Aix*Marseille université

Socialement engagée

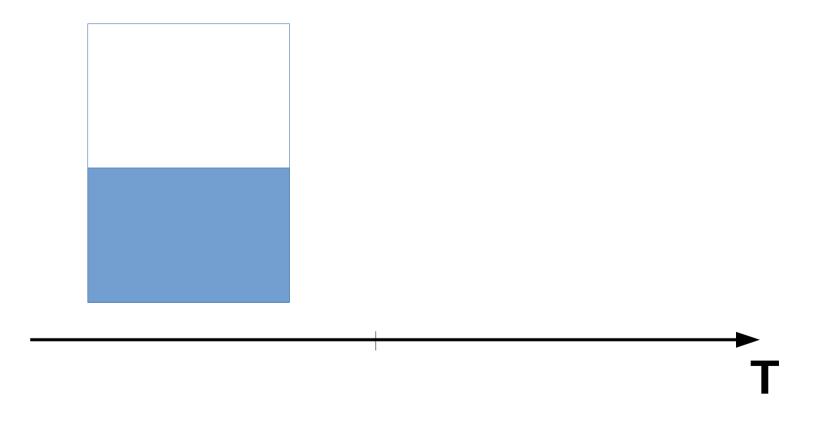
Conceptual
Topological theory
of Phase Transitions
(Just an overview by a non-expert)

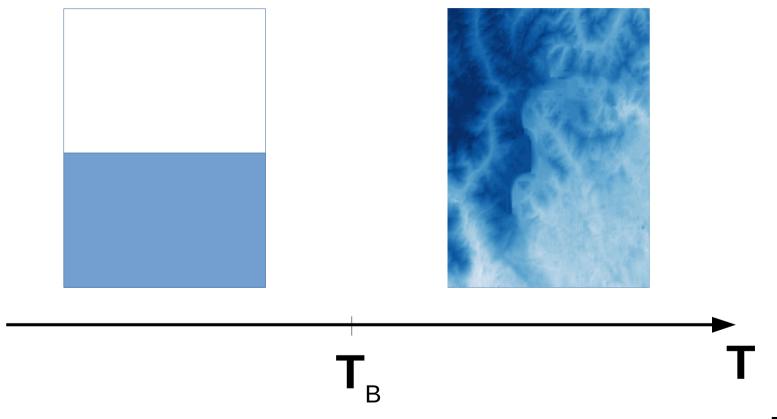
presented by: Abdelhamid Haddad

Supervised by: Pr. Marco Pettini

Outline

- Phase transitions overview :
 - Introduction.
 - Leading theory.
 - Limits and diverse issues.
- BKT transition and XY model.
- Topological point of view :
 - Topological hypothesis.
 - Validations and additional issues.
- Summary.





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Paramagnetic to ferromagnetic transition

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Changes of state (liquid-gas)

Paramagnetic to ferromagnetic transition

Superconductivity

Clustering transitions

Bose-Einstein condensation

..... and many others!

Physical description of a PT

Even if PT encompass a very large number of phenomena that span from the cosmological scale down to the sub-nuclear scale,

A general and complete theory is not yet available.

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The best known (and successful) theory is due to:

Landau (1936)

Associates a PT with a spontaneous symmetry breaking

At higher temperatures correspond to a "higher symmetry" disordered phase;

at lower temperatures, the phases are of ordered "lower symmetry".

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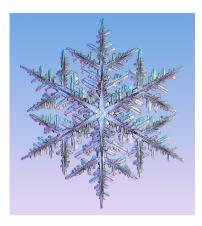
At higher temperatures correspond to a "higher symmetry" disordered phase;

at lower temperatures, the phases are of ordered "lower symmetry".

(To describe the symmetry of the phases Landau introduced a thermodynamic variable, the order parameter ϕ , which vanishes above the transition and, below the transition, it is nonzero.)

Traditionally, phase transitions are defined in the thermodynamic limit only!
 (Thermodynamic limit dogma)

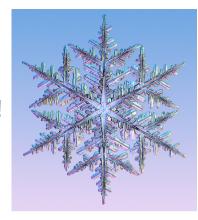
How to characterize PT in small systems?



275 water molecules

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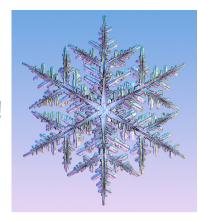


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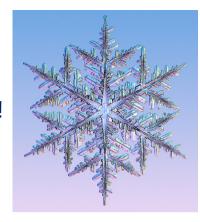


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 - There are systems undergoing PT in the absence of symmetry-breaking.
 - Systems in $d \le 2$ with continuous symmetry which cannot be broken spontaneously at any finite T (Mermin–Wagner theorem).

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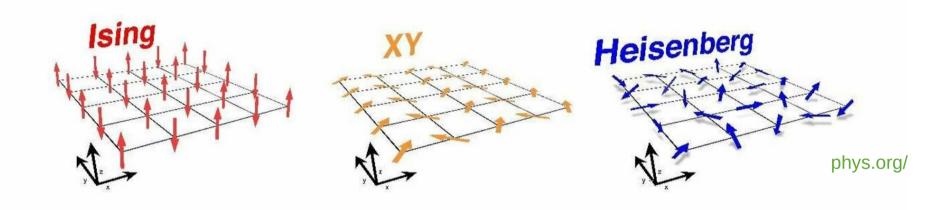
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Even WORSE:

- · There are systems undergoing PT in the absence of symmetry-breaking.
- Systems in $d \le 2$ with continuous symmetry cannot be broken spontaneously at any finite T and then No PT (Mermin–Wagner theorem).
- systems with local symmetries (gauge theories) undergo PT in the absence of an order parameter (Elitzur theorem).

XY model

(Rotator model)



$$H = -J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j = -J \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j).$$

In condensed matter physics, we classify matter in terms of the decay of their correlation functions:

- Long range ordered state $(LRO): G(x,x') \longrightarrow c \neq 0$ Johannes Walcher lecture notes, heidelberg university.
- Disordered state : $G(x, x') \xrightarrow{\propto exp(|x-x'|)} 0$ (Exponential decay of the correlation function)
- Quasi long range ordered state $(QLRO): G(x, x') \xrightarrow{\alpha |x-x'|^{-\eta}; \eta \in \mathbb{R}^+} 0$ (Algebraic decay of the correlation function)

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Tomasz Korzec, Comparison of exact and numerical results in the XY model
$$g(\vec{r}_x) = \langle \vec{s}_0 \cdot \vec{s}_x \rangle = \frac{1}{Z} \int \! D\theta \; \cos(\theta_0 - \theta_x) \exp \left[\beta \sum_{\langle l,k \rangle} \cos(\theta_l - \theta_k) \right]$$

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At low temperatures (large β) one expects neighboring spins to point into similar directions. (spin-wave approximation)

$$g(|\vec{r}_x|) \approx \left| \frac{\vec{r}_x}{r_0} \right|^{\frac{1}{2\pi\beta}}$$

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At high temperatures (small β) the exponential in the partition function can be expanded in β and higher order terms may be neglected

$$g(|\vec{r}|) \propto 2\pi\beta^{|\vec{r}|} = e^{\ln(2\pi\beta)|\vec{r}|}$$

The correlations decay exponentially.

The correlations decay according to a power law

The Berezinsky, Kosterlitz, Thouless PT

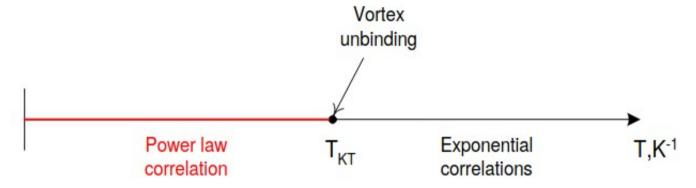


Figure 1: Schematic of the Kosterlitz-Thouless transition.

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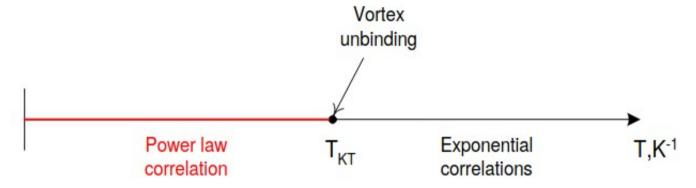
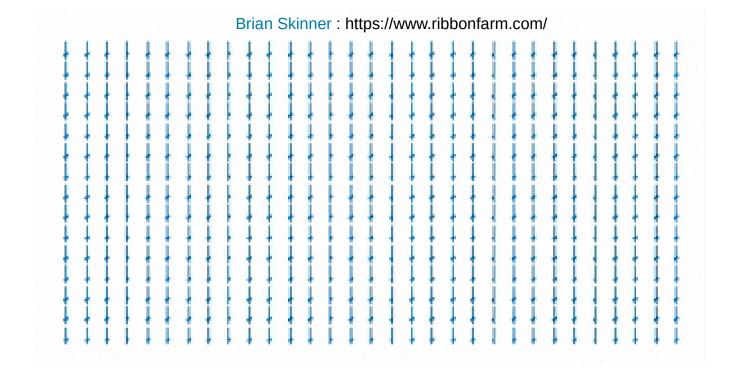


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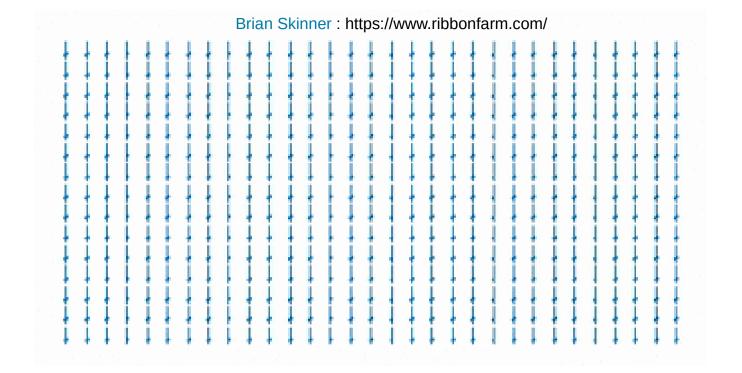
They proposed a solution: Topological defects to explain the Phase transition!

The Defects = Vortices

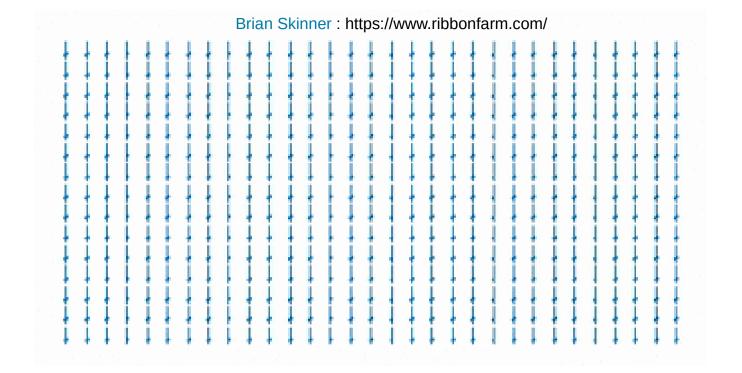


At low temperatures, it contain a dilute 'gas' of vortex-antivortex pairs. Each vortex will stick to an antivortex, since it takes a lot of energy to separate them

As we heat it up, we get more and more vortex-antivortex pairs, since there's more energy available to create them up to their unbinnding.



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Hamiltonian dynamics

$$\mathcal{H}(\{\varphi, \pi\}) = \frac{1}{2} \sum_{i} \pi_{i}^{2} + V(\{\varphi_{i}\})$$

$$\dot{q}_{i} = \frac{\partial H}{\partial p_{i}},$$

$$\dot{p}_{i} = -\frac{\partial H}{\partial q_{i}}, \quad i = 1, 2, \dots, N$$

The coordinates (q, p) are canonical variables, and the space of canonical variables is known as phase space.

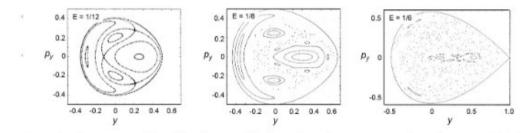


Figure 2: Poincare cross sections of the plane x = 0 for three values of parameter E: regular motion at E = 1/24, mix of regular and irregular motion at E = 1/8, and chaotic motion at E = 1/6. The particles are placed with the initial y = 0. The dots, which appear at random for E = 1/8 and E = 1/6, are generated by a single particle trajectory [1].

As E increases, the dynamics look increasingly chaotic

This dynamical approach brings us new observables such as the Lyapounov eponent and the curvature properties

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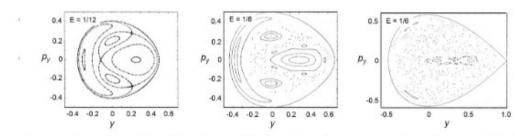


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$$H(\mathbf{p}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{p_{(i,j)}^{2}}{2} + J \left[\cos(\theta_{(i,j)} - \theta_{(i,j+1)}) + \cos(\theta_{(i,j)} - \theta_{(i+1,j)}) - 2 \right]$$

Topological hypothesis

Pettini et al. Geometry of Dynamics, Lyapunov Exponents, and Phase Transitions, PHYSICALREVIEWLETTERS (1997)

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"A thermodynamic transition might be related to a change in the topology of the configuration space, and the observed singularities in the statistical-mechanical equilibrium measure and in the thermodynamic observables at the phase transition might be interpreted as a "shadow" of this major topological change that happens at a more basic level."

(Numerical) confirmations

Pettini et al. Geometry of Dynamics, Lyapunov Exponents, and Phase Transitions, PHYSICALREVIEWLETTERS (1997)

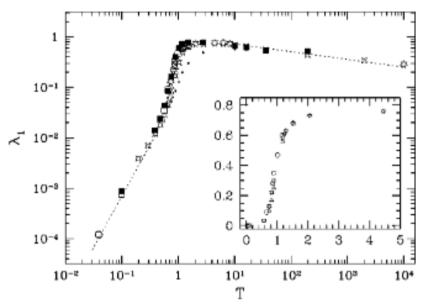


FIG. 1. Lyapunov exponent λ_1 vs temperature T for the d=2 case. Numerical results correspond to lattice size: $N=10^2$ (starred open squares), $N=20^2$ (open triangles), $N=40^2$ (open stars), $N=50^2$ (open squares), and $N=100^2$ (open circles). Full squares are analytic results according to Eq. (4); dots are analytic results without correction (see text). In the inset symbols have the same meaning.

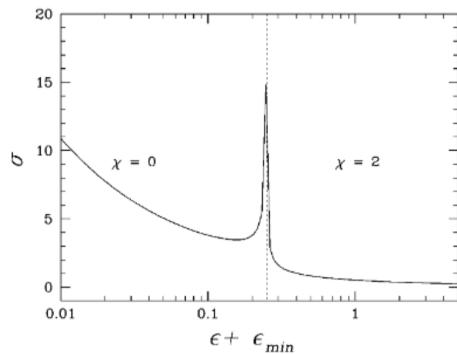


FIG. 5. Fluctuations amplitude, σ , of Gauss curvature of a family of surfaces parametrized by ϵ . For graphical reasons ϵ is shifted by its minimum value $|\epsilon_{\min}| = 0.25$; thus the cusp corresponds to $\epsilon = 0$, the critical value separating two families of different Euler characteristic χ , i.e., of different topology.

Gori et al., Topological Theory of Phase Transition, HAL Id: hal-03410854 (2021)

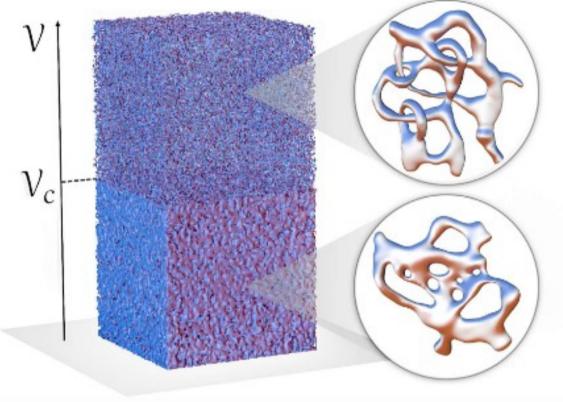


Figure 1. Low-dimensional pictorial representation of the transition between complex topologies as a metaphor of the origin of a phase transition. From the ground level up to the crossover level v_c , the manifolds M_v have a genus which increases with v. Above the crossover level v_c , the manifolds M_v have also a nonvanishing linking number which increases with v

Additional issues

"no topology change in phase space, no phase transition." However, there is at present no theorem that gives a sufficient topological condition for the occurrence of a phase transition.

Summary

- In 2d, continuous spin models cannot have magnetically ordered state. (Mermin-Wagner theorem).
- The XY model, however, has a strange type of phase transition that does not break the symmetry. (BKT transition).
- What kinds of topological transitions are related to phase transitions?
- What is, from a topological point of view, the difference between various types of phase transitions?

Thanks for your Attention!

Your questions are more than welcomed:)