

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

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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
   ✓ Ginzburg-Landau mean-field theory
- Monte Carlo simulation in three and two dimensions
- Berezinskii-Kosterlitz-Thouless phase transition
  - ✓ Wegener's model (Gaussian model)
  - ✓ Topological excitation and BKT phase transition
  - ✓ Nelson-Kosterlitz relation (universal jump in superfluid density)
  - ✓ Renormalization group analysis
- What is superfluidity
  - ✓ Hallmarks of superfluidity
  - ✓ 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 fundamentalprinciples for advancement.— P. W. Anderson

# **Emergent Phenomena**

#### Emergent scale invariance at 2<sup>nd</sup>-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

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

## Macroscopic matter state

• gas, liquid, solid



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### Macroscopic matter state

- 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

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

Thermodynamic relation

$$F = E - TS$$

E - internal energy  $S = k_{\text{B}} \ln \Omega - \text{ entropy}$  $\Omega - \text{ number of microscopic configurations}$ 

#### 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**

1

The XY model

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

✓ U(1) symmetry: Hamiltonian remains unchanged if all the spins are rotated by fixed angle  $\theta$ 

Partition sum

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

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

- 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

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

- ✓ Order parameter is just a complex number  $\Psi \equiv M$ . In the context of superfluidity,  $n_0$  is the density of Bose-Einstein condensation
- ✓  $\mu(T)$  is chemical potential;  $\lambda > 0$  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

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

Research tools

- ✓ 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  

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



• d=2  

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

✓ No BEC in 2D  $g(r \rightarrow \infty) = 0$ 

No spontaneous symmetry breaking for 2D XY model



Topologically distinct configurations

Vorticity 
$$v = \frac{1}{2\pi} \oint_C d\vec{r} \cdot \vec{\nabla} \theta(\vec{r})$$
  
 $\nu = +1$   $\nu = 0$ 

"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

● *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  $\varepsilon(T) = \frac{1}{V} \langle U_{total}(T) \rangle$ 







#### Superfluid density $\rho_s$



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

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

✓ spin-wave excitation (gapless)

Wegner's model (1967)
 Taylor expand till 2<sup>nd</sup> 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

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

✓ 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  $g_D(r)$  is calculated for large distances r in a low-temperature approximation (taking into account shortrange order):

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

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

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

- ✓ No long-range order for  $D \le 2$
- ✓ Correlation function algebraically decays for any T≠ 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**

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

Yes for $T=0$ in 2D	
No for $I=0$ in 1D (quantum fluctua)	tion

#### Explaination

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 ( $\theta$  period) be ignored?

• Energy of a single vortex

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

• Entropy of a vortex

$$S_{\rm v} = 2k_{\rm B} \ln \frac{L}{a}$$
  $\checkmark$  also logarithm of L

• Free energy F = E - TS (energy-entropy balance)  $\Delta F = (\pi J - 2k_{\rm B}T) \ln \frac{L}{a} \implies k_{\rm B}T_c = \frac{\pi J}{2}$  Vortex: a topological defect



**BKT phase transition** is "one of the 20<sup>th</sup> 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  $E = 2\pi J \ln \frac{r}{a}$
- ✓ 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  $T_{\rm c}$ 

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



#### Renormalization group analysis

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

#### **RG** equation:

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



- ✓ y=0 accounts for the "vacuum" states free of vortices, but with various Gaussian fluctuation modes
- ✓ 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 $T_{\lambda}$

- 1908, <sup>4</sup>He liquefied (Onnes)
  1911, "supraconductivity" of mercury (Onnes) <sup>4</sup>He stops boiling below certain temperature (Onnes)
  1922, peculiarity of specific heat (Dana, not published)
  1927-1937, phase transition (*T<sub>A</sub>*=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 $T_{\lambda}$

Liquid <sup>4</sup>He stops boiling < 2.3K. J.C. McLennan *et al.* (1932)



The helium below the  $\lambda$ -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  $\omega_c = \frac{\hbar}{mR^2} \equiv$  quantum unit of rotation (10<sup>-4</sup> Hz for 1cm)



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



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

#### Quantized vortices

 ✓ 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

✓ USTC: <sup>6</sup>Li-<sup>41</sup>K supercluid mixture



Vortex lattice in single-species superfluid

#### Quantized vortices

#### ✓ USTC: <sup>6</sup>Li-<sup>41</sup>K supercluid mixture



Vortex lattice in two-species superfluid

### Vortex ring in 3D and its metastability

A sidedish (superlink) — <u>Crazy pool vortex</u>

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





#### 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 Complex matter field:  $\psi(\vec{r}) = |\psi(\vec{r})| e^{i\Phi(\vec{r})}$ 

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



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

- $\checkmark$  leads to superfluidity
- can be destroyed *only* by **topological** defects (vortices)

## 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

 $T < T_c: f_{k=0} / N > 0$ 

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

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  $\Psi(\vec{r}) = |\Psi(\vec{r})| e^{i\Phi(\vec{r})}$ 

• For low *T*, one has  $\mu \to 0^-$  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. Bosz erdachten Betrachtungsweise, auf welche dieser Autor eine höchst beachtenswerte Ableitung der PLANCKSchen Strahlungsformel gegründet hat<sup>1</sup>.

"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."

 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

<sup>87</sup>Rb

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

✓ <u>BEC cartoon</u>

## 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"  $\rho(\mathbf{r}_1, \mathbf{r}_2) = \left\langle \psi^{\dagger}(\mathbf{r}_2) \,\psi(\mathbf{r}_1) \right\rangle \rightarrow \psi_0^*(\mathbf{r}_2) \,\psi_0(\mathbf{r}_1) \quad \text{at} \quad \left| \mathbf{r}_1 - \mathbf{r}_2 \right| \rightarrow \infty$

"Paradox" for 2D finite-temperature system,

- Mermin-Wegner theorem states that no long-range order occurs
- 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: <sup>3</sup>He-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

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



- BKT phase transition in 2D (Berezinskii 1971, Kosterlitz-Thouless 1972, Nelson Kosterlitz 1976)
- ✓ 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**

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

- ✓ Super-heat-conductivity
- ✓ Fountain effect
- ✓ Escaping from a Dewar



 Heat is transported mechanically by flow of normal component



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



1913	Heike Kamerlingh Onnes	Netherlands	for his investigations on the properties of matter at low temperatures which led, inter alia, to the production of liquid helium.
1921	Albert Einstein	Germany	for his services to Theoretical Physics, and especially for his discovery of the law of the photoelectric effect
1962	Lev Davidovich Landau	Soviet Union	for his pioneering theories for condensed matter, especially liquid helium



1973	Leo Esaki	Japan	for their experimental discoveries regarding tunneling phenomena in semiconductors and superconductors, respectively
	Ivar Giaever	Norway, USA	
	Brian David Josephson	UK	for his theoretical predictions of the properties of a supercurrent through a tunnel barrier, in particular those phenomena which are generally known as the Josephson effects









# **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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