(1) Small \( k \) (long wavelengths) sound-like dispersion \( \omega \approx ck \), where \( c = \sqrt{n_0 V_0/m} \) is sound velocity. Quasiparticles – phonons.

(2) Large \( k \) (short wavelengths) particle-like dispersion \( \omega \approx \frac{\hbar k^2}{2m} \)
Trapped BECs

\[ i\hbar \psi_t(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_0|\psi|^2\psi + V_{ext}(r)\psi - \mu \psi \]

(1) Standard “magnetic” traps \( V_{ext}(r) = V_{tr} = \frac{1}{2}m(\omega_1^2x^2 + \omega_2^2y^2 + \omega_3^2z^2) \), where \( \omega_i \) are trap frequencies.

(2) Other experimental potentials: quartic, periodic optical lattices, disordered potentials...

Strong interactions, large number of particles, shallow trap: kinetic energy negligible compared to trap energy and interaction energy – Thomas-Fermi (TF) limit.

Ground state in Thomas-Fermi limit

\[ V_0 n(r) + V_{ext}(r) = \mu \]

For example, if \( V_{ext} = V_{tr} \)

\[ n(r) \approx |\psi_{TF}(r)|^2 = \frac{\mu}{V_0} \left( 1 - \sum_{j=x,y,z} \frac{x_j^2}{R_j^2} \right) \]

where \( R_j^2 = 2\mu/m\omega_j^2 \) are the three condensate radii.
Rotating condensates [Tsubota et al PRA (2002)]

For a sufficiently large angular velocity, $\Omega$, the state with superfluid at rest becomes energetically unfavorable. In frame rotating with $\Omega$ the energy to minimize is $E_r = E - \Omega \cdot L$, where $L$ is angular momentum $\Rightarrow$ vortices are created.
Vortex motion on uniform backgrounds

Assumptions: $N$ vortices in $(x, y)$-plane, no external potential, vortices separated by distances far exceeding the healing length $\xi$.

Dimensionless form of the GP equation is

$$-2i\psi_t = \nabla^2 \psi + (1 - |\psi|^2)\psi,$$

where time is measured in units of $m\xi^2/\hbar$ and distance in healing lengths $\xi$.

Introduce a small parameter $\epsilon = \xi/L$, where $L$ is an average inter-vortex distance. Scale $\nabla \rightarrow \epsilon \nabla$, $\partial_t \rightarrow \epsilon^2 \partial_t$ From the GP equation we get to the leading order

$$n = 1 - O(\epsilon^2), \quad \nabla^2 S = 0.$$

Vortex motion is according to classical inviscid irrotational (except at the vortex positions $x = x_i$) incompressible flow dynamics. The velocity potential for a point vortex at origin, with the winding number $s$, is $s\theta$, so

$$\mathbf{v} = s\nabla \theta = s\frac{\mathbf{e}_z \times x}{|x|^2} = s\mathcal{J} \frac{x}{|x|^2},$$

where $\mathcal{J}$ denotes rotation through $\pi/2$. 
Laplace’s equation is linear, so we can linearly superpose a finite number \( N \) of point vortices with different strengths and positions \( x_i \) \((i = 1, \ldots N)\), thus

\[
v = \sum_i s_i \frac{e_z \times (x - x_i)}{|x - x_i|^2}.
\]

Each vortex is moved by the velocity field due to all the other vortices.

The dynamical system of vortex motion

\[
\dot{x}_i(t) = \sum_{j \neq i} s_j \frac{e_z \times (x_i - x_j)}{|x_i - x_j|^2} \quad (i = 1, \ldots N).
\]

Remarkably, the equations of vortex motion have a Hamiltonian structure:

\[
s_i \dot{x}_i(t) = \mathcal{J} \frac{\partial H}{\partial x_i}; \quad H = \frac{1}{2} \sum_j \sum_{j \neq i} s_i s_j \ln |x_i - x_j|.
\]

Two more invariants of motion: the dipole momentum \( P \) and the angular momentum \( Q \)

\[
P = \sum_i s_i x_i, \quad Q = \sum_i s_i x_i \cdot x_i.
\]
Some classical results on point-vortex motion Aref (1983)

• An unlike-charged pair with the same winding numbers separated by a distance $d$ propagates normally to their common axis with speed $|s|/d$.

• Method of “images” to deal with boundaries. No mass flux across the boundary implies $v \cdot n = 0$, where $n$ is the normal to the boundary. This condition is satisfied by placing vortices and removing the boundary.

• Chaotic dynamics with the minimum of four vortices in the infinite plane; three in a half-plane or circle, and two in an arbitrary closed region.

Challenge to understand vortex motion in condensates: nonuniform background, interactions with sound, boundaries etc.

Methods:

• boundary-layer theory: vortex problem solved exactly in the inner region (close to the core) and in the outer region (far away from the core); the asymptotics of two solutions are matched in the intermediate region.

• variational approach: trial function that depends on some parameters is used to evaluate the Lagrangian of the GP equation; the Euler-Lagrange equations are used to determine the dynamical evolution of parameters.

• Hamiltonian approach: approximation of a vortex solution is used to evaluate $U = \frac{\partial E}{\partial p}$.

• numerical simulations.
Numerical methods

(A) numerical integration of the GP equation forward in time;
Methods: finite differences, spectral methods;
careful treatment of boundaries to minimize sound emission (open boundaries, dissipative boundaries).
Use: to study dynamics, interactions, nonlinear effects.
Problems: nonexact solutions, sensitivity to resolution, grid effects, etc.

(B) fixed point problems via numerical discretization using finite differences; the resulting nonlinear matrix equation is solved via Newton-Raphson iteration procedure.
Methods: standard linear solvers; infinite domains can be mapped onto finite domains.
Use: stationary (in some reference frame) solutions.
Problems: limited range of problems, but solutions are very accurate.
Vortex motion in trapped BECs

\[ i\hbar \psi_t (r, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi + V_0 |\psi|^2 \psi + V_{\text{ext}}(r) \psi \]

Harmonic trapping potential \( V_{\text{ext}} = \frac{1}{2} m (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \)

**Eric Cornell group (JILA) 2000**

**Wolfgang Ketterle group (MIT) 2001**

**Question:** how does a vortex move in trapped condensates?

**Partial answer:** [Rubinstein & Pismen (1994)]

*Drift across the density gradient:* \( \mathbf{v} = \mathbf{v}_s - J \mathbf{f} \ln \frac{\alpha}{|\mathbf{f}|}, \quad \mathbf{f} = \nabla \ln \rho_0. \)
Vortex motion near the boundary of a semi-infinite condensate [Mason, Berloff and Fetter, PRA 2006]

Dynamics of a BEC in the presence of the solid wall at $y = 0$ is described by the Gross-Pitaevskii (GP) equation (distance is measured in healing lengths $\xi$ and time in $m\xi^2/\hbar$)

$$-2i\psi_t = \nabla^2\psi + (1 - |\psi|^2)\psi,$$

subject to the boundary conditions

$$\psi(x, y = 0, t) = 0, \quad 0 \leq y < \infty, \quad |x| < \infty.$$ 

In the absence of vortices, the exact solution is

$$g(y) = \tanh(y/\sqrt{2}).$$

The condition of zero mass flux through the wall is $\rho \mathbf{u} \cdot \mathbf{n} = 0$. This is automatically satisfied at the wall.

Are image vortices relevant?
Numerical solutions for the vortex motion near the boundary

We seek solitary-wave solutions of the GP equation that preserve their form as they move with fixed velocity $U: \partial_t \rightarrow -U \partial_x$. The GP equation becomes

$$2iU \psi_x = \nabla^2 \psi + (1 - |\psi|^2) \psi.$$

$$p = \frac{1}{2i} \int [ (\psi^* - g(y)) \partial_x \psi - (\psi - g(y)) \partial_x \psi^* ] \, dx \, dy,$$

$$E = \frac{1}{2} \int \left[ |\nabla \psi|^2 + \frac{1}{2} (1 - |\psi|^2)^2 - \text{sech}^4(y/\sqrt{2}) \right] \, dx \, dy.$$

Motion of vortex is faster than that generated by an image vortex. What is the velocity?
Hamiltonian relationship between $U, E, p$ and $y_0$.

$$2iU \psi_x = RHS = \nabla^2 \psi + (\mu - V_{\text{ext}} - V_0|\psi|^2)\psi.$$

$$p = \frac{1}{2i} \int [(\psi^* - g(y))\partial_x \psi - (\psi - g(y))\partial_x \psi^*] \, dx \, dy,$$

$$E = \frac{1}{2} \int |\psi_x|^2 \, dx \, dy + \frac{1}{2} \int |\psi_y|^2 \, dx \, dy + E_{\text{int}}(|\psi|^2).$$

Perform the variation $\psi \rightarrow \psi + \delta \psi$ and some integration by parts to get

$$\delta p = \frac{1}{i} \int [\delta \psi^* \partial_x \psi - \delta \psi \partial_x \psi^*] \, dx \, dy, \quad \delta E = \frac{1}{2} \int [\delta \psi^*(-RHS) + \delta \psi(-RHS^*)] \, dx \, dy.$$

Thus, stationary values of $E$, for fixed $p$ and all $\delta \psi$, require the GP equation and its c.c to be satisfied, with $U$ as Lagrange multiplier:

$$\delta (E - Up) = 0 \quad \text{or} \quad U = \frac{\partial E}{\partial p} = \frac{dE/dy_0}{dp/dy_0}.$$

Useful integral identity: if $x \rightarrow bx$, then

$$\left. \frac{\partial (E - Up)}{\partial b} \right|_{b=1} = -\frac{1}{2} \int |\psi_x|^2 \, dx \, dy + \frac{1}{2} \int |\psi_y|^2 \, dx \, dy + E_{\text{int}}(|\psi|^2) = 0.$$

Therefore,

$$E = \int |\psi_x|^2 \, dx \, dy.$$
**Vortex velocity via Hamiltonian relationship.**

The question we pose is: *What is the position of the vortex \((0, y_0)\) moving parallel to the solid wall with the same velocity as the vortex pair at \((0, y_0 - l)\) in the uniform flow?*

Thus we seek the solution of

\[
U_1(y_0 - l(y_0)) = \frac{1}{2(y_0 - l)} = U_2(y_0) = \frac{\partial E_2}{\partial y_0} \frac{\partial p_2}{\partial y_0}.
\]

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**Trial function:** \(\psi_1 = \psi_0(x, y - y_0)\psi_0^*(x, y + y_0), \quad \psi_2 = g(y)\psi_1,\)

where a Padé approximant (e.g. \(\psi_0 = (x + iy)/\sqrt{x^2 + y^2 + 2}\)) was used.

Integrals \(\partial E_1/\partial y_0\) and \(\partial p_1/\partial y_0\) can be evaluated exactly, and integrals \(\int dE = \partial (E_2 - E_1)/\partial y_0\) and \(\int dp = \partial (p_2 - p_1)/\partial y_0\) for large values of \(y_0\).

To the leading order in \(y_0\) we get

\[
l(y_0) = y_0 - \frac{1}{2} \frac{4\pi + \tilde{d}p}{2\pi/y_0 + dE} \approx \int_0^\infty 1 - g(y)^2 \, dy = \sqrt{2}, \quad U_2 = \frac{1}{2(y_0 - \sqrt{2})}.
\]
Red line – numerics;
Blue line – our Hamiltonian approach;
Black line – $U = 1/(2y_0)$

**Conclusion:** depleted surface layer induces an effective shift in the position of the image equal to the integral of the displaced density!

More generally: In trapped condensates in TF regime (large number of particles / shallow trap) a vortex close to the center of the trap moves mostly due to “shifted” image(s)!
Vortices on varying density backgrounds

Semi-infinite condensate; TF ground state

Trapping potential \( V(y) = \frac{1}{A^2} (y - A)^2 \) if \( y < A \) and \( V(y) = 0 \) otherwise.

\[
V(y) = \begin{cases} 
\frac{1}{A^2} (y - A)^2 & \text{if } y < A \\
0 & \text{otherwise}.
\end{cases}
\]

Density

Motion due to “shifted” image. Motion due to density gradient

If \( y_0 > A \), then \( U \approx (2(y_0 - A/3))^{-1} \) for large \( y_0 \).
If \( y_0 < A \) the velocity is calculated exactly as \( U = \partial E / \partial p \).

Velocity vs \( y_0 \)

Red – numerics
Blue – Hamiltonian for large \( y_0 \)
Green – exact Hamiltonian

Conclusion: “Shifted” images at small density gradient backgrounds & \( U = \partial E / \partial p \) at large density gradient backgrounds.
GP for superfluid helium: Electron bubble

Experiments:

Rayfield and Reif (1964): Above some critical velocity moving ions produce vortex rings;
Packard and Sanders (1972): Vortex lines trap electrons.

Can we model the electron capture by vortex line?

Theory: Berloff & Roberts JPA (2001)

Model on wavefunctions of condensate $\psi$ and electron $\phi$:

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + (U_0|\phi|^2 + V_0|\psi|^2 - E)\psi, \quad \int |\psi|^2 dV = N, \]
\[ i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m_e} \nabla^2 \phi + (U_0|\psi|^2 - E_e)\phi, \quad \int |\phi|^2 dV = 1 \]

$m$ – mass of boson; $E$ – single particle energy of boson; $m_e$ – mass of electron; $E_e$ – energy of electron; $U_0 = 2\pi l\hbar^2/m_e$ – effective interaction potentials between boson and electron; $V_0 = 4\pi d\hbar^2/m$ – effective interaction potentials between bosons; $l$ – boson-impurity scattering length; $d$ – boson diameter.
Capture of electron by vortex line

Energy density of complex

\[ \mathcal{E}(z) = \frac{\rho \kappa^2}{4\pi} \left( \ln \frac{L}{\xi} + L_0(z) \right) \]

Substitution energy

\[ \Delta V = \frac{\rho \kappa^2 \xi}{2\pi} \int_0^\infty \left[ L_0(z) - 0.38 \right] dz \]

Preliminary experiments at Manchester on detecting vortices/turbulence in pure superfluid $^4$He at $T \ll 1 \text{ K}$
New Nonlocal Model

Shortcomings of the GP equation (when applied to superfluid helium):

• GP: only two-body interactions; superfluid $^{4}\text{He}$: many-body interactions;
• GP: $c \propto \sqrt[4]{\rho}$; superfluid $^{4}\text{He}$: $c \propto \rho^{2.8}$;
• dispersion curves

\[
\omega^2 = c^2 k^2 + \left(\frac{\hbar}{2m}\right)^2 k^4
\]

• scaling problem

Conclusion: need new accurate models!
Instead of \( E_{\text{int}} = \frac{V_0}{2m^2} \int \rho^2 \, dr \)

we take \( E_{\text{int}} = \frac{1}{m^2} \int \left[ \frac{1}{2} \int \rho(r') V(r' - r) \rho(r) \, dr' + \frac{W_1}{2+\gamma} \rho^{2\gamma+1} \right] \, dr \)

\[
i\hbar \frac{\partial \psi}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \int V(|r - r'|)|\psi(r', t)|^2 \, dr' + W|\psi|^{4\gamma} \right] \psi
\]

Realistic potential \( V \);
Many-body theory;
roton minimum;
correct speed of sound.

![Vortex core density](image)

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Our model
Monte Carlo calculations Chester et al (1968)
and DF prediction by Dalfovo (1992)
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Solitary waves in condensates

Questions:

- Complete families of solitary waves in various superfluid systems.
- Mechanisms of their formation.

(1) Gross-Pitaevskii equation (Bose-Einstein Condensate)

\[ i\hbar \frac{\partial \psi}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_0 |\psi|^2 \right] \psi \]

(2) Nonlocal Nonlinear Schrödinger equation (Superfluid Helium)

\[ i\hbar \frac{\partial \psi}{\partial t} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \int V(|x - x'|)|\psi(x', t)|^2 dx' + W |\psi|^{2(1+\gamma)} \right] \psi \]

(3) Coupled Gross-Pitaevskii equations (Two-component BECs)

\[ i\hbar \frac{\partial \psi_1}{\partial t} = \left[ -\frac{\hbar^2}{2m_1} \nabla^2 + V_{11}|\psi_1|^2 + V_{12}|\psi_2|^2 \right] \psi_1, \]
\[ i\hbar \frac{\partial \psi_2}{\partial t} = \left[ -\frac{\hbar^2}{2m_2} \nabla^2 + V_{12}|\psi_1|^2 + V_{22}|\psi_2|^2 \right] \psi_2, \]
Solitary waves in GP equation

Localised disturbance moving with constant velocity $U$ in $z$-direction

$$2iU \frac{\partial \psi}{\partial z} = \nabla^2 \psi + (1 - |\psi|^2)\psi, \quad |\psi| \to 1 \quad \text{as} \quad |r| \to \infty$$

Distance in healing lengths $\xi$ and time in $m\xi^2/\hbar$. Velocity of sound $c = 1/\sqrt{2}$.

Summary:

- Solitons in 1D: gray and dark solitons;
- Solitary waves in 2D: vortex pairs and rarefactions pulses; one branch;
- Solitary waves in 3D: vortex rings and rarefactions pulses; two branches.
Solitary waves in GP equation: 1D [Tsuzuki, 1971]

Multiply GP equation by \( \psi^* \) and subtract c.c, look for solutions with constant \( Im(\psi) \).

From compatibility of equations for real and imaginary parts obtain

\[
Im(\psi) = \sqrt{2}U = U/c,
\]

\[
\sqrt{2}\frac{Re(\psi)}{dz} = \left( 1 - \frac{U^2}{c^2} - Re(\psi)^2 \right).
\]

Gray soliton (in stationary frame and dimensional units)

\[
\psi(z - Ut) = \sqrt{n_0} \left( i\frac{U}{c} + \sqrt{1 - \frac{U^2}{c^2}} \tanh \left[ \frac{z - Ut}{\sqrt{2}\xi} \sqrt{1 - \frac{U^2}{c^2}} \right] \right).
\]

Properties:

1. Minimum at \( n(0) = n_0 U^2 / c^2 \)
2. Width of soliton \( \sqrt{2}\xi / \sqrt{1 - U^2 / c^2} \)
3. Phase of wavefunction \( \Delta S = 2 \arccos(U/c) \)
4. As \( U \rightarrow c \), \( E \) decreases: dissipative effects result in an acceleration of soliton and its disappearance.
Solitary waves in GP equation: 2D and 3D

Family of solitary waves [Jones & Roberts, J.Phys A (1982)]

3D

\[ p = \frac{1}{2i} \int \nabla \psi (\psi^* - 1) - \nabla^* \psi^* (\psi - 1) \ dV \]
\[ \mathcal{E} = \frac{1}{2} \int |\nabla \psi|^2 + \frac{1}{2}(1 - |\psi|^2)^2 \ dV. \]

Stability: Lower branch is linearly stable. Upper branch is linearly unstable to axisymmetric infinitesimal perturbations, but the growth rates are small. Spectrum \( \sigma^2 \) is real and changes sign at the cusp.

[Berloff & Roberts JPA (2004)]
Nonlocal model; superfluid helium

Roton can be pictured as “the ghost of a vanished vortex ring” (Onsager)

Families of solitary waves:
only lower branch of the dispersion curve, which terminates at $U = U_L$
Coupled Gross-Pitaevskii system

Atoms in distinct spin or hyperfine levels $^{87}\text{Rb}$ (JILA, NIST) or of different atomic species $^{41}\text{K}-^{87}\text{Rb}$ (LENS).


\[
\begin{align*}
\frac{i\hbar}{\partial t} \psi_1 &= \left[-\frac{\hbar^2}{2m_1} \nabla^2 + V_{11} |\psi_1|^2 + V_{12} |\psi_2|^2 \right] \psi_1, \\
\frac{i\hbar}{\partial t} \psi_2 &= \left[-\frac{\hbar^2}{2m_2} \nabla^2 + V_{12} |\psi_1|^2 + V_{22} |\psi_2|^2 \right] \psi_2,
\end{align*}
\]

$m_i$ is the mass of the atom of the $i$th condensate; coupling constants $V_{ij} = 2\pi \hbar^2 a_{ij}/m_{ij}$; $a_{ij}$ are scattering lengths; $m_{ij} = m_im_j/(m_i + m_j)$ is the reduced mass.

Dispersion relation $(\omega^2 - \omega_1^2)(\omega^2 - \omega_2^2) = \omega_{12}^4$, where $\omega_i^2(k) = c_i^2k^2 + \hbar^2k^4/4m_i^2$ with sound velocity $c_i^2 = |\psi_{i\infty}|^2V_{ii}/m_i$ and $\omega_{12}^2 = c_{12}^2k^2$ where $c_{12}^2 = |\psi_{1\infty}|^2|\psi_{2\infty}|^2V_{12}/m_1m_2$.

Acoustic branches are $\omega \approx c_{\pm}k$ with $2c_{\pm}^2 = c_1^2 + c_2^2 \pm \sqrt{(c_1^2 - c_2^2)^2 + 4c_{12}^4}$.

Dynamical stability $V_{11}V_{22} > V_{12}^2$
Governing equations

\[2iU \frac{\partial \psi_1}{\partial z} = \nabla^2 \psi_1 + (1 - |\psi_1|^2 - \alpha_1 |\psi_2|^2) \psi_1\]

\[2iU \frac{\partial \psi_2}{\partial z} = \gamma \nabla^2 \psi_2 + (1 - \alpha_1 |\psi_1|^2 - \frac{\alpha_1}{\alpha_2} |\psi_2|^2 - \Lambda^2) \psi_2,
\]

\[\psi_1 \to \psi_{1\infty}, \quad \psi_2 \to \psi_{2\infty}, \quad \text{as} \quad |x| \to \infty.\]

where \(\alpha_i = V_{12}/V_{ii}\), \(\gamma = m_1/m_2\) and \(\Lambda^2 = (\mu_1 - \mu_2)/\mu_1\).

Dimensionless units:

\[x \to \frac{\bar{h}}{(2m_1\mu_1)^{1/2}} x, \quad t \to \frac{\bar{h}}{2\mu_1} t, \quad \psi \to \sqrt{\frac{\mu_1}{V_{11} n_i}} \psi.\]

Cylindrical coordinates \((s, \theta, z)\). Map infinite domain onto the box \((0, \frac{\pi}{2}) \times (-\frac{\pi}{2}, \frac{\pi}{2})\) by \(\hat{z} = \tan^{-1}(Dz')\) and \(\hat{s} = \tan^{-1}(Ds')\).

Transformed equations are expressed in second-order finite difference form. Newton-Raphson iteration procedure using banded matrix linear solver based on bi-conjugate gradient stabilised iterative method with preconditioning.
The momentum (or impulse) of the \(i\)-th component

\[
p_i = \frac{1}{2i} \int [(\psi_i^* - \psi_i\infty) \nabla \psi_i - (\psi_i - \psi_i\infty) \nabla \psi_i^*] \, dV.
\]

Form the energy, \(\mathcal{E}\):

- energy of the system with a solitary wave
- energy of an undisturbed system of the same mass

\[
\mathcal{E} = \frac{1}{2} \int \left\{ |\nabla \psi_1|^2 + \gamma |\nabla \psi_2|^2 + \frac{1}{2} (\psi_{1\infty}^2 - |\psi_1|^2)^2 + \frac{\alpha_1}{2\alpha_2} (\psi_{2\infty}^2 - |\psi_2|^2)^2 \right\} \, dV
\]

\[
+ \frac{\alpha_1}{2} \int \prod_{i=1}^2 (\psi_{i\infty}^2 - |\psi_i|^2) \, dV.
\]

Perform the variation \(\psi_i \rightarrow \psi_i + \delta \psi_i\)

Discard surface integrals that vanish provided \(\delta \psi_i \rightarrow 0\) for \(|x| \rightarrow \infty\):

\[
U = \partial \mathcal{E} / \partial (p_1 + p_2)
\]

Let \(z \rightarrow bz\).

\[
\left. \frac{\partial (\mathcal{E} - U(p_1 + p_2))}{\partial b} \right|_{b=1} = 0 \quad \Rightarrow \quad \mathcal{E} = \int |\psi_{1z}|^2 + \gamma |\psi_{2z}|^2 \, dV.
\]
Coupled GP system: Solitary wave complexes [Berloff PRL (2005)]

Vortex Ring – Vortex Ring; Vortex Ring – Rarefaction Pulse;
Vortex Ring – “Slaved Wave”; “Slaved Wave” – Rarefaction pulse

\[ m_1 = m_2, \quad \Lambda = 0.1, \quad \alpha = 0.1 \]
Solitary waves in cylindrical BEC [Komineas and Papanicolaou PRA 2003]

\[ i2U \psi_z = \nabla^2 \psi + (\mu - (x^2 + y^2) \psi - V_0 |\psi|^2) \psi. \]

Single parameter \( \gamma = V_0 / 2\pi \) as \( \mu(\gamma) \) is determined by fixing the ground state density \( \int |\psi_{gr}(x, y)|^2 \, dx \, dy = 1. \)

Lower interactions strength

Higher interactions strength
Mechanisms of vortex ring formation

(1) Critical superflow velocities:
[Frisch et al PRL (1992)] Superflow around a disk releases vortices from the perimeter of the disk creating a net drag force beyond a critical velocity. Nucleation was related to transonic transition.

From the Madelung transformations $\psi = R \exp[iS]$ of the GP equation one gets the following hydrodynamical equations for the number density $n = R^2$ and the phase $\phi = \tilde{n}.S/m$ for the superflow with $\phi = u_\infty x$ as $x^2 + y^2 \to \infty$

$$\frac{\partial n}{\partial t} + \nabla \cdot (n \nabla \phi) = 0$$

$$\frac{\partial \phi}{\partial t} + \frac{1}{2} |\nabla \phi|^2 - \frac{1}{2} u_\infty^2 + c^2 \left( \frac{n}{n_\infty} - 1 \right) = c^2 \xi^2 \frac{\nabla^2 n^{1/2}}{n^{1/2}},$$

where $c = \sqrt{V_0 n_\infty/m}$ is the speed of sound. Consider a stationary flow and neglect the quantum pressure term. We fix a point outside of the disk at which the components move with velocities $u$, introduce the local orthogonal coordinates such that the $x$—axis is tangent to the flow and expand $\phi$ in the neighbourhood of this point as $\phi \approx u x + \epsilon \tilde{\phi}$, where $\epsilon$ is a small parameter.

$$\partial_u (n(u)u) \partial_{xx} \phi + n(u) \partial_{yy} \phi = 0.$$  

At low velocities this equation is elliptic and becomes hyperbolic beyond a critical velocity. This happens when $\partial_u (n(u)u) = 0$ on the equator of the disk.
Superflow around positive ion – formation of vortex rings. Subcritical steady flow is found by asymptotic expansions for $\epsilon =$ healing length/ion radius.

Two-component condensates: [Berloff (2005)]

Nucleation Condition:

$$\frac{\partial (n_1 u_1)}{\partial u_1} \frac{\partial (n_2 u_2)}{\partial u_2} \leq u_1 u_2 \frac{\partial n_1}{\partial u_2} \frac{\partial n_2}{\partial u_1}. $$
Mechanisms continued

(2) transverse “snake” instability [Kuznetsov & Rasmussen PRE (1995)]; Velocity of grey soliton depends on its depth → in multi-dimensions solitons break due to transverse perturbation along the front leading to vortices.

(3) collapsing ultrasound bubbles [Berloff & Barenghi PRL (2004)]

Experiment: *Lene Hau group, Harvard (2005)*
Mechanisms continued

Trap with a laser beam

\[ V_{ext} = \frac{1}{2} \omega^2 (x^2 + y^2) + a \exp \left( -b(x^2 + \frac{1}{4}y^2) \right) \]
Mechanisms continued

(4) interactions of vorticity-free solutions [Berloff JPA (2004)]
(5) during strongly nonequilibrium BEC formation in a macroscopically large uniform weakly interacting Bose gas [Berloff & Svistunov (2002); Berloff & Yin (2006)]
Superfluid turbulence using GP equation

General scenario of turbulence at low temperature: [Kozik & Svistunov (2004; 2005)]

Vortex line reconnections → Kelvin Wave cascade → cusps → kinks → sound (phonons) \( \omega = \frac{k^{2} \pi}{4} \left[ \ln(ka) + c \right] \)

Vortex line self-crossing → Fragmentational Kelvin Wave cascade (LIA) → Pure Kelvin Wave cascade (BSL) → phonons

Decay of superfluid turbulence can be studied in context of GP equation [Nore et al 1997]

Energy spectrum of superfluid turbulence consistent with Kolmogorov law [Kobayashi & Tsubota PRL (2005)]

Vortex rings collisions and Kelvin-wave radiation lead to vortex line decay according to Vinen’s law:

\[ d(L/V) / dt \sim -\chi_{2}(L/V)^{2} \] [Leadbeater, Samuels, Barenghi, Adams (2003)]
Superfluid turbulence: normal fluid

Problem: How to model the normal fluid component?

Nonlinear Schrödinger (NLS) equation describes evolution of all highly occupied modes $n_k \gg 1!$ [Levich and Yakhot, JPA (1978); Kagan and Svistunov, PRL (1997)]

Therefore, NLS equation gives an accurate microscopic description of

- formation of a BEC from a strongly degenerate gas of weakly interacting bosons;
- interactions of vortex tangle with normal fluid (above-the-condensate modes)

Two theoretical limits of mathematical analysis of NLS:

- “weak turbulence” [Zakharov et al (1985), Svistunov (1991)]
  NLS → Boltzmann kinetic equation → self-similar solution for motion of quasi-particles from high energies to low energies
- superfluid turbulence [Nore et al (1997); Kobayashi & Tsubota (2005)]
  start with ad hoc tangle of vortices → tangle decays → energy spectrum

NLS can be used to unify these results!
Unification of the above theoretical limits

[Berloff & Svistunov PRA (2002); Berloff PRA (2004)]

(1) NLS with initial state as random field: \( \psi(x, t = 0) = \sum_k a_k \exp(i\mathbf{k} \cdot \mathbf{x}) \),
(2) Initial evolution according to self-similar solution of Boltzmann kinetic equation on occupation numbers \( n_k = |a_k|^2 \);
(3) **Characteristic time** and **characteristic wave vector** at the beginning of the coherent regime;
(4) Criteria for the number of particles in quasi-condensate;
(5) Formation of vortex tangle;
(6) Decay of superfluid turbulence via interactions with normal fluid.

\[ \eta_i(t) = \sum (\text{shell } i) n_k(t) / M_i, \text{ where } M_i \text{ is the number of harmonics in the } i \text{-th shell} \]

Evolution of the integral distribution of particles

\[ F_k = \sum k' \leq k n_k \]
Number of particles in condensate depends on the total number density $\rho = N/V$ and the energy density of the system [Connaughton, Josserand, Picozzi, Pomeau, Rica PRL 2005]. Total energy is

$$E = \sum_k k^2 a_k^* a_k + \frac{V_0}{2V} \sum_{1234} a_{k_1}^* a_{k_2}^* a_{k_3} a_{k_4} \delta_{k_1+k_2-k_3-k_4}.$$ 

Bogoliubov transformation [Bogoliubov (1947)]

$$\begin{pmatrix} a_k \\ a_{-k}^* \end{pmatrix} = \begin{pmatrix} u_+ & u_- \\ u_- & u_+ \end{pmatrix} \begin{pmatrix} b_k \\ b_{-k}^* \end{pmatrix}, \quad u_\pm = (1 \pm \Gamma_k^2)/2\Gamma_k, \quad \Gamma_k = \sqrt{\frac{k^2}{\omega(k)}}$$

is used to diagonalize the quadratic (in $k \neq 0$) term to

$$\sum_{k \neq 0} \omega(k) b_k^* b_k, \quad \omega(k) = \sqrt{k^4 + 2V_0 \rho_0 k^2}, \quad \rho_0 = n_0/V$$

$\omega(k)$ is the Bogoliubov dispersion relation that takes into account nonlinear interactions. Density of particles

$$\rho = N/V = \sum_k \langle a_k^* a_k \rangle = \rho_0 + \sum_{k \neq 0} (u_+^2 + u_-^2) \langle b_k^* b_k \rangle$$
The equilibrium distribution of non-condensed particles is found from the kinetic equation modified by the presence of condensate: \( n_{k}^{\text{eq}} = T / \omega(k) \) where \( T \) is a temperature.

In the new basis, the uncondensed mass and energy density become

\[
\rho - \rho_0 = \frac{T}{V} \sum_{k \neq 0} \frac{k^2 + V_0 \rho_0}{\omega(k)^2}.
\]

\[
\frac{E}{V} = \frac{1}{2} V_0 \left[ \rho^2 + (\rho - \rho_0)^2 \right] + \frac{T}{V} \sum_{k \neq 0} 1.
\]

\( T/V \) can be eliminated to yield the expression for the density of the condensed particles as function of the energy density for given total number density.

\[
n_0/N
\]
Evolution of topological defects: superfluid turbulence

[Berloff and Svistunov (2002)]

High-frequency wave suppression

Averaging in time

Superfluid turbulence decay: Nore et al (1997); Kobayashi & Tsubota (2005)
Dissipative dynamics of superfluid vortices at non-zero temperatures [Berloff and Youd (2007)]

Main idea: Insert a vortex ring into a state of thermal equilibrium and follow its decay due to the interactions with the non-condensed particles

(1) At all temperatures, the square of the vortex line length decays linearly with time,
\[ \frac{dL^2}{dt} = -\gamma(\rho, T/T_\lambda). \]

(2) \[ \gamma = K\rho_nT/T_\lambda \]

(3) \( \gamma \) is related to mutual friction coefficient, \( \alpha \), in HVBK:
\[ \mathbf{v}_L = \mathbf{v}_{sl} + \alpha \mathbf{s}' \times (\mathbf{v}_n - \mathbf{v}_{sl}) - \alpha' \mathbf{s}' \times [\mathbf{s}' \times (\mathbf{v}_n - \mathbf{v}_{sl})], \]
where \( \mathbf{v}_{sl} \) is the local superfluid velocity (ambient superflow + self-induced velocity \( \mathbf{u}_i \)), \( \mathbf{v}_n \) is the normal fluid velocity, \( \mathbf{s} \) is position vector, \( \mathbf{s}' \) is the unit tangent.
For a single vortex ring \( \frac{dR}{dt} = -\alpha u_i \), where \( u_i = \kappa \frac{\log(8R/\xi) - \delta + 1}{4\pi R} \)
and \( \delta \) is the vortex core parameter.

For the GP vortices \( \delta \approx 0.38 \). In dimensionless units used \( u_i = \frac{\log(8R) - \delta + 1}{R} \).

Integrate the equation for \( \dot{R} \) to get
\[
\alpha t = \frac{R_0^2 - R^2}{2(\log(8\hat{R}) + \delta - 1)}
\]
where \( \hat{R} \) is the mean radius of the ring.

Relationship between \( \gamma \) and \( \alpha \): \( \gamma = 8\pi^2 (\log(8\hat{R}) + \delta - 1) \alpha \).

No transverse force! \( \alpha' = 0 \)
Extras: Vortons, springs, etc. [Berloff & Yin (2006)]

Solitary waves moving along the vortex line.

Ansatz $\psi_1 = (R_1(r) + \chi_1(r, z)) \exp(i\theta)$, $\psi_2 = R_2(r) + \chi_2(r, z)$, where

$$
R''_1 + \frac{R'_1}{r} - \frac{R_1}{r^2} + (1 - R_1^2 - \alpha R_2^2)R_1 = 0,
$$

$$
R''_2 + \frac{R'_2}{r} + (1 - \alpha R_1^2 - R_2^2 - \Lambda^2)R_2 = 0.
$$

$R_1 \sim \psi_1 \infty - \frac{1}{2\psi_1 \infty r^2}$, $R_2 \sim \psi_2 \infty \pm K_0(2\psi_2 \infty r) \sim \psi_2 \infty \pm \exp(-2\psi_2 \infty r)$
\[ 2i\ U \frac{\partial \chi_1}{\partial z} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \chi_1}{\partial r} \right) + \frac{\partial^2 \chi_1}{\partial z^2} - \frac{\chi_1}{r^2} \]

\[ + (1 - |R_1 + \chi_1|^2 - \alpha |R_2 + \chi_2|^2)(R_1 + \chi_1) - (1 - R_1^2 - \alpha R_2^2)R_1. \]

\[ 2i\ U \frac{\partial \chi_2}{\partial z} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \chi_2}{\partial r} \right) + \frac{\partial^2 \chi_2}{\partial z^2} \]

\[ + (1 - \alpha |R_1 + \chi_1|^2 - |R_2 + \chi_2|^2 - \Lambda^2)(R_2 + \chi_2) - (1 - \alpha R_1^2 - R_2^2 - \Lambda^2)R_2. \]
Vortices in the regime of phase separation

\( \psi_1 = R_1(r) \exp(i\theta), \psi_2 = R_2(r), \) and \( |\alpha| > 1. \)

\[
R_1'' + \frac{R_1'}{r} - \frac{R_1}{r^2} + (1 - R_1^2 - \alpha R_2^2) R_1 = 0,
\]

\[
R_2'' + \frac{R_2'}{r} + (1 - \alpha R_1^2 - R_2^2 - \Lambda^2) R_2 = 0.
\]

Boundary conditions are \( R_1(0) = 0, R_1(\infty) = 1, R_2'(0) = 0, R_2(\infty) = 0. \)

For large \( r \) we have \( R_2'' + \frac{R_2'}{r} + (1 - \alpha - \Lambda^2) R_2 = 0. \)

This modified Bessel equation has solution

\( R_2 \sim K_0(\sqrt{\alpha + \Lambda^2 - 1}r) \sim \exp(-\sqrt{\alpha + \Lambda^2 - 1}r). \) This indicates that the distance over which the second component condenses is of order \( 1/\sqrt{\alpha + \Lambda^2 - 1} \)

\( \Lambda^2 = 0, \alpha = 1.03, 1.1, 1.2, 1.5 \)
Vortex rings and phase boundaries [Yin, Ko & Berloff (2007)]

Two-component condensate in the regime of phase separation \( \alpha = \frac{V_{12}}{V_{ii}} \)

A single component vortex ring interacting with a phase boundary.

Four possible outcomes in the second component:
1. One-component vortex ring;
2. Two-component vortex ring;
3. Bubble;
4. No solitary wave.

Vortex rings can be used to insert a controlled amount of one type of atoms into another.
Future directions

(1) New mathematical models of superfluids;
(2) Hierarchies of new [stochastic] models of vortex motion and turbulence;
(3) Mathematical models of interactions of various components at various conditions;
(4) Modelling beyond “mean field”;
(5) Modelling of novel systems - optical lattices, Fermi gasses, Bose-Fermi mixtures, Feshbach resonance, BCS-BEC cross-over, etc.
(6) Unique opportunity to model the physics of quantum matter in general – table-top experiments promise insights into the mechanisms of high-temperature superconductivity, physics of neutron stars, quark-gluon plasma, high energy physics, cosmology (COSLAB initiative).
References

[42] C. Yin, C. Ko, N.G. Berloff in prepararion (2007); preprint is available upon request.