

# BEREZINSKII-KOSTERLITZ-THOULESS TRANSITION AND THE HALDANE CONJECTURE: HIGHLIGHTS OF THE PHYSICS NOBEL PRIZE 2016

## LA TRANSICIÓN DE BERZINSKII-KOSTERLITZ-THOULESS Y LA CONJETURA DE HALDANE: HECHOS DESTACADOS DEL PREMIO NOBEL DE FÍSICA 2016

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The 2016 Physics Nobel Prize honors a variety of discoveries related to topological phases and phase transitions. Here we sketch two exciting facets: the groundbreaking works by John Kosterlitz and David Thouless on phase transitions of infinite order, and by Duncan Haldane on the energy gaps in quantum spin chains. These insights came as surprises in the 1970s and 1980s, respectively, and they have both initiated new fields of research in theoretical and experimental physics.

El premio Nobel de Física 2016 honra una variedad de descubrimientos relacionados con fases topológicas y transiciones de fases. Aquí tratamos dos de estas interesantes facetas: los trabajos seminales de John Kosterlitz y David Thouless en transiciones de fases de orden infinito, y por Duncan Haldane sobre los “gaps” de energía en cadenas cuánticas de espín. Estos hallazgos constituyeron una sorpresa en los 1970s y 1980s, respectivamente, e iniciaron nuevos campos de investigación en la física teórica y experimental.

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### I CLASSICAL SPIN MODELS

When we hear the word “spin” we usually think of Quantum Mechanics, where particles are endowed with an internal degree of freedom, which manifests itself like an angular momentum. So what does a “classical spin” mean?

It is much simpler: it is just a vector (or multi-scalar)  $\vec{e}$ , say with  $N$  components; here we assume them to be real,

$$\vec{e} = \begin{pmatrix} e^{(1)} \\ \vdots \\ e^{(N)} \end{pmatrix} \in \mathbb{R}^N. \quad (1)$$

Models which deal with such *classical spin fields* are usually formulated on a lattice (or grid), such that a spin  $\vec{e}_x$  is attached to each lattice site  $x$ . In solid state physics,  $\vec{e}_x$  might represent a collective spin of some crystal cell. If it is composed of many quantum spins, it appears classical [1].

If the spin directions are fixed on all sites  $x$ , we obtain a *configuration*, which we denote as  $[\vec{e}]$ .

In a number of very popular models, the length of each spin variable is normalized to  $|\vec{e}_x| = 1, \forall x$ . Then the spin field maps the sites onto a unit sphere in the  $N$ -dimensional spin

space,  $x \rightarrow S^{N-1}$ . We are going to refer to this setting, and (for simplicity) to a lattice of unit spacing, with sites  $x \in \mathbb{Z}^d$  in  $d$  dimensions.

To define a model, we still need to specify a *Hamilton function*  $\mathcal{H}[\vec{e}]$  (no operator), which fixes the energy of any possible spin configuration. Its standard form reads

$$\mathcal{H}[\vec{e}] = J \sum_{\langle xy \rangle} (1 - \vec{e}_x \cdot \vec{e}_y) - \vec{H} \cdot \sum_x \vec{e}_x, \quad (2)$$

where the symbol  $\langle xy \rangle$  denotes nearest neighbor sites.  $J$  is a coupling constant, and we see that  $J > 0$  describes a *ferromagnetic* behavior: (approximately) parallel spins are favored, since they minimize the energy.<sup>1</sup>  $\vec{H}$  is an external “magnetic field” (in a generalized sense), which may or may not be included;<sup>2</sup> its presence favors spin orientations in the direction of  $\vec{H}$ .

Thus we arrive at a set of highly prominent models in statistical mechanics, depending on the spin dimension  $N$ :

$N$	Vector Space	Model
1	$e_x \in \{-1, +1\}$	Ising
2	$\vec{e}_x^T = (\cos \varphi_x, \sin \varphi_x)$	XY
3	$\vec{e}_x^T = (\sin \theta_x \cos \varphi_x, \sin \theta_x \sin \varphi_x, \cos \theta_x)$	Heisenberg

<sup>1</sup>Vice versa,  $J < 0$  describes anti-ferromagnets, which also occur in models (cf. Section 3) and in Nature, e.g. Cr, Mn, Fe<sub>2</sub>O<sub>3</sub> and NiS<sub>2</sub>.

<sup>2</sup>In field theory one usually deals with “source fields”, which correspond to a space dependent external field of this kind, i.e. to a term  $\sum_x \vec{H}_x \cdot \vec{e}_x$ .

where  $\varphi_x, \theta_x \in \mathbb{R}$ . These models are discussed in numerous text books, such as Refs. [1–3].

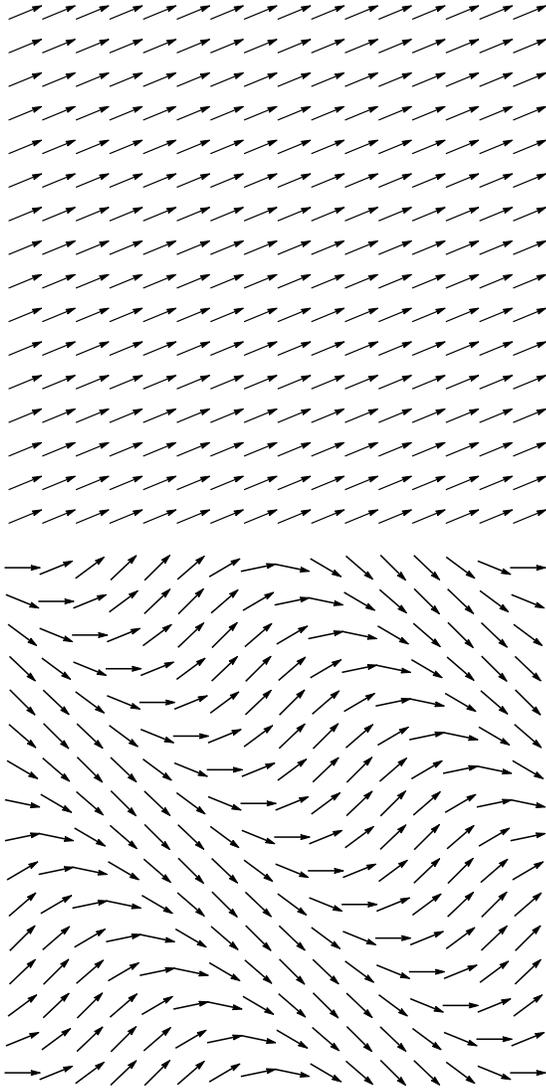


Figura 1. Examples for a uniform configuration of minimal energy (top) and for a non-uniform configuration of higher energy (bottom), in the 2d XY model.

Although it might seem ridiculously simple, the *Ising model* is incredibly successful in describing a whole host of physical phenomena. The *XY model* will be addressed in Section 2; its best application is to model superfluid Helium. The *Heisenberg model* captures actual ferromagnets, like iron, cobalt and nickel. Section 3.1 refers to its 2D version, which is also a toy model for Quantum Chromodynamics (QCD), since it shares fundamental properties like asymptotic freedom, topological sectors, and a dynamically generated mass gap. The *large N limit* also attracts attention, since it

<sup>3</sup>The  $O(4)$  model is of interest as well, in particular due to the local isomorphy  $O(4) \sim SU(2) \otimes SU(2)$ . The latter is the flavor chiral symmetry of QCD with two massless flavors. Here the magnetic field corresponds to the small masses of the quark flavors  $u$  and  $d$ , which break the symmetry down to  $O(3) \sim SU(2)$ .

<sup>4</sup>We express the temperature in units of the Boltzmann constant  $k_B$ , which amounts to setting  $k_B = 1$  throughout this article.

<sup>5</sup>In  $N \geq 2$  the number of configurations is infinite. For the Ising model in a lattice volume  $V$ , *i.e.* with  $V$  lattice sites, their number is  $2^V$ . Even for a modest volume, say a  $32 \times 32$  lattice, this is a huge number of  $O(10^{308})$ , so straight summation is not feasible, not even with supercomputers. Hence to compute expectation values (see below) one resorts to *importance sampling* by means of Monte Carlo simulations. For a text book and a recent introductory review, see Refs. [4].

leads to simplifications, which enable analytical calculations, see *e.g.* Ref. [3].

They are also called non-linear  $\sigma$ -models, or  $O(N)$  models, since — with the Hamilton function (2) at  $\vec{H} = \vec{0}$  — they have a global  $O(N)$  symmetry (or  $Z(2)$  symmetry in case of the Ising model): the energy remains invariant if we perform the same rotation on all spins,  $\vec{e}_x \rightarrow \Omega \vec{e}_x$ ,  $\Omega \in O(N)$ .<sup>3</sup>

If the system has temperature  $T$ , the probability for a configuration  $[\vec{e}]$  is given by<sup>4</sup>

$$p[\vec{e}] = \frac{1}{Z} e^{-\mathcal{H}[\vec{e}]/T}, \quad \text{with} \quad Z = \sum_{[\vec{e}]} e^{-\mathcal{H}[\vec{e}]/T} = e^{-F/T}. \quad (3)$$

The *partition function*  $Z$  is obtained by summing (or integrating) over *all* possible configurations,<sup>5</sup> and  $F = -\frac{1}{T} \ln Z$  is the *free energy*.

For  $J > 0$  the uniform configurations are most probable, since they have the minimal energy  $-VH$  (where  $H = |\vec{H}|$ ). An example is shown in Fig. 1 (left), and in the limit  $T \rightarrow 0$  the system will take such a uniform configuration. For increasing  $T$ , fluctuating configurations — like the one in Fig. 1 (right) — gain more importance. They carry higher energy, so the exponential  $\exp(-\mathcal{H}[\vec{e}]/T)$  suppresses them. On the other hand, there are *many* of them, and the combinatorial factor is relevant too. This is the *entropy effect*, which also matters for their impact, and which plays a key role in Section 2.

### 1.1 *n*-point functions and phase transitions

What does it mean to have an “impact”? What physical quantities are affected? In exact analogy to field theory, the physical terms are expectation values of some products of spins; if they involve  $n$  factors, they are called *n*-point functions.

The most important observable is the 2-point function, or *correlation function*,

$$\langle \vec{e}_x \cdot \vec{e}_y \rangle = \frac{1}{Z} \sum_{[\vec{e}]} \vec{e}_x \cdot \vec{e}_y e^{-\mathcal{H}[\vec{e}]/T}. \quad (4)$$

One often focuses on its “connected part”, which — in most cases — decays exponentially in the distance  $|x - y|$ ,

$$\langle \vec{e}_x \cdot \vec{e}_y \rangle_{\text{con}} = \langle \vec{e}_x \cdot \vec{e}_y \rangle - \langle \vec{e}_x \rangle \cdot \langle \vec{e}_y \rangle = \langle \vec{e}_x \cdot \vec{e}_y \rangle - \langle \vec{e} \rangle^2 \propto e^{-|x-y|/\xi}. \quad (5)$$

With the Hamilton function (2) the system is lattice translation invariant, so the 1-point function  $\langle \vec{e}_x \rangle$  does not depend on the site  $x$ , and we can just write  $\langle \vec{e} \rangle$ ,

$$\langle \vec{e}_x \rangle = \frac{1}{Z} \sum_{[\vec{e}]} \vec{e}_x e^{-\mathcal{H}[\vec{e}]/T} = \langle \vec{e} \rangle. \quad (6)$$

The decay rate of  $\langle \vec{e}_x \cdot \vec{e}_y \rangle_{\text{con}}$  is given by the *correlation length*  $\xi$ , which serves as *the* scale of the system: any dimensional quantity is considered “large” or “small” based on its comparison with (the suitable power of)  $\xi$ . Regarding the energy spectrum,  $\xi$  represents the inverse *energy gap*,  $1/\xi = E_1 - E_0$ . In quantum field theory, this is just the *mass* of the particle, which emerges by the minimal (quantized) excitations of the field under consideration.

The phase transitions that we are interested in are of order 2 or higher, and they are characterized by the property that  $\xi$  *diverges*. In a phase diagram, with axes like  $T$  and  $H$ , this happens in a *critical point*,<sup>6</sup> in particular at a *critical temperature*  $T_c$ . The way how  $\xi$  diverges in the vicinity of a critical point defines the *critical exponent*  $\nu$ ,

$$\lim_{T \rightarrow T_c} \xi \propto (T - T_c)^{-\nu}, \quad (7)$$

where we assume the same power regardless whether  $T_c$  is approached from above or from below (which usually holds). There are a number of critical exponents, which characterize the system close to a critical point; we will see further examples below.

In the limit  $\xi \rightarrow \infty$ , the spacing between the lattice points becomes insignificant (it is negligible compared to  $\xi$ ), so this is the *continuum limit*. This is why the vicinity of a critical point is so much of interest.

Intuitively it is clear that high temperature gives importance to “wild fluctuations”, which suppress long-distance correlations, inducing a short  $\xi$ . So, does  $\xi$  diverge only in the limit  $T \rightarrow 0$ ? This is indeed the case for the 1D Ising model [5]. It does not have an actual transition (with phases on both sides), and the model is considered uninteresting. However, the Ising model does have a finite critical temperature in dimension  $d = 2$  [6] or higher, and the same applies to  $N > 1$ .

The simplest observable is the 1-point function, or *condensate*, of eq. (6), which also defines the *magnetization*  $M$  (in some lattice volume  $V$ ),

$$\vec{m}[\vec{e}] = \sum_x \vec{e}_x, \quad M = |\langle \vec{m} \rangle| = V |\langle \vec{e} \rangle|. \quad (8)$$

$M > 0$  indicates that the  $O(N)$  symmetry is broken. An external field  $H > 0$  causes an explicit breaking. If we start with an external field and gradually turn it off, the destiny of the system depends on the temperature:

- At low  $T$ , the system keeps a dominant orientation in the direction of  $\vec{H}$ , at  $T \rightarrow 0$  it will pick the corresponding uniform configuration. This is known as “spontaneous symmetry breaking”, it reduces the symmetry group to  $O(N - 1)$ .
- At high  $T$ , the system allows for wild fluctuations, and after turning off  $\vec{H}$  it hardly “remembers” its direction.

In this case, the  $O(N)$  symmetry is restored, since the dominant contributions to an expectation value are due to configurations without such a preferred orientation.

Thus the magnetization  $M$  discriminates the scenarios where the  $O(N)$  symmetry is broken ( $M > 0$ ) or intact ( $M \simeq 0$ ). Therefore it is an *order parameter*: it is finite (it vanishes) below (above) the critical temperature  $T_c$  (which is also called “Curie temperature”). The way how it converges to 0, as  $T$  approaches  $T_c$  from below, defines another critical exponent  $\beta$ ,

$$\lim_{T \nearrow T_c} M \propto (T_c - T)^\beta. \quad (9)$$

The follow-up example is the critical exponent  $\gamma$ , which characterizes the divergence of the magnetic susceptibility  $\chi_m$ , at a temperature  $T$  close to  $T_c$ ,

$$\chi_m = \frac{1}{V} (\langle \vec{m}^2 \rangle - \langle \vec{m} \rangle^2) \propto |T - T_c|^{-\gamma}. \quad (10)$$

As in the case of  $\nu$ , also the exponent  $\gamma$  is usually the same for  $T \gtrsim T_c$  and for  $T \lesssim T_c$ .

There are classes of systems, which may look quite different, but which share the same critical behavior, so we say that they belong to the same *universality class*. This means in particular that the critical exponents coincide within a universality class. The enormous success of the Ising model is due to the fact that there are many models — and real systems — in the same universality class, so the Ising model captures their behavior next to a continuum limit.

## II BEREZINSKII-KOSTERLITZ-THOULESS TRANSITION IN THE 2D XY MODEL

This section deals with the 2D XY model, which is among the classical spin models introduced in Section 1. We can imagine a 2D square lattice, where each site  $x = (x_1, x_2)$ ,  $x_\mu \in \mathbb{Z}$ , carries a “watch hand”  $\vec{e}_x$ , like an arrow from the origin to some point on a unit circle. These vectors are parameterizable by an angle  $\varphi_x$ ,  $\vec{e}_x = (\cos \varphi_x, \sin \varphi_x)$ , as we mentioned before.

We formulate the angular difference between two spins as

$$\Delta\varphi_{x,y} = (\varphi_y - \varphi_x) \bmod 2\pi \in (-\pi, \pi], \quad (11)$$

*i.e.* the modulo operation acts such that it picks the minimal absolute value.

Now let us consider one *plaquette*, *i.e.* one elementary square of the lattice with corners  $x, x + \hat{1}, x + \hat{2}, x + \hat{1} + \hat{2}$ , where  $\hat{\mu}$  is a unit vector in  $\mu$ -direction. For a given configuration, each plaquette has a *vortex number*  $v_x$ ,

$$v_x = \frac{1}{2\pi} (\Delta\varphi_{x,x+\hat{1}} + \Delta\varphi_{x+\hat{1},x+\hat{1}+\hat{2}} + \Delta\varphi_{x+\hat{1}+\hat{2},x+\hat{2}} + \Delta\varphi_{x+\hat{2},x}) \in \{-1, 0, +1\}. \quad (12)$$

If the configuration is smooth (close to uniform) in the range of this plaquette, we expect  $v_x = 0$ . In case of sizable angular differences  $|\Delta\varphi_{x,x+\hat{\mu}}|$ , however, we might encounter

<sup>6</sup>Phase transitions of first order are more frequent, and they do not correspond to a critical point, but we won't discuss them.

a *topological defect*: this could be a *vortex*, which we denote as V, or an *anti-vortex*, AV. We assign them vortex number +1 and -1, respectively,

vortex	V	$v_x = +1$
anti-vortex	AV	$v_x = -1$ .

Examples for a configuration with one V or one AV are shown in Fig. 2. On the other hand, the configurations in Fig. 1 do not contain any topological defects.

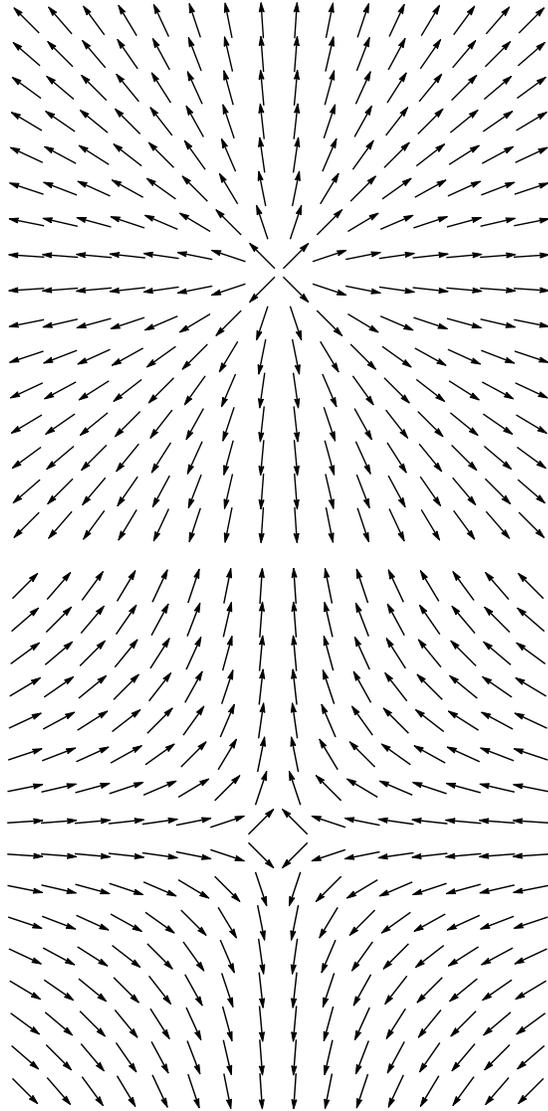


Figura 2. Examples for configurations with one vortex V (left), and with one anti-vortex VA (right), in the 2d XY model.

In numerical studies, we have to deal with a finite lattice volume  $V$ , and we usually implement periodic boundary conditions in both directions; this provides lattice translation invariance. Then, the volume represents a torus, and the total vorticity vanishes,  $\sum_x v_x = 0$ , due to Stokes' Theorem. So, the number of vortices must be equal to the number of anti-vortices,  $n_V = n_{AV}$ , and the configurations of Fig. 2 are actually incompatible with periodic boundaries.

In fact, the global system does not have topological sectors, since its homotopy group is trivial,  $\Pi_2(S^2) = \{0\}$ . Nevertheless, the *local* topological defects V and AV are the crucial degrees of freedom for its phase transition.

### II.1 First look

A first look suggests the following picture:

- The presence of many V and AV, *i.e.* a *high vorticity density*

$$\rho = \langle n_V + n_{AV} \rangle / V = 2 \langle n_V \rangle / V,$$

means that strong fluctuations are powerful, and they destroy the long-range correlations. Hence the corresponding smooth configurations are suppressed, the correlation function  $\langle \vec{e}_x \cdot \vec{e}_y \rangle$  decays rapidly, as in relation (5), and we obtain a correlation length  $\xi$  of a few lattice spacings. Due to the interpretation of  $1/\xi$  as a mass, this is called the *massive phase*.

- On the other hand, for a *low vorticity density*,  $\rho \ll 1$ , long-range correlation dominates. It is not disturbed significantly by the few V and AV that are floating around, and we are in the *massless phase*, where  $\xi = \infty$ . Here the correlation function  $\langle \vec{e}_x \cdot \vec{e}_y \rangle$  does not decay exponentially, but only with some negative power of  $|x - y|$ .

If we start from low temperature and increase  $T$  gradually, this gives more importance to “rough” rather than smooth configurations — they are far from uniform, with strong fluctuations. This increases the vorticity density  $\rho$ , and at the critical temperature  $\rho$  is large enough to mess up the long-range correlations, so the system enters its massive phase.

To make this point more explicit, we estimate the energy that it takes to implement one V or one AV in an otherwise smooth configuration. We do so in a simplified scheme of a quasi-continuous plane: close to the transition this can be justified since  $\xi$  (the relevant scale) is much larger than the lattice spacing. Then the angular field  $\varphi(x)$  of the simplest (rotationally symmetric) V or AV, with its core at  $x = 0$ , obeys

$$|\vec{\nabla}\varphi(x)| = \frac{1}{r}, \quad r = |x|, \quad (13)$$

with opposite gradient directions for a V or an AV, see Fig. 2. In this continuum picture, the vorticity  $v$  is given by a curl integral, anti-clockwise around the core,

$$v = \frac{1}{2\pi} \oint d\vec{x} \cdot \vec{\nabla}\varphi(x) = \frac{1}{2\pi} \int_0^{2\pi} r d\varphi \left( \pm \frac{1}{r} \right) \quad (14)$$

$$= \pm 1 \text{ for } \left\{ \begin{array}{l} \text{a vortex} \\ \text{an anti-vortex.} \end{array} \right\} \quad (15)$$

Regarding the energy, we note that the Hamilton function (2) (at  $\vec{H} = \vec{0}$ ) can be considered as a kinetic term, made of discrete derivatives,

$$J \sum_{\mu=1}^2 (1 - \vec{e}_x \cdot \vec{e}_{x+\hat{\mu}}) \approx \frac{J}{2} \sum_{\mu=1}^2 \Delta \varphi_{x,x+\hat{\mu}}^2 \approx \frac{J}{2} \vec{\nabla} \varphi(x) \cdot \vec{\nabla} \varphi(x). \quad (16)$$

Here we switched from lattice to continuum notation, and we neglect  $O(\Delta \varphi_{x,x+\hat{\mu}}^4)$ .

If we insert relations (13) and (16) into the Hamilton function, we obtain an estimate for the energy requirement for inserting one V or AV into a smooth “background”,

$$E_V = \frac{J}{2} \int d^2x \vec{\nabla} \varphi(x) \cdot \vec{\nabla} \varphi(x) \approx J\pi \int_1^L dr \frac{1}{r} = J\pi \ln L. \quad (17)$$

Note that (despite the continuum notation)  $L$  expresses the system size in lattice units, so it is dimensionless (and taking its logarithm makes sense). The integral over the plane is a bit sloppy regarding the shape of the volume; it is approximated by a circle of radius  $L$ , except for a small inner disc with the radius of one lattice spacing (which we have set to 1). The latter matches the illustrations in Fig. 2, and such an UV cutoff is needed to obtain a finite result.

Even this simplified consideration captures relevant properties. The energy for a single V or VA is considerable: it is enhanced  $\propto \ln L$ , so it takes a high temperature to make such vortex excitations frequent. In the thermodynamic limit,  $L \rightarrow \infty$ , they seem to be excluded, but we will see in Section 2.2 why the topological defects are so important nevertheless. Vadim L. Berezinskii (1935-80) explored these properties in 1971/2 [7]. He was working in Moscow, where he pioneered the vortex picture [8].

## II.2 Refined picture

The picture of Section 2.1 can be criticized for assuming either a single V or a single AV in the entire configuration, although we stressed before that their number must be equal (with periodic boundaries). So the minimal excitation of topological defects leads to one V plus one AV, as illustrated in Fig. 3, and the above calculation has to be revised. In fact, the result is not  $E_{V,AV}^{\text{isolated}} = 2E_V = 2\pi J \ln L$ , but instead

$$E_{V,AV} = 2\pi J \ln r_{V,AV}, \quad (18)$$

where  $r_{V,AV}$  is the distance between the V and AV core. This can be understood qualitatively: if the V–AV pair is tightly bound, its long-range impact cancels; at large distance, the configuration can be practically uniform, as in the absence of any vortices. If we observe the system with a low resolution (corresponding to a large  $\xi$ ), we do not see this pair at all.

Only pulling them far apart leads to “free” V and AV, which are visible to such an observer. When  $r_{V,AV}$  reaches the magnitude of  $L$ , the energy requirement is of the order of  $E_{V,AV}^{\text{isolated}}$ .

From eq. (18) we see that the trend towards minimal energy implies an *attractive force*  $\propto 1/r_{V,AV}$  between the V and AV cores. In  $d = 2$  this is a Coulomb force, so a few V and AV spread over the plane can be considered as a *Coulomb gas*. Its free energy  $F$  consists of the total energy  $E$ , plus an entropy term.

In the period 1972-4, John M. Kosterlitz (born 1942 in Aberdeen), and David J. Thouless (born 1934 in Bearsden), both from Scotland, worked on this issue at the University of Birmingham. They concluded that the driving force of the transition between the massive and the massless phase is not exactly the density  $\rho$  (referred to in Section 2.1), but the density of “free vortices and anti-vortices”, *i.e.* V or AV without any opposite partner nearby. So the phase transition is actually *driven by the (un)binding of V–AV pairs* [9].

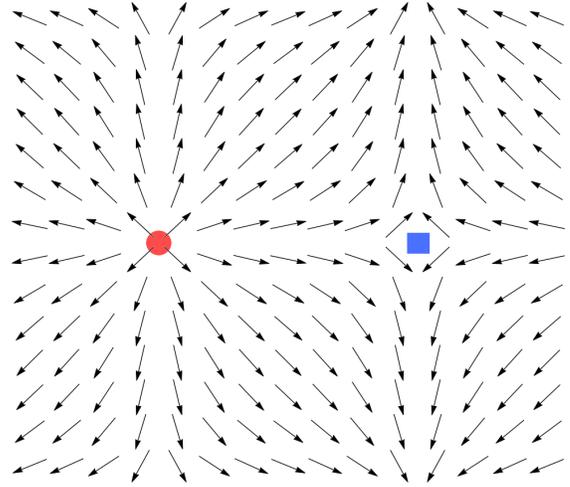


Figure 3. Profile of a configuration with a V–AV pair, with zero total vorticity: the V (AV) core is indicated by a red dot (blue square). Its energy is estimated in eq. (18).

To make this picture more explicit, we consider the free energy  $F$ , say in a sub-volume which is large enough to accommodate one free V. It is convenient to call its size  $L$ , and to recycle formula (17). The entropy  $S$  is the logarithm of the multiplicity of such configurations, here this is just the number of  $L^2$  plaquettes where the vortex could be located. This yields

$$F = E_V - TS = J\pi \ln L - T \ln L^2 = (J\pi - 2T) \ln L, \quad (19)$$

and the phase of the system depends on the question which of these two terms dominates.

- At low  $T$  there are hardly any free V or AV (they are suppressed when  $L$  becomes large), though there might be some tight V–AV pairs.
- At high  $T$  these pairs unbind: due to the dominance of the second term, a large size  $L$  makes it easy to spread free V and AV all over the system.

In this setting, eq. (19) suggests that the critical temperature, where the transition happens, amounts to  $T_c = J\pi/2$  [9].

### II.3 Critical behavior

Kosterlitz and Thouless predicted a type of phase transition, which was unknown before the 1970s. The correlation length diverges at  $T_c$ , as in the well-known phase transitions of second order (at least for  $T \searrow T_c$ ), but in contrast to them *no symmetry breaking is involved*. This means a step beyond Landau's Theory, which successfully describes second order phase transitions with the concept of spontaneous symmetry breaking. In low dimensions ( $D \leq 2$ ), however, thermal fluctuations are powerful enough to prevent spontaneous ordering, like a magnetization  $M > 0$ . This has been explained generally by the Mermin-Wagner Theorem, and specifically for the 2D  $O(N)$  models in Ref. [10]. The characteristics of the BKT transition were also confirmed experimentally, in particular in thin films of superfluid  $^4\text{He}$  [11] and of superconductors [12].

With respect to the critical exponents, this transition was discussed comprehensively by Kosterlitz in 1974 [13], by employing Renormalization Group techniques. He pointed out that this is a phase transition of infinite order, an *essential phase transition*. The correlation length  $\xi$  is not described by a power divergence as in relation (7), but by an essential singularity,

$$\xi \propto \exp\left(\frac{\text{const.}}{(T - T_c)^{\nu_e}}\right), \quad T \gtrsim T_c. \quad (20)$$

Thus one defines a critical exponent  $\nu_e$  for the exponential growth of  $\xi$ ; Kosterlitz derived its value  $\nu_e = 1/2$ .

Since there is no symmetry breaking going on in the BKT transitions, we cannot address the critical exponent  $\beta$ , and the susceptibility  $\chi_m$  does not follow relation (10) either. The critical exponents of Section 1.1 all refer to infinite volume, but in the 2D XY model at  $V = L \times L \rightarrow \infty$ ,  $\chi_m$  diverges throughout the massless phase. Kosterlitz predicted how it diverges as a function of  $L$  (the scale which is left) [13],

$$\chi_m \propto L^{2-\eta_e} (\ln L)^{-2r_e}, \quad \eta_e = 1/4, \quad r_e = -1/16. \quad (21)$$

This prediction is hard to verify numerically: studying the logarithmic term (and further sub-leading logarithms) requires huge volumes. The best confirmation with the standard Hamilton function (2) was given in Ref. [14]. It is based on simulations up to size  $L = 2048$ , and the outcome is consistent with the predicted exponents  $\eta_e$  and  $r_e$ , though  $r_e$  comes with a large error bar.

At this point we mention an alternative and entirely different Hamilton function for the  $O(N)$  spin models. Unlike the term (2), it does not include any (discrete) derivative term, but just a cutoff  $\delta$  for the angular difference between any two nearest neighbor spins,

$$\mathcal{H}[\vec{e}] = \begin{cases} 0 & \text{if } |\Delta\varphi_{x,x+\hat{\mu}}| < \delta \quad \forall x, \mu \\ \infty & \text{otherwise.} \end{cases} \quad (22)$$

Such a *constraint Hamilton function* is *topologically invariant*, which means that most small modifications of a configuration leave the energy exactly invariant. This is highly unusual:

part of the configurations are excluded (those that violate the constraint), while all others have energy 0. Still, it has the same symmetries as the standard action, and it belongs to the same universality class [15–17].

There is no temperature in this formulation, but the constraint angle  $\delta$  plays a role, which bears some analogy. In fact, there is a critical  $\delta_c$ , and the system is in its massive (massless) phase for  $\delta > \delta_c$  ( $\delta < \delta_c$ ). The correlation length exhibits an exponential divergence as in relation (20) when  $\delta$  approaches its critical value within the massive phase [16],

$$\xi \propto \exp\left(\frac{\text{const.}}{(\delta - \delta_c)^{\nu_e}}\right), \quad \delta \gtrsim \delta_c. \quad (23)$$

This observation singles out the critical constraint angle  $\delta_c = 1.775(1)$ . Fig. 4 shows this divergence as  $\delta > \delta_c$  decreases, and the fit yields  $\nu_e = 0.503(7)$ , accurately confirming Kosterlitz' prediction.

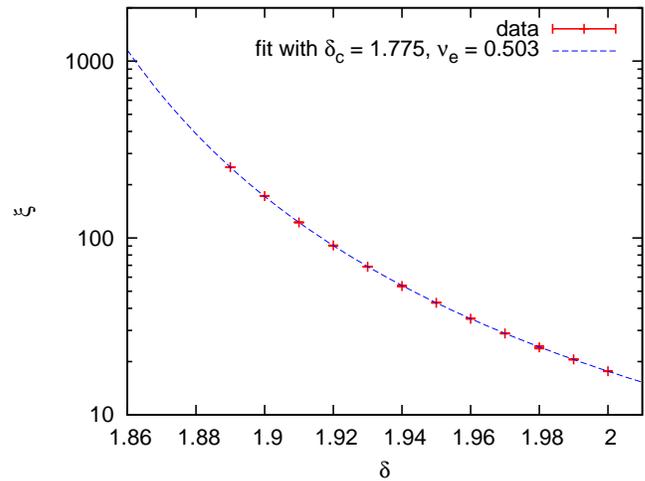


Figure 4. The exponential divergence of the correlation length  $\xi$ , as  $\delta$  decreases towards  $\delta_c \approx 1.775$ . A fit to relation (23) confirms Kosterlitz' prediction for  $\nu_e$ .

Regarding the limit within the massless phase, the divergence of the susceptibility  $\chi_m$  is consistent with the relation (21), and  $\eta_e$  is confirmed to two digits, whereas the value for  $r_e$  is plagued by large uncertainties [16], as in Ref. [14].

Another prediction for the BKT transition in the 2D XY model refers to the *helicity modulus*. In its dimensionless form, it is defined as

$$\Upsilon = \frac{1}{T} \frac{\partial^2 F}{\partial \alpha^2} \Big|_{\alpha=0}, \quad (24)$$

where  $\alpha$  is a twist angle in the boundary conditions. The free energy  $F$  is minimal at  $\alpha = 0$  (periodic boundaries), and  $\Upsilon$  is the curvature in this minimum.

The qualitative picture is illustrated in Fig. 5 (left): in the large volume limit, one expects  $\Upsilon$  to perform a jump at  $T_c$ . Soon after the BKT transition had been put forward, the height of this jump was predicted as  $2/\pi$  [18]. Later a small correction was subtracted to obtain the theoretical value [19]

$$\Upsilon_{c,\text{theory}} = \frac{2}{\pi} \left(1 - 16e^{-4\pi}\right) \approx 0.6365. \quad (25)$$

Regarding the constraint Hamilton function, we can interpret  $\frac{1}{2} \exp(-F(\alpha)/T)$  generally as the probability for a (dynamical) twist angle  $\alpha$ , so the helicity modulus can be studied without the concept of temperature.

Fig. 5 (right) summarizes simulation results for  $\Upsilon_c$  obtained with various lattice Hamilton functions. The standard formulation (2) is very tedious in this regard: even simulations at  $L = 2048$  yielded  $\Upsilon_c = 0.67826(7)$  [14], which is far too high. Somewhat more successful was the use of a “step Hamilton function”, which is also topologically invariant: when  $|\Delta\varphi_{x,x+\hat{\mu}}|$  exceeds  $\delta = \pi/2$ , the energy contributions of this pair of neighboring spins jumps from zero to some finite value, which is varied (instead of varying  $\delta$ ). Here  $L = 256$  led to  $\Upsilon_c = 0.6634(6)$  [20], but it still took faith to accept the compatibility of the large- $L$  extrapolation with the theoretical value in eq. (25).

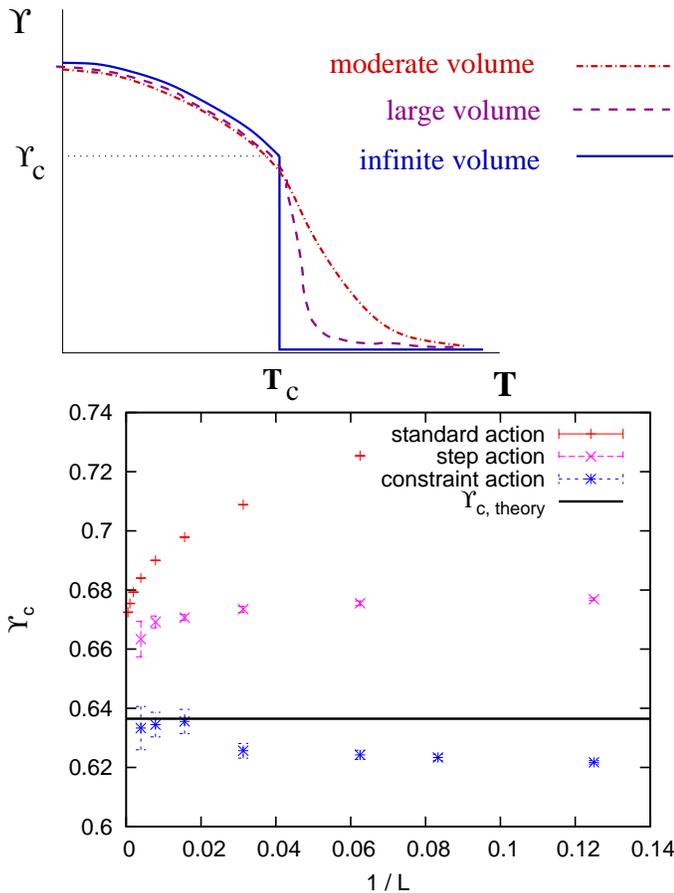


Figure 5. A qualitative picture of the helicity modulus  $\Upsilon$  depending on the temperature (top), and an overview over numerical results for its helicity jump at the critical point,  $\Upsilon_c$  (bottom).

This compatibility was finally demonstrated beyond doubt with the constraint Hamilton function (22). As a function of  $\delta$  (replacing  $T$ ),  $\Upsilon$  behaves exactly as depicted in Fig. 5 (left): a jump is observed around  $\delta_c$ , and it becomes more marked as the volume increases. At  $\delta_c$  the value  $\Upsilon_c = 0.636(4)$  was measured already at  $L = 64$ , and larger volumes confirmed the agreement with eq. (25) [17]. This is one of the clearest pieces of numerical evidence that the BKT transition does occur, and that the corresponding quantitative predictions are valid.

Moreover, the corresponding jump in the superfluid density of thin films has been observed experimentally [11].

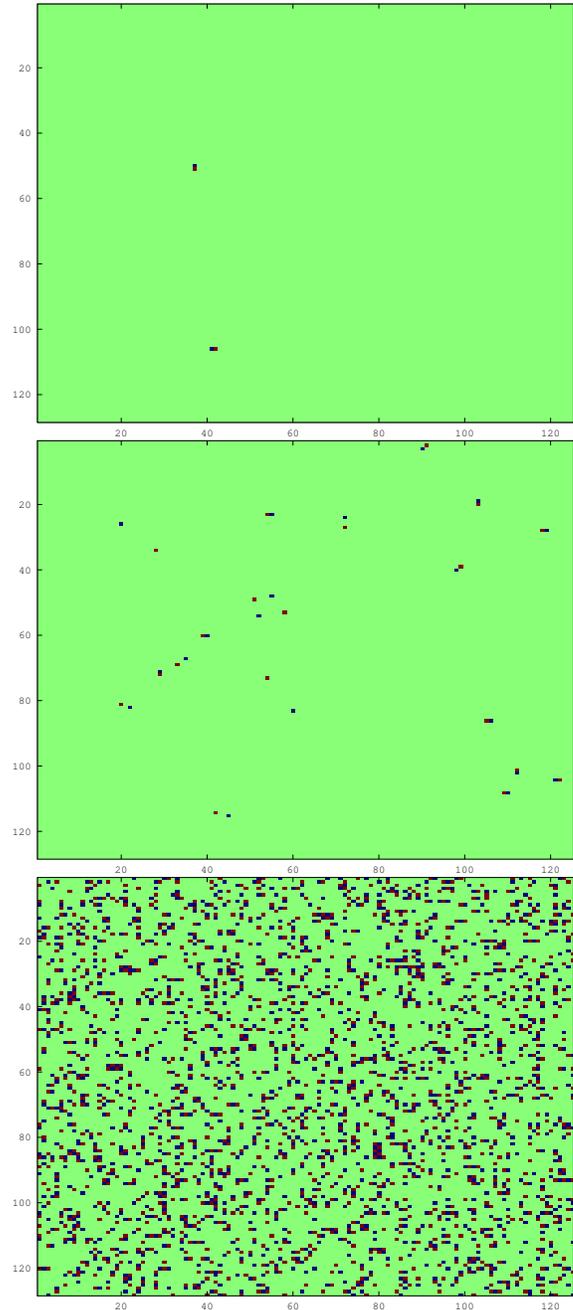


Figure 6. Maps of typical configurations of the XY model on a  $128 \times 128$  lattice, with the constraint Hamilton function (22) and  $\delta = 1.8, 1.9$  and  $2.5$  (from top to bottom). The presence of a V (AV) is indicated by a red (blue) plaquette. As long as there are only few V (for  $\delta \leq 1.9$ ), the effect of V-AV pair formation is evident.

All this seems nicely consistent, but in some sense it is *puzzling*: in Section 2.2 we reviewed the consideration of energy *vs* entropy in the vortex picture, which predicts the BKT transition. This picture is standard, and it has been brought into further prominence by the Nobel Prize Committee. However, in the formulation with the constraint Hamilton function the energy cost for any V or AV is zero, but still the BKT transition is beautifully observed [16,17]. Is this a contradiction?

More to the point, we focus on the question: is the V–AV (un)binding mechanism still at work, even when free V and AV do not require any energy, but only the entropy effect is there?

A first hint is given by Fig. 6, which shows “maps” of the V and AV found in typical configurations at  $\delta = 1.8, 1.9$  and 2.5.

For small  $\delta$ , when only few V and AV show up, the trend to a V–AV pair formation is obvious. At  $\delta = 2.5$  there are numerous topological defects, and it cannot be seen by eye whether or not such a trend persists.

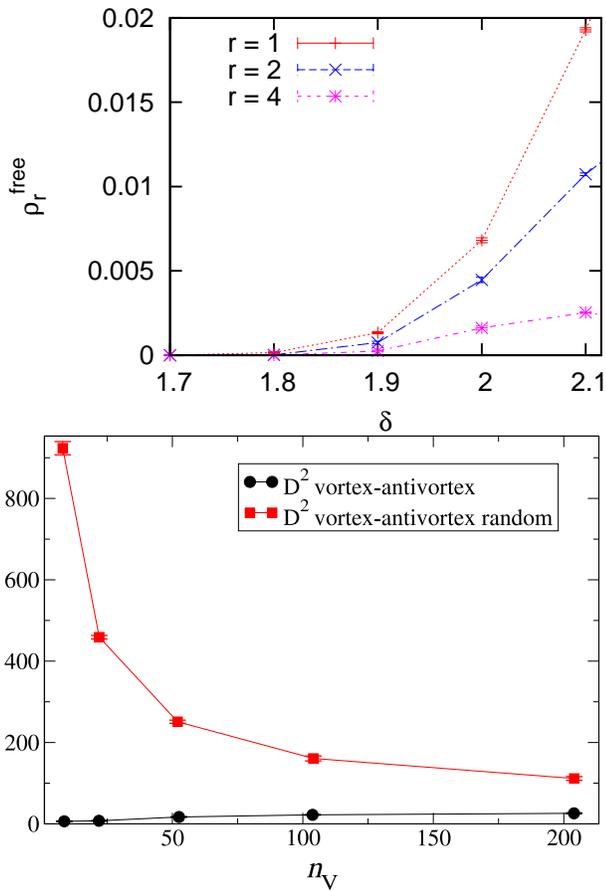


Figura 7. Top: The density of “free vortices”,  $\rho_r^{\text{free}}$ , i.e. of V or AV without an opposite partner within distance  $r = 1, 2$  or 4. We see an onset at  $\delta \geq \delta_c$ , so  $\rho_r^{\text{free}}$  is similar to an (inverse) order parameter. Bottom: The mean distance squared between V–AV pairs,  $D^2$ , for optimal pairing (black line). For small  $n_V$  (few vortices),  $D^2$  is much shorter than the corresponding term for random distributed V and AV (red line). Around  $n_V \geq 50$  (typical for  $\delta \approx 1.9$ ) this striking discrepancy fades away. This confirms the V–AV (un)binding mechanism in the BKT transition.

In any case, Fig. 6 only shows specific configurations, but a conclusive answer requires a statistical analysis. Fig. 7 (top) shows the average density  $\rho_r^{\text{free}}$  of “free V” plus “free AV”, defined by the property that there is no opposite partner within distance  $r$ , with  $r = 1, 2$  and 4. We see an onset around  $\delta \approx 1.8$ , and a sharp increase as  $\delta$  exceeds 1.9. Hence  $\rho_r^{\text{free}}$  behaves indeed like an (inverse) “order parameter” for the BKT transition<sup>7</sup> (although, strictly speaking, there is no ordering).

<sup>7</sup>The finite volume shifts the apparent critical angle somewhat up.

Fig. 7 (top) shows the mean distance squared between nearby V and AV cores,  $d_{V,AV}^2$ , in configurations with  $n_V$  vortices (and  $n_V$  anti-vortices), at  $L = 128$ ,

$$D^2 = \frac{1}{n_V} \sum_{i=1}^{n_V} d_{V,AV,i}^2. \quad (26)$$

The V and AV pairs are formed such that  $D^2$  is minimal. This is compared to  $D^2$  for artificial configurations, where the same number of V and AV are random distributed over the volume. For small  $n_V$  — which corresponds to small  $\delta$  — we see a striking difference for the configurations which are generated by simulating the model. This is clear evidence for a V–AV pair formation. This effect fades away for larger  $\delta$ , when  $n_V$  increases ( $\delta = 1.9$  corresponds to about  $n_V = 50$ ).

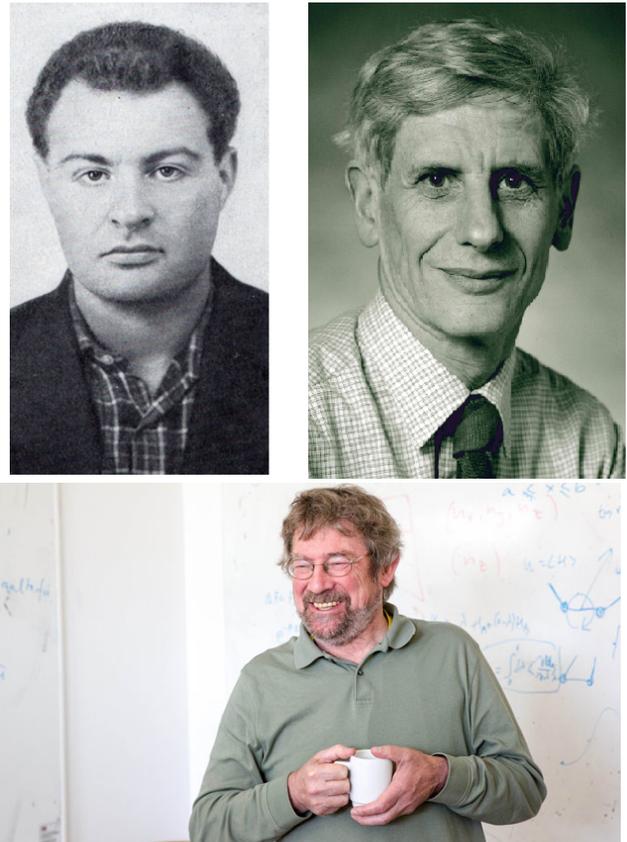


Figura 8. Top left: **Vadim L'vovich Berezinskii** (1935-1980) was born in Kiev (USSR) and graduated 1959 at Moscow State University. After working at the Textile Institute and the Research Institute for Heat Instrumentation, he joined 1977 the Landau Institute of Theoretical Physics in Moscow. Top right: **David James Thouless** was born 1934 in Bearsden (Scotland). He studied at Cambridge University as well, and graduated 1958 at Cornell University, his Ph.D. advisor was Hans Bethe. He worked in Birmingham with Rudolf Peierls, and later with John Kosterlitz. In 1980 he became Professor at the University of Washington in Seattle. Bottom: **John Michael Kosterlitz** was born 1942 in Aberdeen (Scotland), studied at Cambridge University, and graduated 1969 in Oxford. In 1974 he became Lecturer at Birmingham University, and in 1982 Professor at Brown University in Rhode Island, USA.

We conclude that the V–AV (un-)binding mechanism is at work, which confirms once more the elegant picture by Kosterlitz and Thouless for the BKT phase transition. This

observation even holds when topological defects do not cost any energy; then it is a pure entropy effect. Therefore the standard argument for this picture — outlined in Section 2.2 — should be extended.

### III HALDANE CONJECTURE

We now proceed to *quantum spin models*, leaving behind the classical spins (albeit they will be back in Section 3.1). Now the components of a spin vector are Hermitian *operators*, for spin 1/2 they can be represented by the Pauli matrices. For any spin,  $s = 1/2, 1, 3/3, 2, 5/2 \dots$  (in natural units,  $\hbar = 1$ ), we write them as  $\hat{S}_x^a$ , where  $x$  is still a lattice site. These components obey the familiar relations

$$\sum_{a=1}^3 \hat{S}_x^a \hat{S}_x^a = s(s+1), \quad [\hat{S}_x^a, \hat{S}_y^b] = i \delta_{xy} \epsilon^{abc} \hat{S}_x^c, \quad (27)$$

where  $\epsilon$  is the Levi-Civita symbol. If we compare these terms at large  $s$ , we see that the commutator is suppressed as  $O(s) \ll O(s^2)$ , and the spin appears almost classical.

For arbitrary spin we assemble the *Hamilton operator*  $\hat{H}$ , and write down the partition function

$$\hat{H} = -J \sum_{\langle xy \rangle, a} \hat{S}_x^a \hat{S}_y^a, \quad Z = \text{Tr} e^{-\hat{H}/T}. \quad (28)$$

It is analogous to the Hamilton function (2) and partition function (3), now with quantum spins. We recognize a global SU(2) symmetry; its transformation is performed on each component  $\hat{S}_x^a$ .

In addition, this framework differs from the previous sections in the following points:

- We focus on *spin chains*, *i.e.* dimension  $D = 1$ , so now the sites are located on a line.
- We consider *anti-ferromagnets*, with  $J < 0$ , cf. footnote 1.
- We skip the external magnetic field.
- We drop the additive constant (“cosmological constant”) of the Hamilton function (2). This change is irrelevant — what matters are solely energy *differences*.

For commutative spin components it would be trivial to write down a ground state of such an anti-ferromagnetic spin chain: it consists of spins of opposite orientations, in alternating order (say  $|s, -s, s, -s, s, -s \dots\rangle$ ) known as a Néel state. However, this is not an eigenstate of  $\hat{H}$ . Quantum spins are far more complicated, and identifying a ground state is a formidable task, even in  $d = 1$ .

The investigation of these systems has a history of almost 100 years. The ongoing interest has been fueled by the fact that quantum spin chains exist experimentally; we will give examples below. A breakthrough was achieved by Hans Bethe in 1931, who constructed the ground state for spin  $s = 1/2$  [21].

Of course also excited states are of interest, and in particular the question whether or not there is a finite energy gap  $\Delta_s = E_1 - E_0$ . We repeat that a finite gap corresponds to a massive phase, with a correlation length  $\xi = 1/\Delta_s$ .

In the 1950s and 1960s such systems were studied mostly with “spin wave theory”, an approach which was fashion at that time. It predicts a “quasi long-range order” (without Nambu-Goldstone bosons), which means a power decay of the correlation function, *i.e.* the massless case with  $\xi = \infty$ . This was elaborated mostly in higher dimensions,  $d \geq 2$ , doubts remained about the spin chain.

For  $D = 1$ , the expected zero gap for  $s = 1/2$  was proved in 1961 by the Lieb-Schultz-Mattis Theorem [22]. This consolidated the paradigm that anti-ferromagnetic quantum spin chains are always gapless, for any spin  $s = 1/2, 1, 3/2 \dots$ .

Therefore it came as a great surprise when *F. Duncan M. Haldane* (born 1951 in London) contradicted in 1983 [23, 24]. According to the *Haldane Conjecture*, the paradigm was correct only for the half-integer spins, but not for  $s \in \mathbb{N}$ . He conjectured

$$\begin{aligned} s = 1/2, 3/2, 5/2 \dots & \text{ (half-integer) } \Delta_s = 0 \text{ gapless} & (29) \\ s = 1, 2, 3 \dots & \text{ (integer) } \Delta_s > 0 \text{ finite gap.} \end{aligned}$$

Haldane gave topological arguments, which were considered as somewhat cryptic, hence they were initially met with skepticism. We refrain from an attempt to review them, here we refer to Ref. [25].

The zero gap for all half-integer spins was rigorously proved three years later [26], extending the Lieb-Schultz-Mattis Theorem.

The surprising part of this conjecture, which refers to integer spins, was soon supported by numerical studies for  $s = 1$  [27]. Later the existence of a gap  $\Delta_1 > 0$  was proved in Ref. [28], and its value was established to high precision in the early 1990s [29]. A study based on the diagonalization of an  $L = 22$  spin chain, and a large  $L$  extrapolation, obtained  $\Delta_1 = 0.41049(2) J$  [30].

This is in agreement with *experimental* studies. In particular, the material CsNiCl<sub>3</sub> contains quasi-1d anti-ferromagnetic  $s = 1$  spin chains. The scattering of polarized neutrons leads to a multi-peak structure, from which the value  $\Delta_1 \approx 0.4 J$  could be extracted [31]. Similar observations were made with Ni(C<sub>2</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>NO<sub>2</sub>ClO<sub>4</sub> [32], but no gap was found in materials with  $s = 1/2$  spin chains [33].

For higher  $s \in \mathbb{N}$ , it is difficult to observe such a gap: it has a conjectured extent  $\Delta_s \sim \exp(-\pi s)$  [34], so it becomes tiny for increasing  $s$ . The case  $s = 2$  is still tractable numerically: a study up to  $L = 350$  arrived at  $\Delta_2 = 0.085(5) J$  [35].

*In summary, the Haldane Conjecture (30) has been proved rigorously for all half-integer spins, and for  $s = 1$ . Numerical and experimental results for the value of  $\Delta_1$  agree. For  $1 < s \in \mathbb{N}$  we have the conjecture, and specifically for  $s = 2$  also numerical evidence.*

### III.1 Mapping onto the 2D O(3) model

A new perspective occurred by mapping such anti-ferromagnetic quantum spin chains onto the 2D O(3) model, or Heisenberg model. This latter emerged as a low energy effective theory, which was constructed by a large- $s$  expansion, and its validity was conjectured for all  $s$  [24, 36], for a review see Ref. [37].

Thus we are back with a classical spin model of Section 1. We write its Hamilton function in continuum notation,

$$\begin{aligned} \frac{1}{T} \mathcal{H}[\vec{e}] &= \int d^2x \left[ \frac{1}{2g} \partial_\mu \vec{e} \cdot \partial_\mu \vec{e} - \frac{\theta}{8\pi} i \epsilon_{\mu\nu} \vec{e} \cdot (\partial_\mu \vec{e} \times \partial_\nu \vec{e}) \right] \quad (30) \\ &= \frac{1}{T} \mathcal{H}_0 - i \theta Q[\vec{e}]. \end{aligned}$$

The 3-component classical spin field  $\vec{e}(x)$  has the form that we wrote down for the Heisenberg model (below eq. (2)). The term  $\mathcal{H}_0$  is just a continuum version of the form (2) at  $\vec{H} = \vec{0}$ , up to the notation for the coupling constant. At large spin  $s$ , the (approximately classical) spin  $\vec{S}$  can be written as  $\vec{S} \simeq s \vec{e}$ , still with the convention  $|\vec{e}| = 1$ , which leads to a weak coupling  $g \simeq T/(Js^2)$ .

The important novelty is the  $\theta$ -term: its integrated form,  $Q[\vec{e}]$ , counts how many times the configuration  $[\vec{e}]$  covers the sphere  $S^2$  in an oriented manner. Hence it is an integer, namely the *topological charge*, or *winding number*,  $Q[\vec{e}] \in \mathbb{Z}$ .<sup>8</sup> Therefore  $\exp(-\mathcal{H}/T)$  is  $2\pi$ -periodic in  $\theta$ , so it is sufficient to consider  $0 \leq \theta < 2\pi$ .

The Haldane-Affleck map of a anti-ferromagnetic quantum spin chain onto this model relates the quantum spin  $s$  to the *vacuum angle*  $\theta$  as  $\theta = 2\pi s$  (within the large  $s$  construction) [24, 36, 37]. Taking into account the  $2\pi$ -periodicity in  $\theta$ , this amounts to the scheme

		Haldane Conjecture
$s$ integer	$\theta = 0$	gap
$s$ half-integer	$\theta = \pi$	gapless

Under this mapping, the Haldane Conjecture takes a new turn. It is remarkable that the mysterious part flips to the other side: the gap for the 2D O(3) model without a  $\theta$ -term is well established, see e.g. Refs. [38]. On the other hand, it is hard to verify whether the limit  $\theta = \pi$  is indeed gapless. If the mapping were rigorous, we could conclude that everything is accomplished, but of course it is another conjecture. Hence the challenge is to investigate the case  $\theta = \pi$ .

Perturbation theory does not help (cf. footnote 8), so *Ian Affleck* (born 1952 in Vancouver) suggested a non-perturbative topological picture [34], along the lines of our consideration in Section 2. Affleck starts from  $\mathcal{H}_0$  and adds an auxiliary potential term  $\sim \mu^2 (e^{(3)}(x))^2$ , which pushes the field  $\vec{e}$  into the  $(e^{(1)}, e^{(2)})$ -plane; in the limit  $\mu^2 \rightarrow \infty$  we are back with the 2d XY model. We call  $\varphi$  the angle within this

<sup>8</sup>For small variations of the trivial configuration  $\vec{e}(x) = \vec{0}$  we always obtain  $Q[\vec{e}] = 0$ , so the  $\theta$ -term is not visible in the field equations of motion, nor in perturbation theory (expansion in powers of  $g$ ). Still, it does affect the actual physics, which is non-perturbative (finite  $g$ ).

preferred plane (as before), and  $\alpha$  the (suppressed) angle out of it.

Let us consider a sub-volume, where the configuration contains a V or an AV in the preferred plane. Its contribution to the topological charge  $Q$  is given by the vorticity computed in eq. (14), using assumption (13) and Stokes' Theorem, but now normalized by the area of  $S^2$ ,

$$q = \frac{1}{4\pi} \oint d\vec{x} \cdot \vec{\nabla} \varphi(x) = \pm \frac{1}{2}. \quad (31)$$

Local topological defects of this kind, with  $q = 1/2$  and  $q = -1/2$ , are denoted as *merons* and a *anti-merons*, respectively.

The energy estimate is similar to eq. (17), in particular we still obtain the factor  $\ln L/a$  (we now write explicitly a "lattice spacing"  $a$ ). The large  $L$  limit only allows for configurations with total vorticity 0, as before, but it permits meron-anti-meron pairs (cf. eq. (18)). At the end we have to remove the auxiliary potential,  $\mu^2 \rightarrow 0$ ; then the merons and anti-merons can easily avoid the UV divergence in the core, by choosing spin directions out of the previously preferred plane.

Hence we arrive at a picture, which allows for numerous merons and anti-merons, which diffuse the long-range order, and the energy gap occurs. In addition to the meron-anti-meron pairs, there can be an excess of one type by an even number, such that  $Q = (n_{\text{meron}} - n_{\text{anti-meron}})/2 \in \mathbb{Z}$ . However, the meron-anti-meron pairs are mainly responsible for the energy gap.

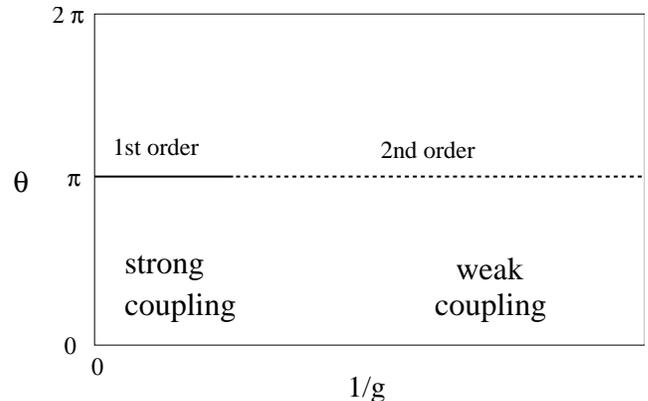


Figure 9. The expected phase diagram of the 2d O(3) model with a topological  $\theta$ -term. At weak coupling, the map from anti-ferromagnetic quantum spin chains, along with Haldane's Conjecture, predicts a finite energy gap at  $\theta = 0$ , but a gapless second order phase transitions for  $\theta \rightarrow \pi$ .

So far this is the picture for  $\theta = 0$ . If we now include a vacuum angle  $\theta$ , we see from eqs. (30), (31) that this attaches to each region with a meron (anti-meron) a factor  $\exp(\pm i\theta/2)$ . Therefore any sub-volume with a meron-anti-meron pair picks up a factor  $\cos(\theta/2)$ , and in particular  $\theta = \pi$  "neutralizes" all these pairs: they do not appear in  $\exp(-\mathcal{H}/T)$ , so they cannot diffuse the long-range order anymore, and the gap vanishes.

This picture refers to rather smooth configurations, which dominate at weak coupling, *i.e.* at small  $g$ . This is the framework of the effective low energy theory [24,36], and we also mentioned that the mapping at large  $s$  leads to a small  $g \propto 1/s^2$ . For the other extreme,  $g \gg 1$ , Seiberg reported a cusp in the free energy, which signals a first order phase transition, at  $\theta = \pi$  [39].

Taking these conjectures together, we arrive at the expected phase diagram shown in Fig. 9. In particular, if we fix a small (or moderate)  $g$ , we should run into a second order phase transition, and therefore into a continuum limit, for  $\theta \rightarrow \pi$ .

A subtle study in Ref. [40] made this interesting feature quantitative. To this end, it related the 2d O(3) model at  $\theta \approx \pi$ , at low energy, to a model of conformal field theory, known as the  $k = 1$  Wess-Zumino-Novikov-Witten model ( $k$  is the central charge) [41], see also Ref. [42]. Assuming both to be in the same universality class (cf. Section 1), the asymptotic behavior of the mass gap was derived as

$$\xi^{-1}(\theta \approx \pi) \propto \frac{|\theta - \pi|^{2/3}}{|\ln(|\theta - \pi|)|^{1/2}}. \quad (32)$$

In a finite volume  $L \times L$ , this translates further into a finite size scaling of the magnetic susceptibility  $\chi_m$  (given in eq. (10)), and the topological susceptibility  $\chi_t = (\langle Q^2 \rangle - \langle Q \rangle^2)/V$ : they are both predicted to exhibit a dominant scaling  $\propto L$ , which is characteristic for a second order phase transition; for a (more abrupt) first order transition one would expect susceptibilities  $\propto L^2$ . The conjectured form, refined by logarithmic corrections, reads

$$\chi_m = L \sqrt{\ln L} g_m(L/\xi), \quad \chi_t = \frac{L}{\sqrt{\ln L}} g_t(L/\xi), \quad (33)$$

where  $g_m$  and  $g_t$  are “universal functions” with respect to variations of  $L$  and  $\xi$ .

This is an explicit prediction, to be verified in order to check the above conjecture about a second order phase transitions for  $\theta \rightarrow \pi$ . The way to study effects beyond perturbation theory, from first principle, are numerical Monte Carlo simulations of the lattice regularized model (we recall footnote 5 and Refs. [4]). Its idea is to generate numerous random configurations with probability  $p[\vec{\sigma}] \propto \exp(-\mathcal{H}[\vec{\sigma}]/T)$ , cf. eq. (3). A large set of such configurations enables the numerical measurement of expectation values of the physical terms.

This is straightforward for  $\mathcal{H}_0$ , but as soon as we include  $\theta \neq 0$ ,  $\mathcal{H}$  and  $\exp(-\mathcal{H}/T)$  become complex, so they do not define a probability anymore. We could generate the configurations using  $|\exp(-\mathcal{H}[\vec{\sigma}]/T)|$ , and include a complex phase *a posteriori* by re-weighting the statistical entries. This is correct in principle, but the re-weighting involves lots of cancellations, hence a reliable measurement requires a huge statistics — the required number of configurations grows exponentially with the volume  $V$ . This is the notorious *sign problem*.

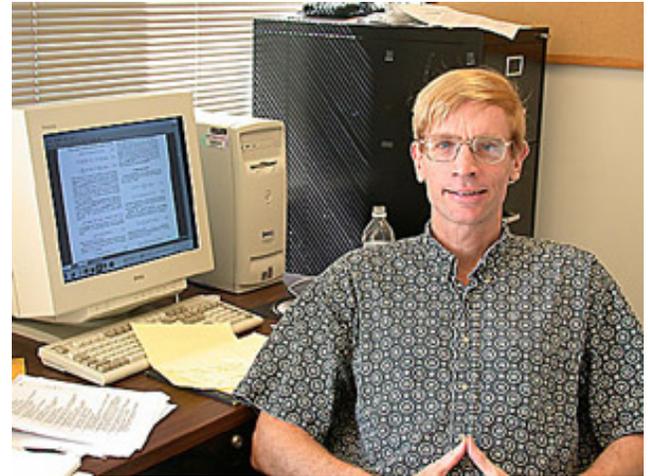


Figura 10. **Frederick Duncan Michael Haldane** (top), was born 1951 in London and studied at Cambridge University, where he graduated in 1978. After working at the University of Southern California, the Bell Laboratories and the University of California, San Diego, he became Eugene Higgins Professor at Princeton University in 1990. **Ian Keith Affleck** (bottom) was born 1952 in Vancouver, studied at Trent University (in Ontario, Canada), and graduated 1979 at Harvard University, his Ph.D. advisor was Sidney Coleman. He worked at Princeton University and Boston University, and since 2003 he is Killam Professor at the University of British Columbia in Vancouver.

In most cases where this problem occurs, in particular in QCD at high baryon density, and also in QCD with a  $\theta$ -term, it has prevented reliable numerical results. However, in the case of the 2D O(3) model, this problem was overcome thanks to the exceptionally powerful *meron cluster algorithm* [43], applied to the constraint Hamilton function (22) at  $\delta = 2\pi/3$ .

This algorithm divides the lattice volume into connected sets of spin variables  $\vec{\sigma}_x$ , the *clusters*, which are updated collectively [44]. This approach provides huge statistics (including many configurations that do not need to be generated explicitly). Hence in this exceptional case, conclusive numerical results were obtained, and they clearly confirmed the predicted large- $L$  scaling of eq. (33), including the  $\ln L$  refinement [43].

In addition, the algorithm also assigns an integer or half-integer topological charge  $q$  to each cluster (they sum up to the topological charge  $Q \in \mathbb{Z}$  of the entire configuration). At weak coupling, most clusters are neutral ( $q = 0$ ), and a few percent carry charge  $q = \pm 1/2$  (higher charges are

very seldom). At this point, we return to Affleck's picture, and interpret the clusters with  $q = 1/2$  ( $-1/2$ ) as merons (anti-merons). Then the picture of pair neutralization appears in a new light: now it is stochastic, and it does not require any  $O(3)$  symmetry breaking (unlike the potential  $\sim \mu^2(e^{(3)})^2$ ). Hence it confirms the result for the second order phase transition, and it even endows the heuristic picture with a neat stochastic interpretation.

#### IV CONCLUSIONS

We described the concept of classical and quantum spin models, the framework of the 2016 Physics Nobel Prize. We addressed aspects related to topology, *i.e.* to quantities which are invariant under (most) small deformations, and which can only change in discrete jumps. We referred to low dimensions,  $D = 1$  and  $2$ , where thermal fluctuations prevent the dominance of ordered structures, and therefore spontaneous symmetry breaking, but smooth phase transitions happen nevertheless.

In the classical 2D XY model we described the BKT phase transition [9], which is essential (of infinite order), and driven by the (un)binding of vortex-anti-vortex pairs. This transition has been observed experimentally, for instance in superfluids [11] and in superconductors [12], and recently also in systems of ultra-cold atoms trapped in optical lattices [45].

Then, we summarized the history of anti-ferromagnetic quantum spin chain studies, in particular the Haldane Conjecture [23, 24] about energy gaps for integer spin vs. gapless chains for half-integer spin. This insight agrees with experimental results as well [31, 32]. We further discussed the mapping onto a classical 2D  $O(3)$  model with a topological  $\theta$ -term (the Haldane-Affleck map [24, 36]), and the manifestation of the Haldane Conjecture in that system.

These are only selected topics of the works, which were awarded with the Physics Nobel Prize 2016. For a review of aspects which have not been covered here — in particular the quantum Hall effect and topological insulators — we refer to Ref. [46].

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