

Berezinskii-Kosterlitz-Thouless Phase Transition and Superfluidity In Two Dimensions

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2016-12-03

Nobelprize.org

2016 Nobel Prize in Physics

Popular Information

Title: **Strange Phenomena in Matter's flatland**

"*Together, they (Thouless and Kosterlitz) took on the problem of phase transitions in the flatlands (the former out of curiosity, the latter out of ignorance, they themselves claim)*."

"*…an entirely new understanding of phase transitions, which is regarded as one of the twentieth century's most important discoveries in the theory of condensed matter physics*."—BKT phase transition

"*The wonderful thing…is that it can be used for different types of materials the KT transition is universal…The theory…also confirmed experimentally*."

2016 Nobel Prize in Physics

Advanced Information

Title: **Topological Phase Transitions and Topological Phases of Matter**

"In 1972 J. Michael Kosterlitz and David J. Thouless identified a completely new type of phase transition in two-dimensional systems where topological defects play a crucial role [35, 36]. Their theory applied to certain kinds of magnets and to superconducting and superfluid films, and has also been very important for understanding the quantum theory of one-dimensional systems at very low temperatures."

"This insight has provided an important link between statistical mechanics, quantum many-body physics and high-energy physics, and these fields now share a large body of theoretical techniques and results."

Goal of this lecture is to address

(1) What is the Berezinskii-Kosterlitz-Thouless phase transition?

(2) What is the superfluidity?

Outline

- Phase transition in high-dimensional XY model \checkmark Ginzburg-Landau mean-field theory
- Monte Carlo simulation in three and two dimensions
- Berezinskii-Kosterlitz-Thouless phase transition
	- \checkmark Wegener's model (Gaussian model)
	- \checkmark Topological excitation and BKT phase transition
	- \checkmark Nelson-Kosterlitz relation (universal jump in superfluid density)
	- \checkmark Renormalization group analysis
- What is superfluidity
	- \checkmark Hallmarks of superfluidity
	- \checkmark Two questions—on its relation to BEC/excitation spectrum

Phase Transition in High-Dimensional XY Model

Emergent Phenomena

Emergent matter state

More is different! Each hierarchical level of science requires its own fundamental principles for advancement. —— P. W. Anderson

Emergent Phenomena

Emergent scale invariance at 2nd-order phase transition

Universal properties!

Universality of Criticality. Critical physics can be captured by a few parameters symmetry of the order parameter, interaction range, and spatial dimensions

Statistical mechanics is to understand emergent (quantum) macroscopic matter state from microscopic interactions. Given a many-body Hamiltonian, the core task is to calculate partition sum

$$
Z = \mathrm{Tr}e^{-H/k_b T} = \sum_i p_i
$$

Macroscopic matter state

• gas, liquid, solid

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- gas, liquid, solid
- magnetism (ferromagnet, antiferromagnet…)

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Macroscopic matter state

• gas, liquid, solid

• …

- magnetism (ferromagnet, antiferromagnet…)
- superfluidity, superconductivity...

Which macroscopic matter state?

Free energy

$$
F = -k_{\rm B}T \ln Z \qquad k_{\rm B} \qquad \text{Boltzmann constant}
$$

Thermodynamic relation

$$
F = E - TS
$$

 $S = k_B ln \Omega$ — entropy E — internal energy Ω — number of microscopic configurations

Thermodynamic law

The stable matter state at a given temperature T is determined by the minima of the free energy

Energy-Entropy Competition/Balance

- At high T, "large entropy" dominates—gas, liquid, plasma
- At low T, "low energy" dominates—crystal, superfluid

Ising Model

"Spontaneous symmetry breaking" is one of the most profound concepts in statistical mechanics and condensed-matter physics.

XY Model

◢

The XY model

$$
H = -\sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = -\sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \qquad \vec{S} = (\cos \theta, \sin \theta) \qquad \boxed{\theta}
$$

 \checkmark U(1) symmetry: Hamiltonian remains unchanged if all the spins *are rotated by fixed angle θ*

Partition sum

$$
Z = \int_{[-\pi,\pi]^\Lambda} \prod_{j\in\Lambda} d\theta_j\; e^{-\beta H({\bf s})}
$$

$$
\checkmark \text{ Local order parameter: } \overrightarrow{M} = \frac{1}{V} \sum_{i} \vec{S}_{i}
$$

- At *T*=0, all spins point to the same direction ferromagnet
- At *T*=infinite, each spin points to a random direction paramagnet

Question

Is there a critical temperature T_c >0 between ferromagnet and paramagnet?

XY Model

Ginzburg-Landau mean-field theory

Free energy density

$$
V(n_0) = -\frac{\mu}{2} |\psi|^2 + \frac{\lambda}{2} |\psi|^4 \qquad (n_0 = |\psi|^2)
$$

- \checkmark *Order parameter is just a complex number* $\Psi \equiv M$. In the context of \longrightarrow *superfluidity,* n_0 *is the density of Bose-Einstein condensation*
- ν μ (T) is chemical potential; λ >0 is for interaction

Solution

XY Model

Mean-field (MF) theory of the XY model

- Ignore fluctuations that are crucial in low-dimensional systems
- For $d>d_{c}=4$, MF critical exponents are correct MF critical point are wrong
- For $d=3$, MF critical exponents are correct MF critical point are wrong
- For $d=2$, the **topological BKT** phase transition is beyond the Ginzburg-Landau mean-field scenario

Complex field model of the XY model

$$
H_{\psi} = -t \sum_{\langle i\mathbf{k}\rangle} \left(\psi_{i}^{*} \psi_{\mathbf{k}} + c.c. \right) + \frac{U}{2} \sum_{i} |\psi_{i}|^{4} - \mu \sum_{i} |\psi_{i}|^{2}
$$

Research tools

- \checkmark Analytical calculation (1D)
- Renormalization group analysis
- Monte Carlo simulation

Monte Carlo Simulation in Three and Two dimensions

Schematic behavior

Two-point correlation function $g(r)$

•
$$
d=3
$$

\n
$$
g(r) = \left\langle \vec{S}_0 \cdot \vec{S}_r \right\rangle = \begin{cases} c_1 e^{-r/\xi} & T > T_c \\ n_0 & T < T_c \\ n_0 \quad -BEC \text{ density} \end{cases}
$$

•
$$
d=2
$$

$$
g(r) = \begin{cases} c_1 e^{-r/\xi} & T > T_c \\ c_2 r^{-\eta(T)} & T \le T_c \end{cases}
$$

 \checkmark No BEC in 2D *g*(*r* → ∞) = 0

No spontaneous symmetry breaking for 2D XY model

Topologically distinct configurations

\n
$$
v = \frac{1}{2\pi} \oint_C d\vec{r} \cdot \vec{\nabla} \theta(\vec{r})
$$
\n

\n\n $\begin{array}{r}\n \text{Matrix: } \n \begin{align*}\n \text{Matrix: } \n \begin{align*}\n \text{Matrix: } \n \begin{align*}\n \text{Matrix: } \n \end{align*} \\
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"Topologically distinct"— two configurations cannot be transformed into each other by a continuous rotation of the spins.

Illustration of MC simulation

• $v = +1$

 $v = -1$

Illustration of MC simulation

• $v = +1$

Illustration of MC simulation

• $v = +1$ $v = -1$

Probability distribution of magnetization in 3D

 $T = 2.0$ $T = 2.1$ $T = 2.2(T_c)$ $T = 2.3$ $T = 2.4$

Energy density $\varepsilon(T) = \frac{1}{N}$ *V* $\overline{U}_{total}(T)$

Superfluid density ρ_s

Two-point correlation function $g(r) = \left\langle e^{i(\theta_0 - \theta_r)} \right\rangle$

Berezinskii-Kosterlitz-Thouless Phase Transition in the Two-Dimensional XY Model

Wegner's model (Gaussian model)

• **Hamiltonian of XY model**

$$
H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)
$$

 \checkmark spin-wave excitation (gapless)

• **Wegner's model** (1967) Taylor expand till 2^{nd} order $\&$ ignore 2π -periodicity

$$
H = E_0 - \frac{J}{2} \sum_{\langle ij \rangle} (\varphi_i - \varphi_j)^2 \qquad \varphi \in (-\infty, +\infty)
$$

Lattice Fourier transform

$$
H = E_0 - \frac{J}{2} \sum_{\mathbf{k}} \varepsilon_k |\varphi_{\mathbf{k}}|^2 \qquad \varepsilon_k = \frac{k^2}{2}
$$

 \checkmark ideal gas (in momentum space)

Wegner's model

Spin-Ordering in a Planar Classical Heisenberg Model

FRANZ WEGNER

Max-Planck-Institut für Physik und Astrophysik, München, Germany

Received July 26, 1967

We consider a D-dimensional system of classical spins rotating in a plane and interacting via a Heisenberg coupling. The spin-correlation function $g_p(r)$ is calculated for large distances r in a low-temperature approximation (taking \overline{m} account shortrange order):

$$
g_1(r) = \exp(-C_1 Tr),
$$

\n
$$
g_2(r) \sim r^{-C_2 T},
$$

\n
$$
\lim_{r \to \infty} g_3(r) = \exp(-C_3 T).
$$

- \checkmark No long-range order for D \leq 2
- \checkmark Correlation function algebraically decays for any T \neq 0 in 2D — *algebraic* order or *quasi-long-range* order

Wegner's model

Mermin-Wegner theorem

In one and two dimensions, continuous symmetries cannot be spontaneously broken at finite temperature in systems with **short-range** interactions

Direct consequences

 \checkmark No BEC for $T\neq 0$ in 2D and 1D Yes in 2D harmonic trap

Explaination

 \checkmark ……

It cost very little energy to induce long-range fluctuations which have enormous entropy and are free-energy-preferred

Topological excitation and BKT transition

Can $U(1)$ nature (θ period) be ignored?

Energy of a single vortex

$$
E_{\rm v} = \pi J \ln \frac{L}{a} \quad \checkmark \quad \text{costive} \quad \text{logarithm of } L
$$

Entropy of a vortex

$$
S_{\rm V} = 2k_{\rm B} \ln \frac{L}{a}
$$
 \t\t \check{a} also logarithm of L

• Free energy *F=E-TS* (energy-entropy balance) $\Delta F = (\pi J - 2 k_{\rm B} T) \ln$ *L* $\frac{L}{a} \Rightarrow k_{\text{B}}T_c =$ πJ 2

Vortex: a topological defect

BKT phase transition is "one of *the 20th century's most important discoveries in the theory of condensed matter physics*"

—popular science background for Nobel Prize in Physics, 2016

- Energy of vortex-anti-vortex pair $E = 2\pi J \ln$ *r a*
- \checkmark for $T < T_c$
	- vortex pairs are bound (in order of lattice spacing)
	- spin-wave excitations lead to "*algebraic/quasi-long-range order*"
	- bound vortex pairs lead to renormalization of coupling *K* that determines critical exponent for the algebraic decay of correlation function

Vortex number per site N and its fluctuation X_N in 2D XY model

Nelson-Kosterlitz relation

Universal jump in superfluid density at T_c

$$
\rho(T_c) = T_c \frac{2}{\pi} \frac{m^2 k_B}{\hbar^2}
$$

Renormalization group analysis

Basic idea: *coarse-grain* and integrate out degrees of freedom for vortexantivortex pairs of *short* distance

RG equation:

 $\begin{array}{rcl} \displaystyle{ \frac{dt}{d\ell} }&=&\displaystyle{ 4\pi^3 y^2 }\\ \displaystyle{ \frac{dy}{d\ell} }&=&\displaystyle{ 4ty/\pi } \end{array}$ *y* — fugacity of vortex $t \text{ -deviation } \sim (T - T_c)$ $b = e^{\ell} \approx 1 + \ell$ *RG* scale

- \checkmark y=0 accounts for the "vacuum" states free of vortices, but with various Gaussian fluctuation modes
- \checkmark the vacuum is stable for *t*<0 (superfluid) and unstable for *t*>0 (normal fluid)

What is Superfluidity

- Finie-temperature (thermomechanical) effects
- 1. Superconductivity of heat/Counterflow
- 2. Fountain effect
- 3. Escaping from a Dewar

4. ……

Frictionless flow below *T*^λ

- 1908 , 4 He liquefied (Onnes) - 1911, "supraconductivity" of mercury (Onnes) 4He stops boiling below certain temperature (Onnes)
- 1922, peculiarity of specific heat (Dana, not published)
- $-$ 1927-1937, phase transition (T_n=2.17K); heat-capacity anomaly, huge reduction of viscosity; "Supra-heat-conductivity" (Keesom, Misner, Allen…)
- 1938, **Discovery of superfluidity** (Kapitza; Allen and Misener)
- 1938, fountain effect (Allen and Jones)

It took 20 years to discover "superfluidity"

Frictionless flow below *T*λ

Liquid ⁴He stops boiling \leq 2.3K. J.C. McLennan *et al*. (1932)

The helium below the λ -point enters a special state which might be called a 'superfluid' -P. Kapitsa (1937)

λ-transition of Helium 4. W.H. Keesom and A.P. Keesom (1935)

Hess-Fairbank effect and Persistent current

Define ω_c = \hbar *mR*² \equiv quantum unit of rotation (10⁻⁴ Hz for 1cm)

Hess-Fairbank effect Wall rotates with $\omega \leq \omega_c$, liquid stationary Equilibrium Effect

Persistent current Wall at rest, Liquid rotates with $\omega \gg \omega_c$, Metastable Effect

Quantized vortices

 \checkmark Theoretical predictions of vortices in superfluid (1948, 1955), and superconductor (Abrikosov 1957)

Onsager 1948, Landau-Lifshitz 1955

Onsager 1949, Feynman 1955

 $\oint_C \vec{v}_s \cdot d\vec{l} = 2\pi\gamma \times \text{integer}$
 $\gamma = \hbar / m$

Varmchuk *et al*. 1979

Vortices in ultracold atomic gases

JILA, 1999 ENS, 2000 MIT, 2001 MIT, 2005

Quantized vortices

 V USTC: ⁶Li-⁴¹K supercluid mixture

Vortex lattice in single-species superfluid

Quantized vortices

V USTC: ⁶Li-⁴¹K supercluid mixture

Vortex lattice in two-species superfluid

Vortex ring in 3D and its metastability

A sidedish (superlink) $-$ Crazy pool vortex

- \checkmark In 3D, vortices have to form a closed ring or an open chain ending at the surface.
- \checkmark Vortices, vortex-rings and persistent currents are metastable due to angular momentum.
- \checkmark Unlike classical analogue, quantum vortex has quantized angular momentum

What is Superfludity?

Mordern view of superfluidity: emergent constant of motion

Superfluid is a natural low-T state of a classical complex-valued matter field, arising from an emergent constant of motion—i.e., topological order $\psi($ \rightarrow \vec{r}) = $|\psi($ \rightarrow \vec{r}) $e^{i\Phi(x)}$ \rightarrow Complex matter field: $\psi(\vec{r}) = |\psi(\vec{r})| e^{i\Phi(\vec{r})}$

 \rightarrow Superfluid velocity field: $\vec{v}_s = \gamma \ \nabla \Phi \ \ (\gamma = \hbar/m)$

Emergent constant of motion: quantized circulation $\oint\limits_C \vec{v}_s \cdot d\vec{l} = \gamma \oint\limits_C d\vec{l} \cdot \nabla \Phi = 2\pi \gamma \times \text{integer}$ leads to superfluidity

 \checkmark can be destroyed *only* by **topological** defects (vortices)

Back to Einstein at 1924-1925

Bose-Einstein statistics for an ideal bosonic system

- Single-particle phase space (μ -space): (x, y, z, k_x, k_y, k_z) Phase-space cell: $\delta x \delta y \delta z \delta k_x \delta k_y \delta k_z = h^3$
- Occupation number in each phase-space cell

— for photons/phonon: $\varepsilon = ck = \hbar \omega, \mu = 0$ — for massive bosons: $\varepsilon = k^2 / 2m, \mu \le 0$

• Bose-Einstein condensation

 $T < T_c$: *f*

1

 $e^{\beta(\varepsilon-\mu)}-1$

 $f =$

A macroscopic number of atoms condense into the quantum state of the lowest momentum.

Thermal wavelength $\lambda_{T} \gg d$, BEC is a matter field ψ (\rightarrow \vec{r}) = $|\psi($ $\overrightarrow{1}$ \vec{r}) $e^{i\Phi(\vec{r})}$

• For low *T*, one has $\mu \rightarrow 0^-$ and $f \gg 1$ for small-*k* motions, the classical matter-field description is valid; No BEC (macroscopic occupation) or superfluidity (topological order) is requested.

Back to Einstein at 1924-1925

Quantentheorie des einatomigen idealen Gases.

Von A. EINSTEIN.

Eine von willkürlichen Ansätzen freie Quantentheorie des einatomigen idealen Gases existiert bis heute noch nicht. Diese Lücke soll im folgenden ausgefüllt werden auf Grund einer neuen, von Hrn. D. Bose erdachten Betrachtungsweise, auf welche dieser Autor eine höchst beachtenswerte Ableitung der PLANCKSchen Strahlungsformel gegründet hat1.

"*One can assign a scalar* wave *field to such a gas… It looks like there would be an* undulatory field *associated with each phenomenon of motion, just like the optical undulatory field is associated with the motion of light quanta.*"

 \checkmark Einstein's classical-field idea for quantum gas was forgotten for tens of years, probably due to the advent of rigorous quantum mechanics

Back to Einstein at 1924-1925

2001 Nobel Prize in Physics

E.A. Cornell W. Ketterle C.E. Wieman

87Rb

"*for the achievement of* Bose-Einstein condensation *in dilute gases of alkali atoms, and for early* fundamental studies *of the properties of the condensates***"**

BEC cartoon

What is Superfludity?

Relation of superfluidity to BEC

- 1938, London argues that Einstein's condensation does exist and suggests that the lambda-transition is related to BEC.
- 1938, Tisza introduces the **two-fluid concept**, with the conjecture that the superfluid component is nothing but **BEC**.
- 1955, Penrose introduces the concept of "off-diagonal long-range order" $\rho(\mathbf{r}_1,\mathbf{r}_2) = \langle \psi^{\dagger}(\mathbf{r}_2) \psi(\mathbf{r}_1) \rangle \rightarrow \psi_0^*(\mathbf{r}_2) \psi_0(\mathbf{r}_1)$ at $|\mathbf{r}_1 - \mathbf{r}_2| \rightarrow \infty$

"Paradox" for 2D finite-temperature system,

- \checkmark Mermin-Wegner theorem states that no long-range order occurs
- \checkmark Experiments show no doubt for the existence of superfluidity

BEC is a sufficient but not a necessary condition for superfluidity

Relation of superfluidity to elementary excitation spectrum

- **1941, Landau's critical velocity** dispersion ε(**q**):

- not sufficient: finite-T superfluidity
- not necessary: ³He-A, "supersolidity"

Landau's criterion for superfluidity is instructive, however, it is neither a sufficient nor a necessary condition

What is Superfludity?

Superfluidity: emergent topological order

 $\oint_{G} \vec{v}_s \cdot d\vec{l} = \gamma \oint_{G} d\vec{l} \cdot \nabla \Phi = 2\pi \gamma \times \text{integer}$

- \checkmark BKT phase transition in 2D (Berezinskii 1971, Kosterlitz-Thouless 1972, Nelson Kosterlitz 1976)
- \checkmark direct experimental evidence of topological order in 2D (Telschow and Hallock, 1976)

The value of the persistent current in an annulus is changed by many orders of magnitude—by changing the thickness of the superfluid 4He film (as a response to the chemical potential shared by the film with the vapor in the bulk).

In contrast to a dramatic change in the value of the net persistent current, the velocity of the superflow stays intact.

Thermomechanical effect of superfluidity

Basic equation

$$
\dot{\mathbf{v}}_s = -\nabla \tilde{\mu} \qquad (v_n = 0) \qquad \tilde{\mu} = \mu / m
$$

- \checkmark Super-heat-conductivity
- \checkmark Fountain effect
- \checkmark Escaping from a Dewar
- The superfluid component is of zero entropy
- Heat is transported mechanically by flow of normal component

Counterflow: $T \uparrow$, $\mu(T) \downarrow$

Summary

Take-home message

- Superfluid is the property of a complex-valued matter field, which is inherited by quantum bosonic systems
- BKT phase transition is driven by topological defects—vortices

Lecture note is prepared together with

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Thank You

