Topological quantum matter and Kosterlitz-Thouless transition

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Summary

- Fluids vs superfluids
- Topology in Physics: quantized vortices
- Quantized vortex line in 2D
- BEC and Mermin-Wagner theorem
- 2D systems: Kosterlitz-Thouless transition

Fluids vs superfluids

A **fluid** can be described by the Navier-Stokes equations of hydrodynamics

$$\frac{\partial}{\partial t} n + \nabla \cdot (n\mathbf{v}) = 0 \,, \quad (1)$$

$$m \frac{\partial}{\partial t}\mathbf{v} - \eta \, \nabla^2 \mathbf{v} + \nabla \left[\frac{1}{2} m v^2 + U_{ext} + \mu(n) \right] = m \, \mathbf{v} \wedge (\nabla \wedge \mathbf{v}) \,, \quad (2)$$

where $n(\mathbf{r}, t)$ is the density field and $\mathbf{v}(\mathbf{r}, t)$ is the velocity field. Here η is the viscosity, $U_{ext}(\mathbf{r})$ is the external potential acting on the particles of the fluid, and $\mu(n)$ is the equation of state of the fluid.
A superfluid is characterized by zero viscosity, i.e. $\eta = 0$, and irrotationality, i.e. $\nabla \wedge \mathbf{v} = \mathbf{0}$.
The equations of superfluid hydrodynamics (EoSH) are then

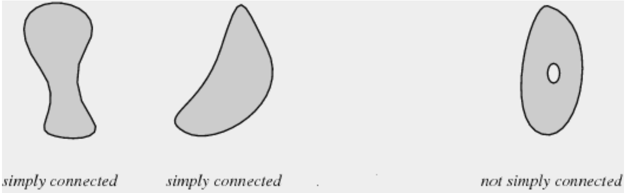
$$\frac{\partial}{\partial t} n_s + \nabla \cdot (n_s \mathbf{v}_s) = 0 \,, \quad (3)$$

$$m \frac{\partial}{\partial t}\mathbf{v}_s + \nabla \left[\frac{1}{2} m v_s^2 + U_{ext} + \mu(n_s) \right] = \mathbf{0} \,. \quad (4)$$

EoSH describe extremely well the superfluid ^{4}He, ultracold gases of alkali-metal atoms, and also several properties of superconductors.

Topology in Physics: quantized vortices (I)

Topology studies objects that are preserved under continuous deformations.



A **connected domain** is said to be simply connected if any closed curve $\mathcal{C}$ can be shrunk to a point continuously in the set.
If the domain is not simply connected, it is said to be multiply connected.

Roughly speaking, a way to produce a multiply connected domain is to introduce **holes**.

Topology in Physics: quantized vortices (II)

In the 1950s **Lars Onsager**, **Richard Feynman** (Nobel 1965), and **Alexei Abrikosov** (Nobel 2003) suggested that for superfluids the circulation of the superfluid velocity field $\mathbf{v}_s(\mathbf{r}, t)$ around a generic closed path $\mathcal{C}$ must be quantized, namely

$$\oint_{\mathcal{C}} \mathbf{v}_s \cdot d\mathbf{r} = \frac{\hbar}{m} \, 2\pi \, q \, , \tag{5}$$

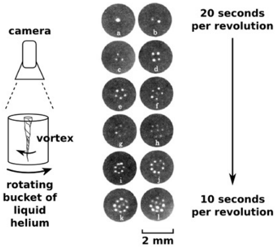
where $\hbar$ is the reduced Planck constant and $q = 0, \pm 1, \pm 2, ...$ is an integer number.
If $q \neq 0$ it means that inside the closed path $\mathcal{C}$ there are topological defects, and the domain where $\mathbf{v}_s$ is well defined is multiply connected.

For a multiply connected domain $\mathcal{D}$, with $\mathbf{r} \in \mathcal{D}$ one gets

$$\boldsymbol{\nabla} \wedge \mathbf{v}_s(\mathbf{r}) = \mathbf{0} \implies \mathbf{v}_s(\mathbf{r}) = \boldsymbol{\nabla}\chi(\mathbf{r}) \text{ with } \chi(\mathbf{r}) \text{ multi-valued scalar field.}$$

Topology in Physics: quantized vortices (III)

A simple example of topological defect is a quantized vortex line along the z axis.



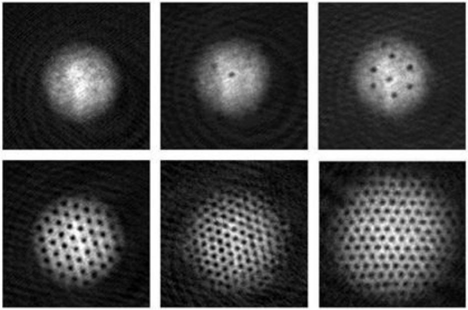
Vortex line: superfluid number density n_s and modulus of the superfluid velocity v_s as a function of the cylindric radial coordinate R.

$$n_s(R) \simeq n_s(\infty) \left(1 - \frac{1}{1 + \frac{R^2}{\xi^2}} \right) \quad \text{and} \quad v_s(R) = \frac{\hbar}{m} \frac{q}{R}$$

Clearly at $R = 0$, i.e. at $(x, y) = (0, 0)$, the superfluid velocity is not defined. q is called charge of the vortex and ξ is the healing length.

Topology in Physics: quantized vortices (IV)

Nowadays quantized vortices are **observed experimentally** in type-II superconductors, in superfluid liquid helium, and in ultracold atomic gases.



Formation of quantized vortices in a Bose-Einstein condensate of ^{87}Rb atoms. The number of quantized vortices grows by increasing the frequency of rotation of the system [J. R. Abo-Shaeer, C. Raman, J.M. Vogels, W. Ketterle, Science **292**, 476 (2001)]. **Wolfang Ketterle**, with **Eric Cornell** and **Carl Wieman** (Nobel 2001).

Topology in Physics: quantized vortices (V)

The quantization of circulation can be explained assuming that the dynamics of **superfluids** is driven by a complex scalar field

$$\psi(\mathbf{r},t) = |\psi(\mathbf{r},t)| \; e^{i\theta(\mathbf{r},t)} \; , \tag{6}$$

which satisfies the nonlinear Schrödinger equation (NLSE)

$$i\hbar \frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + U_{ext} \right] \psi + \mu(|\psi|^2) \; \psi \tag{7}$$

and it is such that

$$n_s(\mathbf{r},t) = |\psi(\mathbf{r},t)|^2 \; , \qquad \mathbf{v}_s(\mathbf{r},t) = \frac{\hbar}{m} \boldsymbol{\nabla}\theta(\mathbf{r},t) \; . \tag{8}$$

In fact, under these assumptions, NLSE is practically equivalent to EoSH and the angle variable $\theta(\mathbf{r},t)$ is such that

$$\oint_{\mathcal{C}} d\theta = \oint_{\mathcal{C}} \boldsymbol{\nabla}\theta(\mathbf{r},t) \cdot d\mathbf{r} = 2\pi \sum_j q_j \; , \tag{9}$$

with q_j the quantum number, also called topological charge, of the j-th vortex.

Topology in Physics: quantized vortices (VI)

The NLSE of the complex scalar field $\psi(\mathbf{r}, t)$ of superfluids

$$i\hbar \frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + U_{ext} \right] \psi + \mu(|\psi|^2)\ \psi \tag{10}$$

admits the constant of motion (energy of the system)

$$E = \int \left\{ \frac{\hbar^2}{2m}|\nabla\psi|^2 + U_{ext}\ |\psi|^2 + \mathcal{E}(|\psi|^2) \right\}\ d^D\mathbf{r}\ , \tag{11}$$

where $\mu(|\psi|^2) = \frac{\partial \mathcal{E}(|\psi|^2)}{\partial |\psi|^2}$. Taking into account that

$$\psi(\mathbf{r}, t) = n_s(\mathbf{r}, t)^{1/2}\ e^{i\theta(\mathbf{r},t)} \quad \text{with} \quad \mathbf{v}_s(\mathbf{r}, t) = \frac{\hbar}{m}\boldsymbol{\nabla}\theta(\mathbf{r}, t) \tag{12}$$

one finds

$$\frac{\hbar^2}{2m}|\nabla\psi|^2 = \frac{\hbar^2}{2m}\ n_s\ (\nabla\theta)^2 + \frac{\hbar^2}{8m}\frac{(\nabla n_s)^2}{n_s}\ , \tag{13}$$

which are phase-stiffness energy and quantum pressure.

Quantized vortex line (I)

For a three-dimensional (3D) time-independent superfluid we have

$$\psi(\mathbf{r}) = |\psi(\mathbf{r})| \; e^{i\theta(\mathbf{r})} \; , \tag{14}$$

where $\mathbf{r} = (x, y, z)$ is the position vector,

$$n_s(\mathbf{r}) = |\psi(\mathbf{r})|^2 \; , \qquad \mathbf{v}_s(\mathbf{r}) = \frac{\hbar}{m} \boldsymbol{\nabla} \theta(\mathbf{r}) \; . \tag{15}$$

A single quantized vortex line with topological charge $q \in \mathbb{Z}$ and located along the z axis is obtained setting $U_{ext} = 0$ and

$$\theta(\mathbf{r}) = q \; \phi = q \arctan\left(\frac{y}{x}\right) \; , \tag{16}$$

where $\phi = \arctan(y/x)$ is the polar angle of cylindrical coordinates. Taking into account that $\boldsymbol{\nabla} = (\partial_x, \partial_y, \partial_z) = (\partial_R, \frac{1}{R}\partial_\phi, \partial_z)$ with $R = \sqrt{x^2 + y^2}$ is the polar radius of cylindrical coordinates, one finds

$$\mathbf{v}_s(\mathbf{r}) = \frac{\hbar}{m} \frac{q}{R} \, \mathbf{u} \; , \tag{17}$$

where $\mathbf{u} = \left(- \frac{y}{\sqrt{x^2+y^2}}, \frac{x}{\sqrt{x^2+y^2}}, 0 \right)$ is a unit vector orthogonal to $\mathbf{r}$.

Quantized vortex line (II)

Let us now consider a stationary two-dimensional (2D) superfluid with a quantized vortex line. We also assume that the modulus of the complex scalar field is uniform, i.e.

$$\psi(\mathbf{r}) = \psi_0 \; e^{i\theta(\mathbf{r})} = \psi_0 \; e^{iq\phi} = \psi_0 \; e^{iq \arctan\left(\frac{y}{x}\right)} \; , \tag{18}$$

where $\mathbf{r} = (x, y) = (r, \phi)$ with $r = \sqrt{x^2 + y^2}$ and $\phi = \arctan(y/x)$. The kinetic energy E_K, with $n_{s0} = |\psi_0|^2$ and $v_s(\mathbf{r}) = (\hbar/m)(q/r)$, is given by

$$\begin{aligned} E_K &= \int \left\{ \frac{1}{2} m \; n_{s0} \; v_s(\mathbf{r})^2 \right\} \; d^2\mathbf{r} = \frac{1}{2} m \; n_{s0} \int \left\{ \frac{\hbar^2 q^2}{m^2 r^2} \right\} \; d^2\mathbf{r} \\ &= n_{s0} \frac{\hbar^2 q^2}{2m} \int_{r_0}^{r_{max}} dr \;\; r \int_0^{2\pi} d\phi \frac{1}{r^2} \\ &= \frac{\pi \hbar^2 n_{s0}}{m} \; q^2 \;\; \ln\left(\frac{r_{max}}{r_0} \right) \; , \end{aligned} \tag{19}$$

where r_0 is the minimal distance, related to the healing length, while r_{max} is the maximal distance. Notice that $E_K = 0$ for $r_{max} = r_0$.

Vortex-antivortex pair (I)

Let us now consider a 2D superfluid system characterized by two (effectively parallel along the z axis) vortex lines at the 2D positions $\mathbf{r}_1 = (x_1, y_1)$ and $\mathbf{r}_2 = (x_2, y_2)$ with opposite topological charge q and $-q$. This is the so-called vortex-antivortex configuration. The corresponding 2D superfluid velocity is given by

$$\mathbf{v}_s(\mathbf{r}) = \mathbf{v}_{s,1}(\mathbf{r}) + \mathbf{v}_{s,2}(\mathbf{r}) = \frac{\hbar}{m}\frac{q}{|\mathbf{r}-\mathbf{r}_1|}\,\mathbf{u}_1 - \frac{\hbar}{m}\frac{q}{|\mathbf{r}-\mathbf{r}_2|}\,\mathbf{u}_2 \ , \tag{20}$$

where

$$\mathbf{u}_j = \frac{1}{|\mathbf{r}-\mathbf{r}_j|}\,(y_j - y, x - x_j) \tag{21}$$

are 2D unit vectors perpendicular (in the plane XY) to the 2D position vectors $\mathbf{r} - \mathbf{r}_j = (x - x_j, y - y_j)$, with $j = 1, 2$.

Vortex-antivortex pair (II)

The kinetic energy of this system then reads

$$E_K = \int \left\{ \frac{1}{2} m \; n_{s0} \; v_s(\mathbf{r})^2 \right\} \; d^2\mathbf{r} = \frac{1}{2} m \; n_{s0} \int \left\{ |\mathbf{v}_{s,1}(\mathbf{r}) + \mathbf{v}_{s,2}(\mathbf{r})|^2 \right\} \; d^2\mathbf{r}$$

$$= \frac{\hbar^2 n_{s0} q^2}{2m} \int \left| \frac{\mathbf{u}_1}{|\mathbf{r} - \mathbf{r}_1|} - \frac{\mathbf{u}_2}{|\mathbf{r} - \mathbf{r}_2|} \right|^2 \; d^2\mathbf{r} \; . \tag{22}$$

After some calculations one finds

$$E_K = E_{K,1} + E_{K,2} + E_{K,12} \; , \tag{23}$$

where

$$E_{K,1} = E_{K,2} = \frac{\pi \hbar^2 n_{s0}}{m} \; q^2 \; \ln \left(\frac{r_{max}}{r_0} \right) \tag{24}$$

$$E_{K,12} = 2\pi \frac{\hbar^2 n_{s0} q^2}{m} \ln \left(\frac{|\mathbf{r}_1 - \mathbf{r}_2|}{r_0} \right) \; . \tag{25}$$

The formation of a vortex-antivortex pair at a distance larger that r_0 has an energy cost. Thus, oppositely charged vortices attract, and they prefer to stay at the minimal distance, i.e. $|\mathbf{r}_1 - \mathbf{r}_2| = r_0$.

BEC and Mermin-Wagner theorem (I)

In three spatial dimensions ($D = 3$), the complex scalar field of superfluids is called order parameter of the system and it is often identified as the **macroscopic wavefunction** of Bose-Einstein condensation (BEC), where a macroscopic fraction of particles occupies the same single-particle quantum state.

BEC phase transition: For an ideal gas of non-interacting identical bosons there is BEC only below a critical temperature T_{BEC}. In particular one finds

$$k_B\, T_{BEC} = \begin{cases} \frac{1}{2\pi\zeta(3/2)^{2/3}} \frac{\hbar^2}{m} n^{2/3} & \text{for } D = 3 \\ 0 & \text{for } D = 2 \\ \text{no solution} & \text{for } D = 1 \end{cases}$$

where D is the spatial dimension of the system, n is the number density, and $\zeta(x)$ is the Riemann zeta function.

BEC and Mermin-Wagner theorem (II)

This result due to Einstein (1925), which says that there is no BEC at finite temperature for $D \leq 2$ in the case of non-interacting bosons, was extended to interacting systems by **David Mermin** and **Herbert Wagner** in 1966.

For the BEC phase transition, the Mermin-Wagner theorem states that

there is no Bose-Einstein condensation at finite temperature in homogeneous systems with sufficiently short-range interactions in dimensions $D \leq 2$.

2D systems: Kosterlitz-Thouless transition (I)

Despite the absence of BEC, in 1972 **Kosterlitz** and **Thouless** (but also **Vadim Berezinskii** (1935-1980)) suggested that a 2D fluid can be superfluid below a critical temperature, the so-called Berezinskii-Kosterlitz-Thouless critical temperature T_{BKT}.
They analyzed the 2D XY model, which was originally used to describe the magnetization in a planar lattice of classical spins. The energy of the continuous 2D XY model is given by

$$E = \int \frac{J}{2} \left(\nabla\theta\right)^2 \; d^2\mathbf{r} \ ,$$

where $\theta(\mathbf{r})$ is the angular field and J is the phase stiffness (rigidity).
This is nothing else than the energy of the 2D NLSE of the complex scalar field

$$\psi(\mathbf{r}) = \psi_0 \, e^{i\theta(\mathbf{r})} \qquad (26)$$

of 2D superfluids with a uniform modulus $\psi_0 = \sqrt{n_{s0}}$, where $J = n_{s0}(\hbar^2/m)$, and neglecting the bulk energy.

2D systems: Kosterlitz-Thouless transition (II)

A simple way to estimate the Berezinskii-Kosterlitz-Thouless (BKT) critical temperature T_{BKT} is to consider the Helmholtz free energy F of the 2D superfluid system characterized by **one vortex line** with topological charge $q = 1$ at temperature T. It is given by

$$F = E - T\ S\ , \tag{27}$$

where the internal energy E reads

$$E = \pi J\ \ln\left(\frac{R}{r_0}\right) \tag{28}$$

with $J = \hbar^2 n_{s0}/m$ the phase stiffness, while the entropy S is given by

$$S = k_B \ln\left(\frac{\pi R^2}{\pi r_0}\right) = 2k_B \ln\left(\frac{R}{r_0}\right)\ , \tag{29}$$

with $(\pi R^2)/(\pi r_0^2)$ the number of possible configurations of the vortex line of size r_0 in a circular domain of size R.

2D systems: Kosterlitz-Thouless transition (III)

It follows that

$$F = (\pi J - 2k_B T) \ \ln\left(\frac{R}{r_0}\right) . \tag{30}$$

This function does not have singularities. The temperature T_c at which F changes sign is then

$$k_B T_c = \frac{\pi}{2} J = \frac{\pi \hbar^2 n_{s0}}{2m} . \tag{31}$$

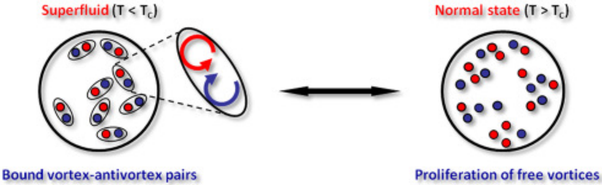
For $T < T_c$ the free energy F is positive and in the limit $R \to +\infty$ it goes to $F \to +\infty$. Instead, $T > T_c$ the free energy F is negative and in the limit $R \to +\infty$ it goes to $F \to -\infty$. Therefore, in the case of a very large system, T_c signals the topological phase transition from a superfluid phase $(0 \leq T < T_c)$ without free vortices to a normal phase $(T > T_c)$ characterized by the proliferation of free vortices.

This is the simplest argument for the Kosterlitz-Thouless transition based on a single vortex. Actually, Eq. (31) gives the same critical temperature T_{BKT} one derives from a more sophisticated approach based on the renormalization group.

2D systems: Kosterlitz-Thouless transition (IV)

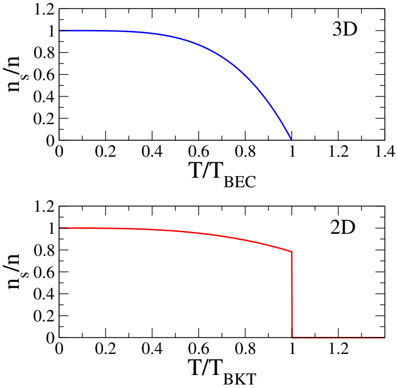
The analysis of **Kosterlitz** and **Thouless** based on the renormalization group shows that:

- As the temperature T increases vortices start to appear in vortex-antivortex pairs (mainly with $q = \pm 1$).
- The pairs are bound at low temperature until at the critical temperature $T_c = T_{BKT}$ an unbinding transition occurs above which a proliferation of free vortices and antivortices is predicted.
- The phase stiffness J is renormalized by the presence of vortices.
- The renormalized superfluid density $n_s = J(m/\hbar^2)$ decreases by increasing the temperature T and jumps to zero above $T_c = T_{BKT}$.



2D systems: Kosterlitz-Thouless transition (V)

An important prediction of the Kosterlitz-Thouless transition is that, contrary to the 3D case, in 2D the superfluid fraction n_s/n jumps to zero above a critical temperature.



For 3D superfluids the transition to the normal state is a BEC phase transition, while in 2D superfluids the transition to the normal state is something different: a topological phase transition.