Advanced Statistical Physics: 2. Phase Transitions

Leticia F. Cugliandolo
leticia@lpthe.jussieu.fr
Sorbonne Université
Laboratoire de Physique Théorique et Hautes Energies
Institut Universitaire de France

September 21, 2020

Contents

2 Phase transitions

Take a piece of material in contact with an external reservoir. The material will be characterised by certain global observables, energy, magnetisation, *etc.*. To characterise macroscopic systems it is convenient to consider densities of energy, magnetisation, *etc*, by diving the macroscopic value by the number of particles (or the volume) of the system. If the system is coupled to its surroundings, this external environment will be characterised by some parameters, like the temperature, magnetic field, pressure, *etc.* In principle, one is able to tune the latter and measure the former as a function of them. In isolated systems, the temperature can also be defined from the entropy-energy relation following the microcanonical prescription, and it can be used as one of the axis in the phase diagram.

Sharp changes in the behaviour of *macroscopic systems* at critical points (lines) in parameter space have been observed experimentally. These correspond to *phase transitions* [1, 2, 3, 4, 5, 6, 7, 8, 9], a non-trivial *collective phenomenon* arising in the thermodynamic limit, $N \to \infty$ and $V \to \infty$. *Phase diagrams* as the one in Fig. 2.1 are used as a visual help to identify the global behaviour of a system according to the values that the *order parameters* (relevant observables) take in different regions of variation of the *control parameters* that give the axes to the phase diagram.

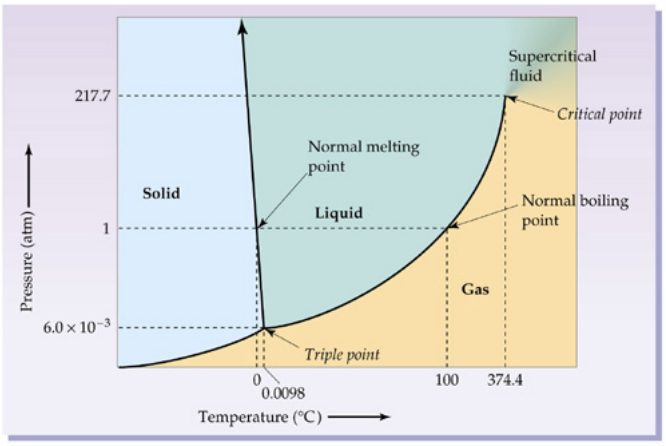

Figure 2.1: A quite generic phase diagram.

The phase diagram in Fig. 2.1 is bidimensional: the temperature-pressure plane. Both temperature and pressure can be thought of as parameters externally controlled. In recent years, it has become popular in atomic physics, in particular in cold atoms experiments, to work in isolation and study the statistical properties of the systems for different values

of the relevant *coupling constants* in the Hamiltonian, which can be tuned with smart experimental techniques.

Macroscopic models of agents in interaction may have *static* and *dynamic phase transitions*. The former are the usual ones studied with statistical physics methods. For example, in the canonical ensemble, one finds the phase transitions by looking for *non-analyticities* of the *free-energy density* (or another relevant thermodynamic potential) as a function of the control parameters, say just $\beta = 1/(k_B T)$,

$$-\beta f(\beta) = N^{-1} \ln \mathcal{Z}(\beta) \qquad \text{with} \qquad \mathcal{Z}(\beta) = \sum_C e^{-\beta H(C)} \tag{2.1}$$

where C represents all the system configurations. One is interested in identifying the *order parameter* (in some cases this is easy, in others it is not), finding the *critical curves* of the control parameters in the phase diagram, studying the *critical phenomenon* that is to say the behaviour of the order parameter and other properties close to the phase transition, *etc.*

Dynamic phase transitions correspond to sharp changes in the dynamic evolution of a macroscopic system. We will not discuss them in these notes.

Mean-field theories have been notably successful in capturing much of the global behaviour of many macroscopic systems. Of course, they cannot reproduce the details such as the functional form of the order parameters or the peculiarities of the critical phenomena. Still, they are notably useful to understand what is going on and get a first feeling of the quantitative behaviour of real systems.

We showed in the figure a phase diagram of a particle system with the usual gas, liquid and solid phases. For the sake of simplicity, it is better to discuss phase transitions in the context of magnetic systems. This is what we shall do in the rest of this Chapter.

2.1 The standard models for magnetic systems

Let us analyse a magnetic system. The Hamiltonian describing all microscopic details is a rather complicated one. It depends on the electrons' magnetic moments giving rise to the macroscopic magnetisation of the sample but also on the vibrations of the atomic crystal, the presence of structural defects, *etc.* If we call α a *microstate*, in the canonical ensemble its probability is $P_\alpha = e^{-\beta H_\alpha}/\mathcal{Z}$ with $\mathcal{Z}$ the partition function, $\mathcal{Z} = \sum_\alpha e^{-\beta H_\alpha}$. It is, however, impossible and not necessarily interesting to keep all details and work with all possible physical phenomena simultaneously. Imagine that we are only interested on the magnetic properties, characterised by the electronic magnetic moments.

The *Ising model* is a simplified mathematical representation of a magnetic system. It describes the magnetic moments as *classical spins*, s_i, taking values ± 1, lying on the vertices of a cubic lattice in d dimensional space, and interacting via nearest-neighbour

couplings, $J > 0$. The energy is then

$$H[\{s_i\}] = -\frac{J}{2}\sum_{\langle ij\rangle} s_i s_j - \sum_i h_i s_i \tag{2.2}$$

where h_i is a local external magnetic field. Most typically one works with a uniform field, $h_i = h$ for all sites. The justification for working with an Ising variable taking only two values is that in many magnetic systems the magnetic moment is forced to point along an *easy axis* selected by crystalline fields. We then need a model that focuses just on these.

There are two external parameters in H, the coupling strength J and the external field h. $J > 0$ favours the alignment of the spin in the same direction (*ferromagnetism*) while $J < 0$ favours the anti-alignement of the spins (*antiferromagnetism*). The magnetic field tends to align the spins in its direction.

In *finite dimensional* cases, the spins lie on a d dimensional *lattice* that can have different geometries. For instance, a cubic lattice is such that each vertex has *coordination number*, or number of neighbours, $z = 2d$. Triangular, honeycomb, *etc.* lattices are also familiar.

The Ising model is specially attractive for a number of reasons:

(i) It is probably the simplest example of modelling to which a student is confronted.

(ii) It can be solved in some cases: $d = 1$, $d = 2$, $d \to \infty$. The solutions have been the source of new and powerful techniques later applied to a variety of different problems in physics and interdisciplinary fields.

(iii) It has not been solved analytically in the most natural case, $d = 3$!

(iv) In $d \geq 2$, it has a phase transition at a finite value of the control parameter T/J, an interesting collective phenomenon, separating two phases that are well-understood and behave, at least qualitatively, as real magnets with paramagnetic disorder at high T/J and ferromagnetic order at low T/J.

(v) There is an *upper*, d_u, and a *lower*, d_l, *critical dimension*. Above d_u mean-field theory correctly describes the critical phenomenon. At and below d_l there is no finite T phase transition. Below d_u mean-field theory fails.

(vi) One can see at work generic tools to describe the critical phenomenon like *scaling* and the *renormalisation group*.

(vii) The phenomenon of *frustration* is illustrated by the antiferromagnetic Ising model on the triangular lattice.

(viii) Generalisations in which the interactions and/or the fields are random variables taken from a probability distribution are typical examples of problems with *quenched disorder*.

(ix) Generalisations in which spins are not just Ising variables but vectors with n components with a local constraint on their modulus are also interesting. Their energy is

$$H[\{\vec{s}_i\}] = -\frac{J}{2}\sum_{\langle ij\rangle} \vec{s}_i \cdot \vec{s}_j - \sum_i \vec{h}_i \cdot \vec{s}_i \tag{2.3}$$

with $n = 1$ (Ising), $n = 2$ (XY), $n = 3$ (Heisenberg), ..., $n \to \infty$ ($O(n)$) as particular

cases. The *local constraint* on the length of the spin is

$$s_i^2 \equiv \sum_{a=1}^{n} (s_i^a)^2 = n \ . \tag{2.4}$$

Note that each component is now a continuous variable bounded in a finite interval, $-\sqrt{n} \leq s_i^a \leq \sqrt{n}$, that actually diverges in the $n \to \infty$ limit. When $n \to \infty$ it is sometimes necessary to redefine the coupling constants including factors of n that yield a sensible $n \to \infty$ limit of thermodynamic quantities.

(x) One can add a dynamic rule to update the spins. We are then confronted to the *kinetic Ising model* (or its multi-component extensions) and more generally to the new World of stochastic processes.

(xi) *Dynamic phase transitions* occur in the properties of the system's evolution. We will not discuss them in these Lectures.

(xii) In the low temperature phase of clean models or even weakly frustrated/disorderd ones, the progressive order is reached via *domain growth*, the simplest example of coarsening.

(xiii) Last but not least, it has been a paradigmatic model extended to describe many problems going beyond physics like *neural networks*, *social ensembles*, *etc.*

Note the difference between the two parameters, N and n. N is the number of spins in the system. n is the number of components that each spin vector has. There is still another dimension, the one of real space, that we call d.

2.2 Concepts

Let us now discuss some important concepts, *symmetries*, *order parameters*, *pinning fields*, *broken ergodicity* and *broken symmetry* [1, 2, 3, 4, 5, 6, 7, 8, 9], with the help of the concrete example of the Ising model. The discussion applies, though, in greater generality.

2.2.1 Symmetries

Let us treat separately the case of continuous and discrete symmetries.

Continuous

In the absence of an applied magnetic field the Hamiltonian (2.3) remains invariant under the simultaneous *rotation* of all spins:

$$\begin{aligned} H[\{\vec{s}_i\,'\}] &= -\frac{J}{2}\sum_{\langle ij\rangle} \vec{s}_i\,' \cdot \vec{s}_j\,' = -\frac{J}{2}\sum_{\langle ij\rangle} R^{ab} s_i^b R^{ac} s_j^c = -\frac{J}{2}\sum_{\langle ij\rangle} R^{T\,ba} R^{ac} s_i^b s_j^c \\ &= = -\frac{J}{2}\sum_{\langle ij\rangle} s_i^b s_j^b = -\frac{J}{2}\sum_{\langle ij\rangle} \vec{s}_i \cdot \vec{s}_j = H(\{\vec{s}_i\}) \end{aligned} \tag{2.5}$$

since R is an orthogonal transformation, such that $R^T R = I$. The model is $O(n)$ symmetric. This symmetry is explicitly broken by the external field. (Summation over repeated a, b indices is assumed.)

Discrete

The Ising model with no applied field is invariant under the simultaneous *reversal* of all spins, $s_i \to s'_i = -s_i$, for all i, a discrete symmetry. The model is invariant under a Z_2 symmetry.

2.2.2 Order parameters

An *order parameter* is generically defined as a quantity – the statistical average of an observable – that typically vanishes in one phase and is different from zero in another one (or other ones). One must notice though that the order parameter is *not unique* (*e.g.*, any power of an order parameter is itself an order parameter) and that there can exist transitions without an order parameter as in the *topological* Kosterlitz-Thouless transition in the $2d$ XY model that we will study later.

In the ferromagnetic Ising model the order parameter is the global magnetisation density

$$m = \frac{1}{N} \sum_{i=1}^{N} \langle\, s_i \,\rangle \qquad \text{and} \qquad \langle\, s_i \,\rangle = \mathcal{Z}^{-1} \sum_{C} s_i \, e^{-\beta H(C)} \tag{2.6}$$

where N is the total number of spins and the angular brackets represent the thermal average in the canonical ensemble (that we adopt henceforth unless otherwise stated).

In Ising antiferromagnetic models one can define *staggered magnetisations* that take into account the periodicity between two possible orientations of the local spins. Generalisations to systems with different internal dimension of the spins are straightforward.

2.2.3 Thermodynamic limit

The abrupt change in the order parameter at particular values of the external parameters, say temperature and magnetic field (T, h), is associated to the divergence of some derivative of the free-energy (we use the canonical ensemble) with respect to one of these parameters. The partition function is a sum of positive terms. In a system with a finite number of degrees of freedom (as, for instance, in an Ising spin model where the sum has 2^N terms with N the number of spins) such a sum is an analytic function of the parameters. Thus, no derivative can diverge. One can then have a phase transition only in the *thermodynamic limit* in which the number of degrees of freedom diverges.

2.2.4 Pinning field

In the absence of a magnetic field, and for pairwise (two-body) interactions, the energy of an Ising model is an even function of the spins, $H(\{s_i\}) = H(\{-s_i\})$ and, consequently,

the equilibrium magnetisation density computed as an average over *all* spin configurations with their canonical weight, $e^{-\beta H(C)}$, vanishes at all temperatures:

$$\langle s_i \rangle = 0 \ \ \forall \ i \quad \text{if} \quad h_i = 0 \ \ \forall \ i \ . \tag{2.7}$$

At high temperatures, $m = 0$ (see Eq. (2.6)) characterises completely the equilibrium properties of the system since there is a unique paramagnetic state with vanishing magnetisation density. At low temperatures instead if we perform an experiment in a, say, ferromagnetic sample, we *do observe* a net magnetisation density. In practice, what happens is that when the experimenter takes the system through the transition he/she cannot avoid the application of tiny external fields – the experimental set-up, the Earth... – and there is always a small *pinning field* that actually selects one of the two possible equilibrium states, with positive or negative magnetisation density, allowed by symmetry. In the course of time, the experimentalist should see the full magnetisation density reverse, to ensure $m = 0$ in equilibrium. However, this is not seen in practice since astronomical time-scales would be needed. We shall see this phenomenon at work when solving mean-field models exactly.

To see $\langle s_i \rangle \neq 0$ one needs to compute

$$\lim_{h \to 0} \lim_{N \to \infty} \langle s_i \rangle_h = m \neq 0 \ , \tag{2.8}$$

that is to say, the average under an applied field that is taken to zero only after the infinite size limit.

2.2.5 Broken ergodicity

Introducing dynamics into the problem,[1] *ergodicity breaking* can be stated as the fact that the temporal average over a long (but finite) time window

$$\overline{A}_t = \lim_{t_0 \ll \tau \ll t} \frac{1}{2\tau} \int_{t-\tau}^{t+\tau} dt' A(t') \tag{2.9}$$

is different from the static statistical one, with the sum running over all configurations with their associated Gibbs-Boltzmann weight:

$$\overline{A}_t \neq \langle A \rangle \ . \tag{2.10}$$

In practice, the temporal average is done in a long but finite interval $\tau < \infty$. During this time, the system is positively or negatively magnetised depending on whether it is in "one or the other degenerate equilibrium states" (see Fig. 2.2). Thus, the temporal average of the orientation of the spins, for instance, yields a non-vanishing result $\overline{A}_t = m_t \neq 0$. If, instead, one computes the statistical average summing over *all* configurations of the spins,

[1] Note that Ising model does not have a natural dynamics associated to it. Convenient dynamic rules can be attributed to the evolution of the spins ensuring the system's approach to canonical equilibrium.

the result is zero, as one can see using just symmetry arguments, explained in Sec. 2.2.4. The reason for the discrepancy is that with the time average we are actually summing over half of the available configurations of the system: if the averaging time-window controlled by τ is not as large as a function of N, the trajectory does not have enough time to visit all configurations in phase space. One can reconcile the two results, in the statistical average, by summing only over the configurations with positive (or negative) magnetisation density and recovering in this way a non-vanishing result. We shall see this at work in a concrete calculation below.

Note that ergodicity breaking is a statement about the dynamics of a system.

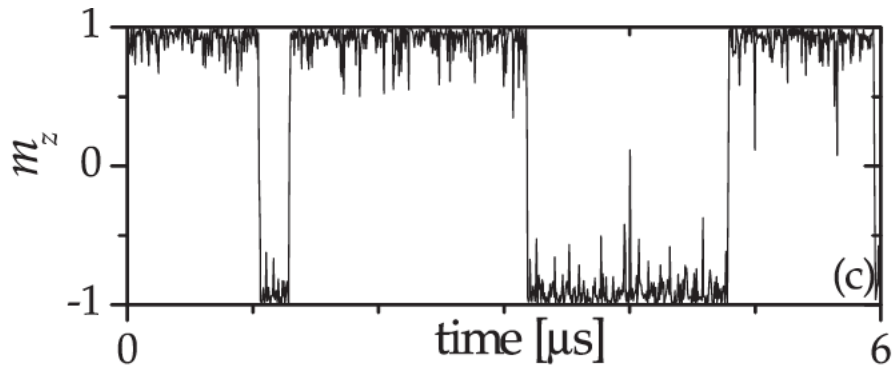

Figure 2.2: Time dependence of the global magnetisation in a magnetic system, with sudden switches from one state to another.

2.2.6 Spontaneous broken symmetry

In the absence of an external field the Hamiltonian is symmetric with respect to the simultaneous reversal of all spins, $s_i \to -s_i$ for all i. The phase transition corresponds to a *spontaneous symmetry breaking* between the states of positive and negative magnetization. One can determine the one that is chosen when going through T_c either by applying a small *pinning field* that is taken to zero only after the thermodynamic limit, or by imposing adequate *boundary conditions* like, for instance, all spins pointing up on the borders of the sample. Once a system sets into one of the equilibrium states this is completely stable in the $N \to \infty$ limit. The mathematical statement of spontaneous symmetry breaking is then

$$\lim_{h\to 0^+} \lim_{N\to\infty} \langle\, s_i \,\rangle = - \lim_{h\to 0^-} \lim_{N\to\infty} \langle\, s_i \,\rangle \neq 0 \,. \tag{2.11}$$

Ergodicity breaking necessarily accompanies spontaneous symmetry breaking but the reverse is not true; an example is provided by systems with quenched disorder. Indeed, spontaneous symmetry breaking generates disjoint ergodic regions in phase space, related

by the broken symmetry, but one cannot prove that these are the only ergodic components in total generality. Mean-field spin-glass models provide a counterexample of this implication, in which many ergodic components not related by symmetry exist.

2.2.7 Landau scheme

Without getting into the details of the Landau description of phase transitions (that you will certain study in the Statistical Field Theory lectures) we just summarise here, in Figs. 2.3 taken from [2], the two scenarii corresponding to second order (the panels in the first row) and first order phase transitions (the next six panels). The figures show the evolution of the free-energy density as a function of the order parameter η when temperature (called T in the first three panels and t in the next six ones) is modified.

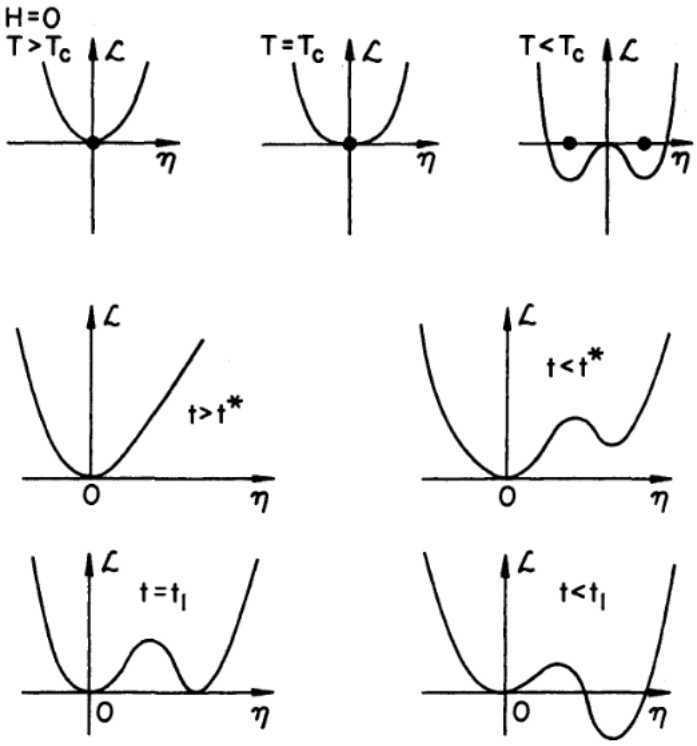

Figure 2.3: Second order (first line) and first order (second and third lines) phase transitions. Figures taken from [2].

In the Landau formalism, the order parameter is determined by a saddle-point equation which typically takes the form $x =$ a sigmoid function. The difference between *second order* and *first order* transitions is the way in which the sigmoid function changes when the control parameter is modified. Figure 2.4 shows two sketches of this evolution for second order (labelled[2] $p = 2$) and first order (labelled $p = 3$) transitions.

[2]the origin of this name lies in a family of models realising this phenomenon and changing character

In a second order phase transition the non-vanishing solutions split from the vanishing one in a continuous way. A possible strategy to find the critical parameters is, then, to look for the values at which the slope of the sigmoid function close to zero equals one.

In a first order phase transition the sigmoid function touches the diagonal axis at a non-vanishing value when the local minimum at $x \neq 0$ first appears. Further changing the parameters this point splits in two and the sigmoid function crosses the diagonal at three points, say $x = 0$, x_1 (a maximum of the free-energy density) and x_2 (the non-zero minimum of the free-energy function). Other two crossings are symmetrically placed on $x < 0$ values if the model is invariant under $x \mapsto -x$.

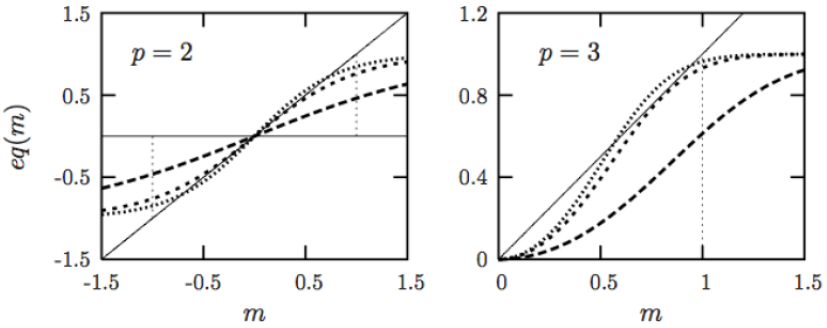

Figure 2.4: Sketch of the graphical solution of the mean-field equation for the order parameter in the ferromagnetic $p = 2$ (left) and $p = 3$ (right) models. The curves represent the sigmoid function (labelled eq) as a function of the order parameter m (in the horizontal axis).

Exercise 2.1 Take the p-spin ferromagnetic Ising model, defined by the Hamiltonian

$$H(\{s_i\}) = -J \sum_{i_1 \neq \cdots \neq i_p} s_{i_1} \dots s_{i_p} \tag{2.12}$$

where p is an integer parameter and the sum runs over all p-uplets of spins that one can construct among the N ones. The variables s_i are Ising like and take two values $s_i = \pm 1$. Consider separately the cases $p = 2$ and $p > 2$. Study the canonical equilibrium properties of the two models. Think about the necessary rescaling of the coupling strength $J > 0$ with the system size N to make the energy extensive. Construct the free-energy density as a function of the global ferromagnetic order parameter m. Identify and study the stability of its extremes. Find the phase transitions and determine their order. Derive the equations that determine the order parameter m and compare them to the plots in Fig. 2.4.

2.2.8 Energy *vs.* entropy - the Peierls argument

Let us use a thermodynamic argument to describe the high and low temperature phases of a magnetic system and argue that for short-range interactions a one dimensional system

depending on a parameter p that takes integer values.

with short-range interactions cannot sustain an order phase a finite temperature while one with sufficiently long-range interactions can.

The *free-energy* of a system is given by $F = U - TS$ where U is the internal energy, $U = \langle H \rangle$, and S is the entropy. The equilibrium state may depend on temperature and it is such that it minimises its free-energy F. A competition between the energetic contribution and the entropic one may then lead to a change in phase at a definite temperature, *i.e.* a different group of micro-configurations, constituting a state, with different macroscopic properties dominate the thermodynamics at one side and another of the transition.

At zero temperature the free-energy is identical to the internal energy U. In a system with nearest-neighbour ferromagnetic couplings between magnetic moments, the magnetic interaction is such that the energy is minimised when neighbouring moments are parallel.

Switching on temperature thermal agitation provokes the reorientation of the moments and, consequently, misalignments. Let us then investigate the opposite, infinite temperature case, in which the entropic term dominates and the chosen configurations are such that entropy is maximised. This is achieved by the magnetic moments pointing in random independent directions.

The competition between these two limits indicates whether a finite temperature transition is possible or not.

Short-range interactions

At zero temperature the preferred configuration is such that all moments are parallel, the system is fully ordered, and for nearest-neighbour couplings $U = -J\#$ pairs.

For a model with N Ising spins, the entropy at infinite temperature is $S \sim k_B N \ln 2$.

Decreasing temperature magnetic disorder becomes less favourable. The existence or not of a finite temperature phase transitions depends on whether long-range order, as the one observed in the low-temperature phase, can remain stable with respect to *fluctuations*, or the reversal of some moments, induced by temperature. Up to this point, the discussion has been general and independent of the dimension d.

The competition argument made more precise allows one to conclude that there is no finite temperature phase transition in $d = 1$ while it suggests there is one in $d > 1$. Take a one dimensional ferromagnetic Ising model with closed boundary conditions (the case of open boundary conditions can be treated in a similar way),

$$H[\{s_i\}] = -J \sum_{i=1}^{N} s_i s_{i+1} \ , \tag{2.13}$$

and $s_{N+1} = s_1$. At zero temperature it is ordered and its internal energy is just

$$U_o = -JN \tag{2.14}$$

with N the number of links and spins. Since there are two degenerate ordered configurations (all spins up and all spins down) the entropy is

$$S_o = k_B \ln 2 \tag{2.15}$$

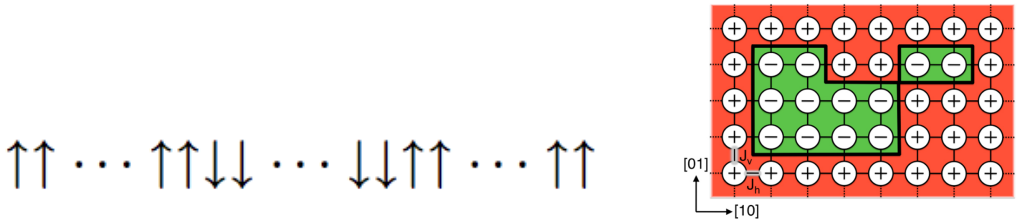

Figure 2.5: Left, a domain wall in a one dimensional Ising system and right, two bidimensional domains in a planar (artificial) Ising system.

The internal energy is extensive while the entropy is just a finite number. At temperature T the free-energy of the completely ordered state is then

$$F_o = U_o - TS_o = -JN - k_B T \ln 2 \; . \tag{2.16}$$

This is the *ground state* at finite temperature or global configuration that minimises the free-energy of the system.

Adding a *domain* of the opposite order in the system, *i.e.* reversing n spins, two bonds are unsatisfied and the internal energy becomes

$$U_2 = -J(N-2) + 2J = -J(N-4) \; , \tag{2.17}$$

for any n. Since one can place the misaligned spins anywhere in the lattice, there are N equivalent configurations with this internal energy. The entropy of this state is then

$$S_2 = k_B \ln(2N) \; . \tag{2.18}$$

The factor of 2 inside the logarithm arises due to the fact that we consider a reversed domain in each one of the two ordered states. At temperature T the free-energy of a state with *two domain walls* is

$$F_2 = U_2 - TS_2 = -J(N-4) - k_B T \ln(2N) \; . \tag{2.19}$$

The variation in free-energy between the ordered state and the one with one reversed domain is

$$\Delta F = F_2 - F_o = 4J - k_B T \ln N \; . \tag{2.20}$$

Thus, even if the internal energy increases due to the presence of the domain walls, the increase in entropy is such that the free-energy of the state with a droplet in it is much lower, and therefore the state much more favourable, at any finite temperature T. One can repeat this argument reversing domains within domains and progressively disorder the sample. We conclude that spin flips are favourable and order is destroyed at any non-vanishing temperature. The ferromagnetic Ising chain does not support a non-zero temperature ordered phase and therefore does not have a finite temperature phase transition.

A similar argument in $d > 1$ suggests that one can have, as indeed happens, a finite temperature transition in these cases (see, *e.g.* [2]).

Note that this argument explicitly uses the fact that the interactions are short-ranged (actually, they extend to first neighbours on the lattice only in the example). Systems with sufficiently long-range interactions can have finite temperature phase transitions even in one dimension, as shown below.

Exercise 2.2 Solve the one dimensional Ising chain and confirm that it only orders at zero temperature. Identify the correlation length, $\xi(T)$, from the decay of the correlation function, $C(r) \sim e^{-r/\xi(T)}$, and its temperature dependence.

Power-law interactions

Take now a one dimensional Ising model

$$H = -\frac{J}{2}\sum_{i\neq j} J_{ij}s_i s_j = -J\sum_{i=0}^{N-1}\sum_{k=1}^{N-i} J_{i\,i+k}s_i s_{i+k} \tag{2.21}$$

with open boundary conditions and algebraically decaying ferromagnetic interactions

$$J_{i\,i+k} \sim J\, r_{i\,i+k}^{-(1+\sigma)} = J\,(ak)^{-(1+\sigma)}\ , \tag{2.22}$$

where $r_{i\,i+k} = |\vec{r}_i - \vec{r}_{i+k}|. = ak$, a is the lattice spacing and we used here the notation in [17] that compared to the one of the Introductory chapter is $\alpha = \sigma + 1$. From the arguments put forward in that chapter, we expect a change in behaviour at $\sigma = 0$ or $\alpha = d = 1$.

In a perfect ferromagnetic configuration the energy is $U_0 = -J\sum_{i=0}^{N-1}\sum_{k=1}^{N-i}(ak)^{-(1+\sigma)}$ that in a continuous limit, $ak \mapsto y$, $a\sum_k \mapsto \int dy$, and $a\sum_i \mapsto \int dx$ reads

$$\begin{aligned} U_0 \;&\mapsto\; -\frac{J}{a^2}\int_0^{L-a} dx \int_a^{L-x} dy\, \frac{1}{y^{1+\sigma}} = \frac{J}{a^2}\frac{1}{\sigma}\int_0^{L-a} dx\, [(L-x)^{-\sigma} - a^{-\sigma}] \\ &= \frac{J}{a^2}\frac{1}{\sigma}\frac{1}{1-\sigma}[-a^{1-\sigma} + L^{1-\sigma} - a^{-\sigma}(L-a)]\ . \end{aligned} \tag{2.23}$$

We see that for $\sigma < 0$ the energy is superextensive, $U_0 \propto -L^{1-\sigma}$. Instead, for $\sigma > 0$ the large system size limit is controlled by the last term and the (still negative) ground state energy is extensive.

We now make an explicit calculation to check whether this system can have long-range order in the cases $\sigma > 0$.

Consider an excitation over the ferromagnetically order state in which n spins on the left point down and $N-n$ spins on the right point up, that is to say, a configuration with a single sharp domain wall (possible because of the open boundary conditions). The excess energy of this excitation with respect to the perfectly ordered ground state in which all spins point up is:

$$\Delta U = 2J\sum_{i=0}^{n}\sum_{j=n-i+1}^{N-i}\frac{1}{(aj)^{1+\sigma}}\ . \tag{2.24}$$

Clearly, if $n = 0$ or $n = N - 1$, $\Delta U = 0$. In the continuous space limit, $a \to 0$, the sums can be transformed into integrals

$$\begin{aligned} \Delta U &\mapsto \frac{2J}{a^2} \int_0^z dx \int_{z-x+a}^{L-x} dy \, \frac{1}{y^{1+\sigma}} \\ &= -\frac{2J}{a^2\sigma} \int_0^z dx \left[(L-x)^{-\sigma} - (z-x+a)^{-\sigma} \right] \\ &= \frac{2J}{a^2\sigma(1-\sigma)} \left[(L-z)^{1-\sigma} - L^{1-\sigma} - a^{1-\sigma} + (z+a)^{1-\sigma} \right] \end{aligned} \tag{2.25}$$

where we called $L = Na$ the length of the chain and z the placement of the domain wall. We now study this expression in the case $L \gg z \gg a$, that is to say, when the domain wall is placed at a finite distance from the origin compared to the infinite size limit. The contribution of the first two terms in the square brackets is proportional to z/L^σ for $z \ll L$ and negligible for $\sigma > 0$. The third term is just a short-length regularisation depending on the lattice size. The last term is the important one that we approximate as

$$\approx \frac{2J}{a^2\sigma(1-\sigma)} \, z^{1-\sigma} \tag{2.26}$$

using $z \gg a$. Therefore, the excitation energy increases with the length to the reversed domain for $0 < \sigma < 1$ (while in the short range case it was independent of it). The reversal of large domains is not favourable energetically and this is an indication that long-range order can exist in such a model with weakly long-range interactions such that $0 < \sigma < 1$. In the case $\sigma < 0$ interactions are strongly long-ranged and order is possible as well. In contrast, for $\sigma > 1$ the energy of a large droplet is bounded and the entropic term at finite temperature will end up destroying the ferromagnetic order.

2.2.9 Exact solutions in low dimension

In one dimension the partition function of a number of magnetic models can be computed exactly and the absence of a finite temperature phase transition see from the absence of non-analyticities in the free-energy. In the two following exercises this fact is made explicit in the one dimensional Ising chain and XY model.

Exercise 2.3 Calculate the free-energy of the one dimensional ferromagnetic Ising chain (no external field applied) $H = -J \sum_{i=1}^{N} s_i s_{i+1}$. Discuss free and periodic ($s_1 = s_{N+1}$) boundary conditions separately.

Exercise 2.4 Calculate the free-energy of the one dimensional ferromagnetic XY chain (no external field applied) $H = -J \sum_{i=1}^{N} \vec{s}_i \cdot \vec{s}_{i+1}$. Discuss free and periodic ($\vec{s}_1 = \vec{s}_{N+1}$) boundary conditions separately.

Exercise 2.5 Study the equilibrium properties of the nearest-neighbour Ising model in one dimension with the addition of a fully connected term: $H = -J_{\text{nn}} \sum_{i=1}^{N} \vec{s}_i \cdot \vec{s}_{i+1} + J_{\text{fc}} \left(\sum_i s_i^2 \right)^2$ with J_{fc} conveniently rescaled with N so as to make the energy extensive. This model can be studied in the canonical and microcanonical ensembles and for certain values of the parameters inequivalence of results are found. See, *e.g.* [17] and references therein for a discussion.

2.2.10 Field theories

A field theory for the magnetic problem can be rather simply derived by coarse-graining the spins over a coarse-graining length ℓ. This simply amounts to computing the averaged spin on a box of linear size ℓ. In the limit $\ell \gg a$ where a is the lattice spacing many spins contribute to the sum. For instance, an Ising bimodal variable is thus transformed into a continuous real variable taking values in $[-1, 1]$. Studying the problem at long distances with respect to ℓ (or else taking a continuum spatial limit) the problem transforms into a *field theory*. This is the route followed by Landau.

Field theories are the natural tool to describe particle physics and cosmology. For example, the Big Bang leaves a radiation-dominated universe at very high temperature close to the Planck scale. As the initial fireball expands, temperature falls precipitating a sequence of phase transitions. The exact number and nature of these transitions is not known. It is often considered that they are at the origin of the structures (galaxies, clusters, *etc.*) seen in the universe at present, the original seeds being due to density fluctuations left behind after the phase transition.

The similarity between the treatment of condensed matter problems and high energy physics becomes apparent once both are expressed in terms of field theories. It is however often simpler to understand important concepts like spontaneous symmetry breaking in the language of statistical mechanics problems.

2.3 Critical phenomena and scaling

The notion of *universality* was originally introduced by experimentalists to describe the observation that several apparently unrelated physical systems were characterised by the same type of singular behaviour near a continuous phase transition. It implies that the emerging long-range correlations of fluctuations of the order parameter are fully specified by the symmetry properties and conservation laws and do not depend on details of the microscopic interactions or dynamics.

Correlation function yield a very useful way to characterise phases and phase transitions. The two-point spatial correlation measures how much the fluctuation of the local (say, scalar) order parameter $O(\vec{r})$ around its averaged value influences the same quantity at a given distance within the system:

$$C(\vec{r}, \vec{r}') = \langle (O(\vec{r}) - \langle O(\vec{r}) \rangle)(O(\vec{r}') - \langle O(\vec{r}') \rangle) \rangle \ . \tag{2.27}$$

The averages $\langle O(\vec{r}) \rangle$ and $\langle O(\vec{r}') \rangle$ are not expected to depend on the space points $\vec{r}$ and $\vec{r}'$ in a homogeneous system but, for completeness, we keep this potential dependence in the notation used. These are also called *connected correlation functions*. In the disorder phase the order parameter vanishes and connected and normal correlation functions coincide. In the ordered phase this is not the case. In models with no order parameter, such as the $2d$ XY model, the correlation function of the would-be order parameter still yields

relevant information about the systems behaviour. Therefore, in the spin models we deal with in this Section

$$C_{ij} = \langle (\vec{s}_i - \langle \vec{s}_i \rangle) \cdot (\vec{s}_j - \langle \vec{s}_j \rangle) \rangle \tag{2.28}$$

that, because of invariance under translations and isotropy, one expects to be a function of the distance between the two spins, $r_{ij} \equiv |\vec{r}_i - \vec{r}_j|$.

Close to a continuous phase transition, a two-point correlation function should behave as

$$C(\vec{r}, \vec{r}') \simeq r^{2-d-\eta}\ e^{-r/\xi_{eq}}\ , \tag{2.29}$$

with $r = |\vec{r} - \vec{r}'|$, and the *correlation length*, the only relevant length scale, diverging at the critical point according to

$$\xi_{eq} \simeq |T - T_c|^{-\nu} \ \text{(2nd order)} \qquad \xi_{eq} \simeq e^{b|T-T_c|^{-\nu}} \ (\infty \text{ order})\ . \tag{2.30}$$

Time-delayed correlation functions characterise the temporal de-correlation of equilibrium fluctuations. The equal space, time delayed connected correlations are defined as

$$C(\vec{r}, t) = \langle (O(\vec{r}, t) - \langle O(\vec{r}, t) \rangle)(O(\vec{r}, t) - \langle O(\vec{r}, t) \rangle) \rangle\ . \tag{2.31}$$

In a *stationary state*, one-time quantities are independent of absolute time $\langle O(\vec{r}, t) \rangle \to \langle O(\vec{r}) \rangle$ and two-time quantities depend upon the time difference only. Close to criticality one expects

$$C(t, t') \simeq\ |t - t'|^{(2-d-\eta)/z_{\rm eq}}\ e^{-|t-t'|/\tau_{eq}}\ . \tag{2.32}$$

In second order cases, the correlation length and *correlation time* are linked by

$$\xi_{eq} \simeq \tau_{eq}^{1/z_{eq}}\ . \tag{2.33}$$

In infinite order cases the relation should be exponential.

At the critical point, the exponents and scaling functions can be derived with the RG analysis of an effective field theory, valid in the vanishing lattice spacing limit.

In experiments it is often easier to measure linear response functions instead of correlation functions. The linear response of the local observable $O(\vec{r})$ is defined as

$$\chi(\vec{r}, \vec{r}') = \left. \frac{\delta \langle O(\vec{r}) \rangle_h}{\delta h(\vec{r}')} \right|_{h=0} \tag{2.34}$$

where the infinitesimal perturbation $h(\vec{r}')$ is applied linearly to the same observable O in such a way that the Hamiltonian of the system is modified as $H \mapsto H - \int d^d r\, h(\vec{r}) O(\vec{r})$. The notation $\langle \cdots \rangle_h$ indicates that the average has to be calculated in the presence of the field, that is to say, with the perturbed Hamiltonian.

A simple calculation yields the *fluctuation-dissipation theorem*

$$\chi(\vec{r}, \vec{r}') = \beta \left(\langle O(\vec{r}) O(\vec{r}') \rangle - \langle O(\vec{r}) \rangle \langle O(\vec{r}') \rangle \right) \tag{2.35}$$

where all averages in the right-hand-side are measured with no applied field. This is a model independent relation since it does not depend on the form of the Hamiltonian H and only relies on the assumption of equilibrium.

Exercise 2.6 Prove eq. (2.35) assuming equilibrium in the canonical ensemble.

In a homogenous case one expects $\chi(\vec{r},\vec{r}') = \tilde{\chi}(\vec{\Delta r})$ with $\vec{\Delta r} = \vec{r} - \vec{r}'$. If the problem is furthermore isotropic then $\chi(\vec{r},\vec{r}') = \tilde{\chi}(r)$ with $r = |\vec{\Delta r}| = |\vec{r} - \vec{r}'|$. Under these assumptions, the integration of the susceptibility or linear response over the full space reads

$$\int d^d r \int d^d r' \, \chi(\vec{r},\vec{r}') = V \int d^d r \, \tilde{\chi}(r) = V \Omega_d \int dr \, r^{d-1} \, \tilde{\chi}(r) = V \Omega_d \beta \int dr \, r^{d-1} \, \tilde{C}_c(r) \, , \tag{2.36}$$

where V is the volume, Ω_d is the angular volume of the d dimensional space, and we used the fluctuation-dissipation relation (2.35). If we now use the critical scaling form of the connected correlation function, eq. (2.29),

$$\begin{aligned} (V\Omega_d)^{-1} \int d^d r \int d^d r' \, \chi(\vec{r},\vec{r}') &= \beta \int_0^L dr \, r^{d-1} \, r^{2-d-\eta} \, e^{-r/\xi_{\rm eq}} \\ &= \beta \, \xi_{eq} \, \xi_{eq}^{d-1} \, \xi_{\rm eq}^{2-d-\eta} \int_0^{L/\xi_{eq}} du \, u^{d-1} \, u^{2-d-\eta} \, e^{-u} \\ &= \beta \, c(L/\xi_{eq}) \, \xi_{eq}^{2-\eta} \, . \end{aligned} \tag{2.37}$$

where $c(L/\xi_{\rm eq})$ is the value of the last integral. In the infinite size limit, $L/\xi_{\rm eq} \to \infty$, $c(L/\xi_{\rm eq})$ reaches a constant and the integrated susceptibility diverges with the correlation length at the critical point.

2.4 Models with continuous symmetry

The energy of spin models with continuous variables, such as the XY, Heisenberg or generic $O(n)$ models introduced in (2.3) and (2.4) in the absence of an applied field ($\vec{h} = \vec{0}$), is invariant under the simultaneous rotation of all the spin variables:

$$s_i^a \mapsto R^{ab} s_i^b \, . \tag{2.38}$$

(R^{ab} are the n^2 elements of a rotation matrix in an n-dimensional space. As all rotation matrices in real space it has real elements and it is orthogonal, that is to say, $R^T = R^{-1}$ with $\det R = \pm 1$.) This is a *continuous global symmetry* to be confronted to the *discrete global* spin reversal invariance, $s_i \mapsto -s_i$, of the Ising case. In group theoretical terms, the continuous symmetry is $O(n)$ and the discrete one is Z_2.

The spontaneous magnetization at zero temperature can point in any of the infinite equivalent directions constrained to satisfy (2.4). This gives rise to an infinite degeneracy of ground states that are translational invariant (in real space). These equilibrium states

are controlled by a continuous variable, determining the direction on the n-dimensional hypersphere of radius 1. The effect of thermal fluctuations depends on the dimensions of the real space d and the vector n. We analyse them below, especially in the case of $d = n = 2$.

2.4.1 The d-dimensional XY model: spin-waves

Let us consider one such equilibrium state and call it $\vec{s}_i^{\,\mathrm{eq}}$. It is clear that if one slightly modifies the angle of the $\vec{s}$ vector on neighbouring space points, the energy cost of such a perturbation vanishes in the limit of vanishing angle. These configurations are called *spin-waves* and they differ from the uniformly ordered state by an arbitrarily small amount.

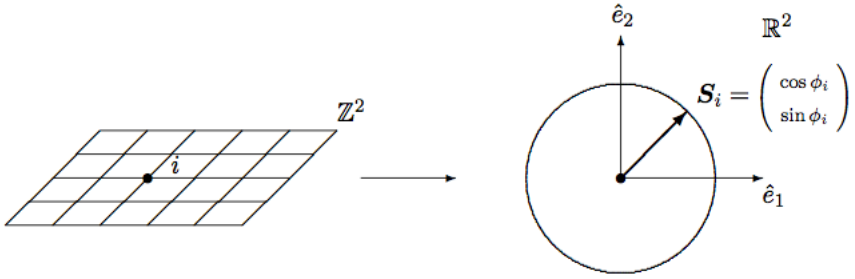

Figure 2.6: A sketch of the $2d$ XY model definition. On the left the square lattice in $2d$, on the right the $n = 2$ spin vector.

In the particular case of the XY model, see Fig. 2.6, the local spins are constrained to rotate on the *plane*; therefore, each spin has only two components ($n = 2$) and it can be parametrised as

$$\vec{s}_i = (s_i^1, s_i^2) = |\vec{s}_i|(\cos\phi_i, \sin\phi_i) = (\cos\phi_i, \sin\phi_i) \tag{2.39}$$

where $0 \leq \phi_i \leq 2\pi$ is the angle with respect to the x axis of the plane on which the spin vector lives, on each d-dimensional lattice site i. The modulus of each vector spin is fixed to one. The Hamiltonian (2.3) then becomes

$$H[\{\vec{s}_i\}] \mapsto H[\{\phi_{ij}\}] = -\frac{J}{2}\sum_{\langle ij\rangle} \cos\phi_{ij} \tag{2.40}$$

where $\phi_{ij} = \phi_i - \phi_j$ is the angle between the spins at neighbouring sites i and j. Equation (2.40) remains invariant under the global translation of all angles, $\phi_i \to \phi_i + \phi_0$ by the same amount, that corresponds to the *global rotational invariance*. The zero-temperature ground state is any of the fully aligned states $\phi_i = \phi$ for all i, with ϕ in

$[0, 2\pi]$. There is, therefore, an *infinite degeneracy* of the ground state, as all possible orientations of the magnetisation $\vec{m}$ are equally probable. Any of these ground states has perfect *long-range order* since all spins point in the same direction. The ground state energy is $E_0 = -JNz/2$ with z the coordination number of the lattice and N the total number of spins in the system.

If one now assumes that at low enough T the angles between contiguous spins can only be small, $|\phi_i - \phi_j| \ll 2\pi$, the cosine in the Hamiltonian can be expanded to second order and

$$\begin{aligned} H[\{\phi_i\}] &\simeq -\frac{Jz}{2}N + \frac{J}{4}\sum_{\langle ij\rangle}(\phi_i - \phi_j)^2 \\ &= E_0 + \frac{J}{4}\sum_{\vec{r},\vec{a}}[\phi(\vec{r}+\vec{a}) - \phi(\vec{r})]^2 = H[\{\phi(\vec{r})\}] \; . \end{aligned} \tag{2.41}$$

In the last member we used a different parametrisation of the lattice sites in which they are identified by their positions $\vec{r}$ with respect to the origin of a coordinate system, and the vectors $\vec{a}$ point along all axes of the lattice. On a square lattice in $d = 2$, $\vec{a} = \hat{e}_k$ with $k = 1, 2$, and has modulus a, the lattice spacing. If $\phi(\vec{r})$ is a slowly varying function of $\vec{r}$ one can approximate the finite difference by a derivative, *e.g.*, along the x axis $\phi(\vec{r}+\vec{a}) = \phi(\vec{r}+a\hat{e}_x) - \phi(\vec{r}) \simeq a\partial_x\phi(\vec{r})$ since typically, $a \ll |\vec{r}|$. Next, the sum over lattice sites is approximated by an integral $\sum_{\vec{r}} \cdots \simeq a^{-d}\int d^d r \ldots$, and we write

$$H[\{\phi(\vec{r})\}] \simeq E_0 + \frac{J}{4a^{d-2}}\int d^d r \; [\vec{\nabla}\phi(\vec{r})]^2 \tag{2.42}$$

where $d = 2$. We ended up with a quadratic form that, if we *relax the angular constraint* $\phi \in [0, 2\pi]$, acts on a *real unbounded field*

$$-\infty < \phi < \infty \; . \tag{2.43}$$

This is also called the *elastic representation*. We note that if we use a Fourier transform $\phi_{\vec{k}} = V^{-1}\int d^d r \; e^{i\vec{k}\cdot\vec{r}}\,\phi(\vec{r})$, where $\phi_{\vec{k}}$ is now a complex function of $\vec{k}$, with $\vec{k} = 2\pi n/L\,\hat{e}_k$ and n an integer (see App. 2.B, the number of variables is not doubled since the Fourier components are constrained to satisfy $\phi^*_{\vec{k}} = \phi_{-\vec{k}}$), the Hamiltonian becomes one of independent harmonic oscillators or *modes*

$$H[\{\phi_{\vec{k}}\}] \simeq E_0 + \frac{(2\pi)^d J}{4a^{d-2}}\sum_{\vec{k}} k^2 |\phi_{\vec{k}}|^2 \; . \tag{2.44}$$

We note that the contribution of the *long wave-length* modes, that is to say, small $k = 2\pi/\lambda$, is expected to be very small due to the k^2 factor.

From the harmonic Hamiltonian, assuming the smooth character of the field $\phi(\vec{r})$, one finds that the equation for the field configurations that minimise the energy is

$$\nabla^2\phi(\vec{r}) = 0 \; . \tag{2.45}$$

This equation is identical to the *Laplace equation* for the electrostatic potential in the absence of any charge density. It admits the trivial solution $\phi(\vec{r}) = \text{cst}$, that is just the ground state configuration.

First of all one may want to compute the average magnetisation $\vec{m} = \langle\, \vec{s}(\vec{r})\,\rangle = \lim_{\vec{h}\to\vec{0}}\langle\, \vec{s}(\vec{r})\,\rangle_{\vec{h}}$ where $\vec{h}$ is a pinning field. Mermin's exact calculation [10, 11] (that we will not present here, see [7] for a description of the proof) leads to $\vec{m} = \vec{0}$ at all non-vanishing temperatures in the thermodynamic limit, excluding usual magnetic order at any finite temperature in this system.

Exercise 2.7 Study Mermin's proof.

The interest is in computing the *spin-spin correlation function*

$$G(\vec{r}) \equiv \langle \vec{s}(\vec{r})\cdot\vec{s}(\vec{0})\rangle = \text{Re}\,\langle e^{i[\phi(\vec{r})-\phi(\vec{0})]}\rangle = e^{-\frac{1}{2}\langle[\phi(\vec{r})-\phi(\vec{0})]^2\rangle} \equiv e^{-\frac{1}{2}g(r)}\ , \tag{2.46}$$

where the second identity holds for Gaussian fields with zero average.[3] $G(\vec{r})$ here is a space-dependent correlation function and its Fourier transform is called the *structure factor*. Since there is no perturbation breaking the systems *isotropy*, one can expect this quantity to be a function of the modulus of the position vector and not of its direction; therefore, one should find that the result is given by a $G(r)$. Next, one should analyse whether the correlation function, at long distances, converges to a finite value (*long-range order*) or zero (no long-range order). Some details of this calculation (which can be found in many textbooks and your statistical field-theory lectures, I presume) are given in App. 2.C. They lead to

$$\frac{Ja^{2-d}}{k_BT}\ g(r) \simeq \begin{cases} \Omega_d/(d-2)\ (\pi/L)^{d-2} & d>2\ , \\ (2\pi)^{-1}\ \ln(r/L) & d=2\ , \\ r/2 & d=1\ , \end{cases}$$

that imply

$$G(r) \simeq \begin{cases} e^{-\text{const}\ k_BT} & d>2 & \textit{long-range order}\ , \\ (r/L)^{-\eta(k_BT/J)} & d=2 & \textit{quasi-long-range order}\ , \\ \exp[-k_BT/(2Ja)\ r] & d=1 & \textit{short-range order} \end{cases}$$

The behaviour is special in $d=2$. Interestingly enough, we find that the $2d$ XY model does not support long-range order but its correlation function decays algebraically at all non-zero temperatures. This is the kind of decay found *at* a critical point, $G(r) \simeq r^{-(d-2+\eta)}$, so the system behaves as at criticality at all temperatures. This does not seem feasible physically (at least at very high temperature the decay should be exponential) and, indeed, we shall see that other excitations, not taken into account by the continuous expansion above, are responsible for a phase transition of a different kind, a so-called *topological phase transition*. After these have been taken care of, the low-T phase remains well described

[3] Gaussian identity: $\int_{-\infty}^{\infty}\frac{dz}{\sqrt{2\pi\sigma^2}}\,e^{-\frac{z^2}{2\sigma^2}}\,e^{iz} = \int_{-\infty}^{\infty}\frac{dz}{\sqrt{2\pi\sigma^2}}\,e^{-\frac{1}{2}\left(\frac{z}{\sigma}-i\sigma\right)^2}e^{-\frac{\sigma^2}{2}} = e^{-\frac{\sigma^2}{2}}$.

by the spin-wave approximation but the high-T one is dominated by the proliferation of topological defects.

The exponent $\eta(k_BT/J)$ continuously depends on temperature, $\eta(k_BT/J) = k_BT/(2\pi J)$. This is a signature of the *criticality of the low-T phase*. The criticality is also accompanied by other special features, such as, for example, the non-trivial fluctuations of the "failed" order parameter $m = N^{-1}\langle|\sum_{i=1}^{N}\vec{s}_i|\rangle$ for finite system size [14]. Indeed, the thermally averaged value of the order parameter m has abnormally large finite size corrections. Within a spin wave calculation one finds $m = (1/(2N))^{k_BT/(8\pi J)}$ with the expected vanishing value in the thermodynamic limit but rather large values at low temperature and finite sizes. Monte Carlo simulations demonstrate that the distribution function, $P(y)$ with $y = N^{-1}|\sum_{i=1}^{N}\vec{s}_i|$ is a universal asymmetric form with interesting characteristics.

2.4.2 The $2d$ XY model: high temperature expansions

A first quantitative hint on the fact that there must be a phase transition in the $2d$ XY model came from the study of the high temperature expansion [15, 16]. The method is very similar to the one used to study Ising spin systems. With the aim of developing a small β Taylor expansion, the partition function is written as

$$Z = \int \prod_i d\phi_i \; e^{\frac{\beta J}{2}\sum_{\langle ij\rangle}\cos(\phi_i-\phi_j)} = \int \prod_i d\phi_i \prod_{\langle ij\rangle} e^{\frac{\beta J}{2}\cos(\phi_i-\phi_j)} \; . \tag{2.47}$$

Exploiting the periodicity of the exponential of the cos, one can use several tricks to derive

$$G(r) = e^{-r/\xi} \qquad \text{with} \qquad \xi = a/\ln(4k_BT/J) \tag{2.48}$$

an exponential decay of the correlation function (see [9] for details). This calculation strongly suggests that there must be a phase transition between the high temperature disordered phase and a low temperature phase, the latter with, possibly, the quasi long-range order predicted by the spin-wave approximation. (It was argued that higher order terms in the gradient expansion around the zero temperature ground state do not destroy the quasi long-range order at low temperatures since they are irrelevant in the RG sense [9].)

2.4.3 The $2d$ XY model: vortices and the Kosterlitz-Thouless transition

The failure of the spin-wave approximation at high temperatures is rooted in that it only allows for small and smooth deviations (*gradient expansion*) about the ferromagnetically ordered state. In particular, it excludes configurations in which the angular field is singular at some isolated point(s). In other words, only *single-valued* functions ϕ satisfying,

$$\sum_{nn\,\vec{r},\vec{r}'\in C}[\phi(\vec{r}) - \phi(\vec{r}')] \mapsto \oint_C d\vec{r}' \cdot \vec{\nabla}\phi(\vec{r}') = 0 \tag{2.49}$$

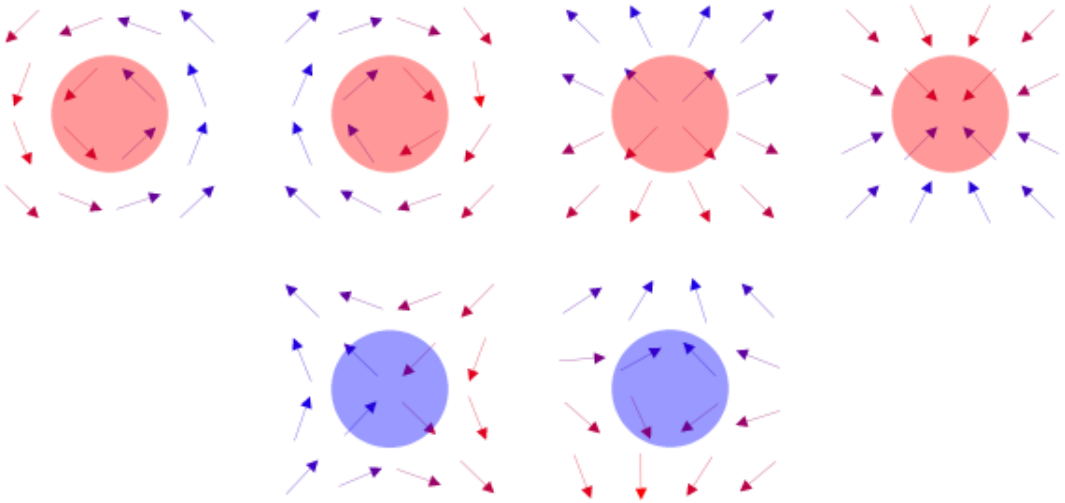

Figure 2.7: Four examples of vortices with charge $q = 1$ (first line) and two examples of anti-vortices with $q = -1$ (second line), see Eq. (2.52) for the definition of q. Figures borrowed from [21].

for any closed path C are admitted in the spin-wave expansion. However, in the $2d$ XY model, only the spin $\vec{s}_i$ should be single-valued and the original Hamiltonian (2.40) defined on the lattice has a *discrete symmetry*

$$\phi_i - \phi_j \to \phi_i - \phi_j + 2\pi q \qquad \text{with} \qquad q \in \mathbb{Z} \tag{2.50}$$

that is lost in the continuous approximation (2.42). This symmetry permits the existence of *vortices*, a particular kind of *topological defects*. These excitations are the ones that kill the simple spin-wave prediction of there being quasi long-range order at all temperatures, as explained by Kosterlitz & Thouless in the series of papers [18, 19, 20]. Kosterlitz & Thouless (together with Haldane) were retributed the Nobel Prize in 2016 for having exhibited a new class of phase and phase transitions, qualified as *topological*.

> *Topological defects* are configurations, in this case spin configurations, that are local minima of the potential energy and that *cannot* be smoothly transformed into the ground state, in this case the configuration in which all the spins are aligned, by a continuous transformation of variables, in this case a continuous rotation of all spins.

In a continuous description of the lattice problem, this means that there is no transformation of the kind

$$\vec{s}(\vec{r}) \mapsto R(\vec{r})\vec{s}(\vec{r}) \tag{2.51}$$

with a continuous rotation matrix $R(\vec{r})$ that transforms the configuration with a topological defect into one of the ground state (continuously transformable into a spin-wave state).

In the $2d$ XY model, the topological defects are *vortices*. On the lattice a vortex configuration is such that

$$\sum_{nn\, i,j\in C} (\phi_i - \phi_j) = 2\pi q \tag{2.52}$$

with q an integer ensuring that the spin be single-valued on each site of the lattice, the *charge* of the vortex. These are spin configurations for which in going around a closed path the angle rotates by $2\pi q$. The discrete nature of the charge, makes impossible to continuously deform the configuration to the uniformly ordered state in which the charge is zero. The center of the vortex is located on a site of the *dual lattice*.

In the continuous limit vortex configurations are *local minima* of the Hamiltonian

$$\frac{\delta H}{\delta\phi(\vec{r})} = 0 \qquad \text{and} \qquad \frac{\delta^2 H}{\delta\phi(\vec{r})\delta\phi(\vec{r}')} \quad \text{positive definite} \tag{2.53}$$

where the second condition ensures their stability. Indeed, $\phi(\vec{r}) = \text{cst}$ is not the only field configuration that minimises the energy. Vortex configurations, $\phi(\vec{r})$, in which the field has a *singularity* at the location of a point-like *charge*, also satisfy the conditions above.

A vortex configuration located at the origin $\vec{r} = \vec{0}$ can be written as

$$\phi(\vec{r}) = q\varphi(\vec{r}) + \phi_0 \tag{2.54}$$

with q the *integer charge* and $\varphi(\vec{r})$ the polar angle (angle with the horizontal x axis) of the space point $\vec{r}$

$$\varphi(\vec{r}) = \arctan\left(\frac{y}{x}\right) \tag{2.55}$$

and ϕ_0 an additive constant. As a example, let us take $q = 1$ and $\phi_0 = 0$. One can easily construct the spin configuration associated with this $\phi(\vec{r})$, that is $\vec{s}(\vec{r}) = (\cos\phi(\vec{r}), \sin\phi(\vec{r}))$. The arrows point as in the third panel in the first line in Fig. 2.7. Another choice is to use $q = 1$ and $\phi_0 = \pi/2$, leading to a configuration in which the spins turn anti-clockwise as in the left Fig. 2.10. Finally, one can use $q = 1$ and $\phi_0 = \pi$ to construct a configuration in which all spins point inwards, as in the last snapshot in the first line in Fig. 2.7.

All the configurations with the same q can be continuously transformed into one another. In the cases listed in the previous paragraph, $q = 1$, and

$$\vec{s}(\vec{r}, t) = (\cos(\varphi + t), \sin(\varphi + t)) \tag{2.56}$$

with t a real parameter, taking the values $t = 0, \pi/2$ and π in these particular cases. However, there is no parameter t that makes this configuration be one with another charge q'; this excludes the transformation into a constant field with $q' = 0$.

The *divergence at the origin of the gradient* of the configuration $\phi(\vec{r}) = q\varphi(\vec{r}) + \phi_0$ with $\varphi)\vec{r})$ in (2.54) is

$$\begin{aligned}
\vec{\nabla}\phi(\vec{r}) &= q\vec{\nabla}\varphi(\vec{r}) = q\vec{\nabla}\arctan\left(\frac{y}{x}\right) = -q\frac{y}{x^2}\frac{1}{1+\frac{y^2}{x^2}}\hat{e}_x + q\frac{1}{x}\frac{1}{1+\frac{y^2}{x^2}}\hat{e}_y \\
&= -q\,\frac{y}{x^2+y^2}\,\hat{e}_x + q\,\frac{x}{x^2+y^2}\,\hat{e}_y = -q\,\frac{r\sin\varphi}{r^2}\,\hat{e}_x + q\,\frac{r\cos\varphi}{r^2}\,\hat{e}_y
\end{aligned}$$

and

$$\boxed{\vec{\nabla}\phi(\vec{r}) = \frac{q}{r}\,\hat{e}_\varphi} \tag{2.57}$$

where we used $\hat{e}_\varphi = \cos\varphi\,\hat{e}_y - \sin\varphi\,\hat{e}_x$. One clearly sees the divergence for $r \to 0$. The problem is *spherically symmetric* in the sense that the modulus of the gradient of the field only depends on the modulus of r, $|\vec{\nabla}\phi(\vec{r})| = f(r)$. Moreover, $\vec{\nabla}\phi(\vec{r})$ points along a circle around the center of the vortex, that is to say, perpendicularly to the radius ($\hat{e}_\varphi \cdot \hat{e}_r = 0$).

We now check that the *Laplacian of the angular field* ϕ vanishes for all $r \neq 0$:

$$\vec{\nabla}\cdot\vec{\nabla}\phi(\vec{r}) \;=\; q\,\frac{2xy}{(x^2+y^2)^2} - q\,\frac{2xy}{(x^2+y^2)^2} = 0\;.$$

At the origin one has to be more careful because of the divergence of the gradient. We proved in this way that the proposed configuration satisfies the extremisation equation. One can also check that it is a *local minimum* of the energy.

Taking a circle with radius R and centred at the centre of the vortex, the *circulation of the angular field* ϕ in (2.54)-(2.63) around C yields

$$\oint_C d\phi(\vec{r}) = \oint_C d\vec{l}\cdot\vec{\nabla}\phi(\vec{r}) = \int_0^{2\pi} R\,d\varphi\,\hat{e}_\varphi\cdot\frac{q}{R}\,\hat{e}_\varphi = 2\pi q\;. \tag{2.58}$$

Note that this result is independent of the radius of C. Actually, in a single vortex configuration the angle winds around the topological defect for any contour C around the centre of the vortex[4]

$$\boxed{\oint_C d\phi(\vec{r}) = \oint_C d\vec{l}\cdot\vec{\nabla}\phi(\vec{r}) = 2\pi q\;.} \tag{2.59}$$

(Note that the spin has to point in the same direction after coming back to the starting point of the circulation, this condition implies that q must be an integer.) The integral yields this non-vanishing result for all paths C that encircle the centre of the vortex and vanishes on paths that do not. The position of the vortex corresponds to a singularity in the field that is constructed with the *coarse-graining* procedure (the continuous space limit we used to build the field). The discrete nature of the charge makes it impossible to find a continuous deformation which returns the state to the uniformly ordered configuration in which the charge is zero. (One justifies the continuous treatment of the spin rotation by taking a curve around the vortex core with a sufficiently large "radius" so that the variations in angle will be small and the lattice structure can be ignored. The continuous approximation fails close to the core of the vortex.) A vortex creates a distortion in the phase field $\phi(\vec{r})$ that persists infinitely far from the centre of the vortex.

[4]Recall Gauss' divergence theorem $\int dV\;\vec{\nabla}\cdot\vec{F} = \int dS\;\hat{n}\cdot\vec{F}$, where the volume integral on the left transforms into the surface integral on the right. Applied to a volume in two dimensions and $\vec{F} = \vec{\nabla}\phi$, one goes from eq. (2.57) to eq. (2.59) for a single vortex with charge q.

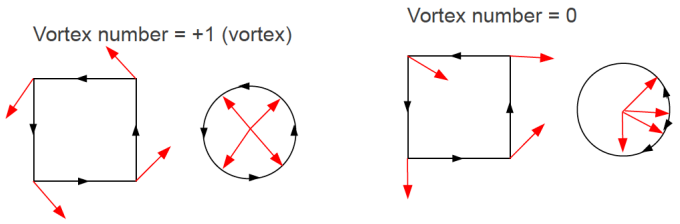

Figure 2.8: A graphical way to visualise the charge of a vortex. One places on the circle an arrow corresponding the the "firs" (arbitrary choice) spin. One takes the next spin on the plaquette, conventionally turning in anti-clockwise order, and places a second arrow on the circle. One repeats the procedure until the last spin on the plaquette. The points on the circle are numbered according to the order of the spins on the plaquette, $1, \ldots, 4$ in these examples. If the points make one turn on the circle the charge is $q = 1$. If it has made an anti-turn the charge is $q = -1$. If they make more than one turn the charge is higher than 0.

The electromagnetic analogy, that is explained in detail in the book by Chaikin & Lubensky [25], is such that

$$\begin{array}{rrcl} \text{magnetic induction} & \vec{B} & \leftrightarrow & \vec{\nabla}\phi \\ \text{electric current density} & \vec{J} & \leftrightarrow & \vec{\mathcal{M}} = \vec{\nabla} \times \vec{\nabla}\phi \\ \text{vector potential} & \vec{\nabla} \times \vec{A} & \leftrightarrow & \vec{\nabla}\phi \end{array} \tag{2.60}$$

The current density is singular at the location of the centre of the vortices as

$$\vec{\mathcal{M}}(\vec{r}) = 2\pi \sum_i q_i \delta(\vec{r} - \vec{r}_i)\ \hat{e}_z = 2\pi\rho(\vec{r})\ \hat{e}_z \tag{2.61}$$

where $\vec{r}$ lives on the two dimensional plane and $\hat{e}_z$ is perpendicular to it. $\rho(\vec{r})$ is the charge density constituted by point-like charges located at positions $\vec{r}_i$.

Several singular configurations are shown in Fig. 2.7, with vortices ($q = 1$) in the first row and antivortices ($q = -1$) in the second row (figures borrowed from [21]). A simple visualisation of the winding angle is sketched in Fig. 2.8. Vortices with higher charge are also possible (though as they have a higher energetic cost they are less common), see Fig. 2.9. A vortex and a nearby anti-vortex configuration are shown in Fig. 2.10 and some constant spin lines around vortex-antivortex pairs are shown in Fig. 2.11. The latter appear bounded in the low temperature phase, see Fig. 2.12.

An angular configuration with M vortices with charge q_i situated at the points $\vec{r}_i$ is

$$\boxed{\phi(\vec{r}) = \textstyle\sum_i^M\ q_i\ \arctan\left(\frac{(\vec{r}-\vec{r}_i)_y}{(\vec{r}-\vec{r}_i)_x}\right)} \tag{2.62}$$

where the sub-scripts $_x$ and $_y$ indicate the horizontal and vertical components.

Let us evaluate the *energy of a single vortex* configuration. We have already argued that the vortex configuration satisfies

$$\vec{\nabla}\phi(\vec{r}) = \frac{q}{r}\,\hat{e}_\varphi \tag{2.63}$$

where, without loss of generality, we set the origin of coordinates at the center of the vortex, φ is the angle of the position $\vec{r}$ with respect to the x axis, and q is the charge of the vortex. Using the expression (2.42) where $\vec{\nabla}\phi(\vec{r})$ is replaced by (2.63),

$$E_{1\ vortex} = \frac{J}{2}\int d^2r\ [\vec{\nabla}\phi(\vec{r})]^2 = \frac{J}{2}q^2\int_0^{2\pi} d\varphi \int_a^L dr\ r\ \frac{1}{r^2} = \pi J q^2 \ln\frac{L}{a} \tag{2.64}$$

with L the linear dimension of the system. The energy of a single vortex

- increases quadratically with its charge
- diverges logarithmically in the infinite size limit

and one might conclude that these configurations cannot exist in equilibrium at any temperature. However, as already discussed when presenting Peierls argument applied to the Ising chain, at finite T one needs to estimate the *free-energy* difference between configurations with and without a vortex to decide for their existence or not. The *configurational entropy of a single vortex* is $S = k_B \ln\mathcal{N} = k_B \ln(L/a)^2$ since in a $2d$ lattice the centre of the vortex can be located on $(L/a)^2$ different sites. Then

$$\boxed{\Delta F = F_{1\ vortex} - F = (\pi J q^2 - 2k_B T)\ln(L/a)} \tag{2.65}$$

Both energy and entropy of a single vortex configuration grow as $\ln L$. The variation of the free-energy changes sign at $k_B T = \pi J q^2/2$ therefore *there cannot be isolated vortices in equilibrium below*

$$\boxed{k_B T_{KT} = \pi J/2} \tag{2.66}$$

but they can at higher temperatures. Indeed, at $T > T_{KT}$, isolated vortices proliferate (favoured by the entropic contribution), destroy the quasi long-range order and make correlations decay exponentially on a length-scale given by the typical spacing between vortices

$$G(r) \simeq e^{-r/\xi(T)} \qquad\qquad \xi(T) \simeq e^{b|T-T_{KT}|^{-1/2}} \tag{2.67}$$

close to T_{KT}. This very fast divergence of the correlation length, $\nu \to \infty$, can be rigorously proven with an RG analysis [20] that we shall not present here.

The estimate of T_{KT} just given represents only a bound for the stability of the system towards the condensation of topological defects. Pairs (dipoles) of defects may appear at larger couplings or lower temperatures.

Although the energy of a single vortex diverges as $\ln L$, the energy of a *bound pair* of vortex-antivortex does not diverge, since, the total vorticity of the pair vanishes, see the Fig. 2.11 taken from [6]. Below T_{KT} vortices exist only in bound pairs with opposite vorticity held together by a logarithmic confining potential

$$E_{pair}(\vec{r}_1, \vec{r}_2) = -\pi J q_1 q_2 \ln(|\vec{r}_1 - \vec{r}_2|/a)\ . \tag{2.68}$$

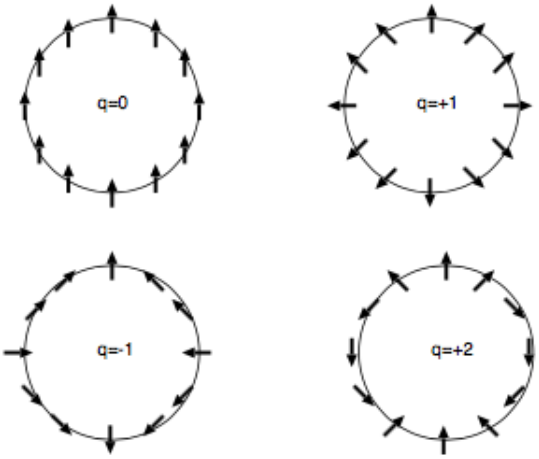

Figure 2.9: Four vortices with charges $q = 0, 1, -1, 2$.

This expression follows uniquely from the fact that at distances much larger than the pair's size there is no net vorticity, so the energy of the pair must be finite, and as the pair's size diverges E_{pair} should yield the sum of the energies for an isolated vortex and an isolated antivortex. (A more detailed calculation uses an integral over a contour in the $2d$ plane that excludes the centers of the vortices. In particular, this approach allows one to show that a sum over the energies of the single vortices appears multiplied by $\sum_i q_i$ and this divergence is eliminated if the total vorticity is zero, i.e. $\sum_i q_i = 0$.) Such pairs can thus be thermally excited, and the low temperature phase will host a gas of such pairs. The insight by Kosterlitz and Thouless was that at a certain temperature T_{KT} the pairs will break up into individual vortices. It is this vortex pair unbinding transition that will take the system to a high temperature phase with exponentially decaying correlations.

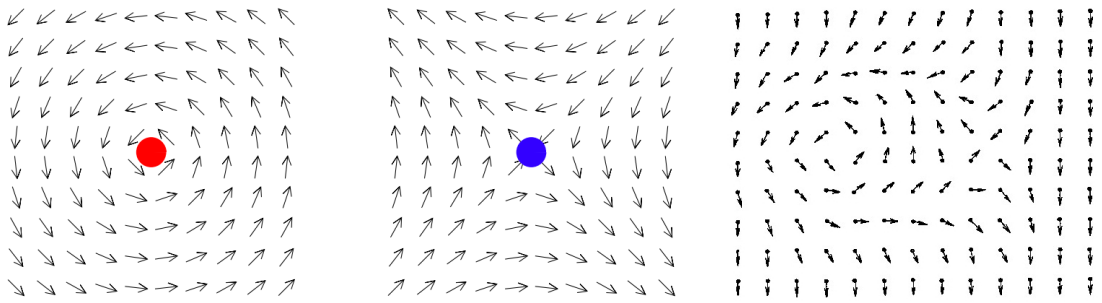

Figure 2.10: A vortex and a near-by anti-vortex configuration as they may appear bounded in the low temperature phase.

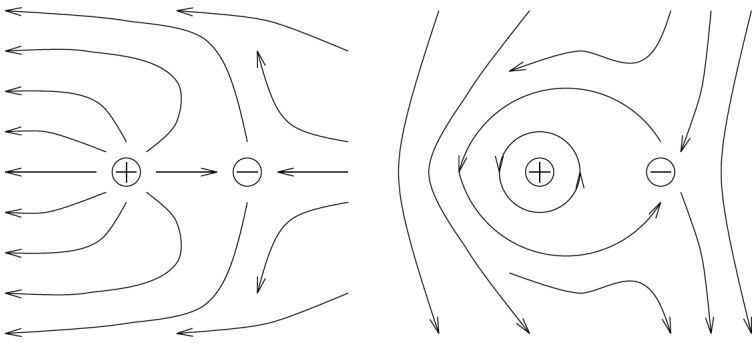

Figure 2.11: Lines of spin direction close to a vortex-antivortex pair. As one observes the spin configurations far from the vortex cores, the lines of constant spin are smooth.

The (single) vortices and anti-vortices act as if they were two point particles with charges $q = +1$ and $q = -1$ interacting with a $1/r$ force. Since this corresponds to the Coulomb interaction in two dimensions, the physics of the topological defects is just like the physics of a two-dimensional *neutral Coulomb gas*. Note that the energy increases if one tries to unbind – separate – the vortices in the pair. The vortices remain paired and do not change much the behaviour in the low temperature phase. The correlation still decays as a power-law and there is no spontaneous symmetry breaking in this phase since the order parameter vanishes – in agreement with the Mermin-Wagner theorem that we discuss below. In terms of the electrostatic analogy, the high temperature phase is a plasma. A detailed description of the vortex influence on the equilibrium properties of the $2d$ XY goes beyond the scope of these Lectures. A detailed description can be found in several book, in particular in [7].

This argument shows that two qualitatively different equilibrium states exist at high and low T but it does not characterize the transition. The naive order parameter vanishes on both sides of the transition but there is still a topological order, with the spin-spin correlation decaying exponentially on one side (high T) and as a power law on the other (low T) of the transition. In contrast to usual continuous phase transitions, the KT-transition does not break any symmetry.

2.4.4 The $2d$ XY model: numerical evaluation

Distinguishing a second order phase transition from a Kosterlitz-Thouless one is a daunting challenge. See, *e.g.*, [26] for a recent effort to verify the scalings expected. A useful method is based on the scaling properties of the kurtosis of the (pseudo) order parameter or Binder parameter [27, 28].

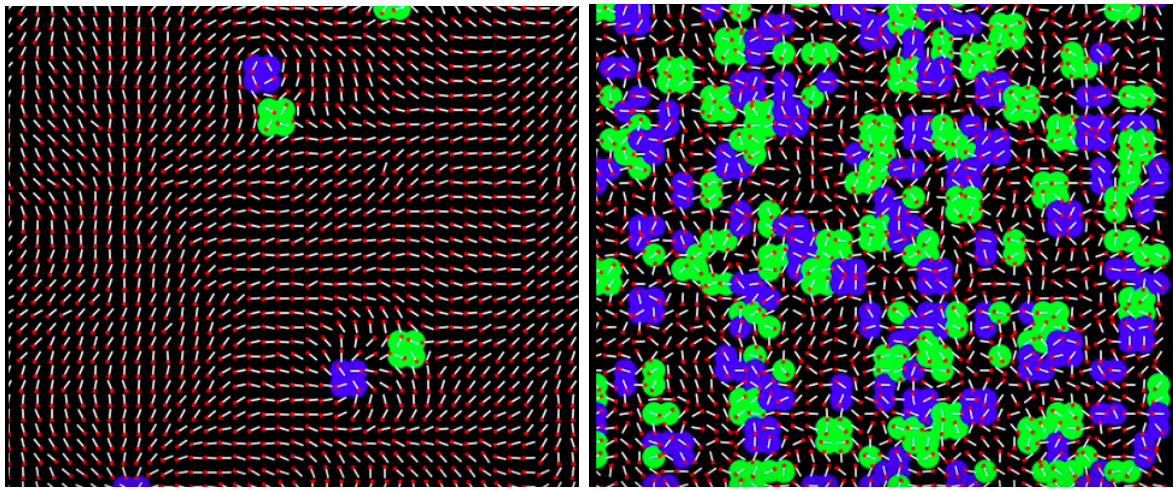

Figure 2.12: At low T there are few vortices and they are bound in pairs. At high T there are many more vortices, they are free and can separate apart. Image taken from [22].

2.4.5 The $2d$ XY model: Nobel Prize and applications

From the Nobel Lecture: *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. 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.*

Other two dimensional systems, notably those of particles in interaction that would like to form solids at sufficiently low temperature and high densities, also fall into the scheme of the Kosterlitz-Thouless phase transitions. Indeed, in 1934, Peierls argued that thermal motion of *long-wave length phonons* will destroy the long-range order or a two dimensional solid in the sense that the mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system [**?**]. He also proposed a model, just atoms sitting on a lattice in $2d$ and linked together by Hookean springs, that has quasi long-range order at all temperatures [23]. Quasi long range order means in this context that he mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system. It was later understood that the mechanism for destabilising this critical phase is through the unbinding of topological defects that are of a different kind from the ones we studied here. (For more details, see, for example the slides that I included in my web page and the Subsection below.)

For similar reasons, the expectation value of the *superfluid order parameter* in a two dimensional Bose fluid is zero. In 1978, Bishop and Reppy studied the superfluid transition of a thin two dimensional helium film absorbed on an oscillating substrate. The observation results on superfluid mass and dissipation supported the Kosterlitz-Thouless

picture of the phase transition in a two dimensional superfluid. The jump in the superfluid density at the transition given by Kosterlitz and Thouless is in good agreement with estimates from experiment.

2.4.6 The Mermin-Wagner theorem

What happens in $d = 2$ and below? Indeed, the logarithmic behaviour of the angle correlation function in the XY model or the transverse correlation in the generic $O(n)$ model, see below, are signatures of the fact that this is a special dimension.

In 1968, using a mathematical inequality due to Bogoliubov, Mermin showed that the magnetisation density m is strictly zero at all $T > 0$ in the $2d$ XY model. This proof is part of what is nowadays called the Mermin-Wagner theorem.

The *Mermin-Wagner theorem* is often quoted as stating that for any system with short-range interactions there is a *lower critical dimension* below which no spontaneous broken symmetry can exist at finite temperature [11]. In other words, fluctuations are so large that any ordering that breaks a continuous symmetry is destroyed by thermal fluctuations. $d_c = 1$ for discrete symmetries and $d_c = 2$ for systems with continuous symmetries. The absence of long-range order in the $2d$ XY case, for example, is demonstrated by the fact that the finite temperature correlation decays to zero at long distances – albeit as a power law – and thus there is no net magnetisation in the system.

However, the statement above is not totally correct. What Mermin proved is that some order parameters (like the magnetisation for the $2d$XY model or the one associated to translational order in $2d$ particle systems in interaction) cannot take a non-zero value at any non-vanishing temperature. This does not exclude that *other* order parameters could do it. This is indeed what happens in the problem of $2d$ melting, where the translational order parameter vanishes at all non-zero temperatures but a less obvious order parameter, associated to orientational order, does not. The system can therefore sustain long-range orientational order at finite temperatures while it cannot maintain translational order.

The Mermin-Wagner theorem [11] is known as Coleman-Weinberg theorem/result in field theory [12]. Independently of Mermin & Wagner, Hohenberg developed a similar argument in the context of Bose quantum liquids and superconductors [13].

2.4.7 About universality

The picture described above has been developed based on the analysis of the 2d XY model in which planar spins are placed on the vertices of a regular lattice, with nearest neighbour pairwise interactions $-Jcos\theta_{ij}$ with θ_{ij} the angle between the two spins. Interestingly enough, the nature of the transition can change dramatically if the interaction term takes other forms that still respect rotational invariance. The potential $2[1 - \cos^{2p^2}(\theta_{ij}/2)]$, that interpolates between the conventional one for $p = 1$ and a much steeper well for large p^2 was used by Domany, Schick and Swendsen [29] to show that the transition crosses over from BKT to first order for large p^2. In particular, for $p^2 = 50$ the

transition is very sharp with a huge peak in the specific heat and many other elements of a first order phase transition. The reason for this behaviour is that the typical temperature for the unbinding of vortex-antivortex pairs is pushed to very high values, beyond the ones at which other kinds of excitations drive the discontinuous transition. Similarly, other examples of models expected to have BKT transitions, such as the 2d Coulomb gas, were shown to comply with the expectations only at low density and depart towards a first order phase transition at higher density.

The phenomena just described seem to be in contradiction with the picture that emerges from the renormalisation group theory according to which systems in the same universal class (having the same symmetry of the order parameter and same dimensionality) should exhibit the same type of phase transition with identical values of critical exponents. However, a rigorous proof that planar spin models of the XY kind with a sufficiently narrow potential undergo first order phase transitions was provided by van Enter & Shlosman [30] and the fact that with a simple change of parameter one can change the order of the transition was thus confirmed.

2.4.8 On interface energies

In a continuous spin model the cost of an interface is proportional to its surface divided by its thickness (note that spins can smoothly rotate from site to site to create a thick interface). The thickness of the interface depends on the details of the model, temperature, *etc.* This means that interfaces are much easier to create in continuous spin models than in discrete ones. One can then expect to have lower lower critical dimensions for continuous spin models than for discrete ones.

2.4.9 O(n) model: Ginzburg-Landau field theory and Goldstone modes

We lift here the constraint on the modulus of the vector spins and we let it fluctuate. It is simple to derive a continuum limit of the lattice model in analogy with the Landau approach. One first coarse-grains the two-component spin to construct a n-component field

$$\vec{\psi}(\vec{r}) = \ell^{-d} \sum_{i \in V_{\vec{r}}} \vec{s}_i \ . \tag{2.69}$$

Let us first focus on the *d dimensional O(2) model*, where the field has just two components. One proposes a Landau ψ^4 action for the field $\vec{\psi}$,

$$F[\vec{\psi}] = \int d^d r \left[\frac{1}{2} [\vec{\nabla} \vec{\psi}(\vec{r})]^2 + \frac{T - T_c}{T_c} \psi^2(\vec{r}) + \frac{\lambda}{4!} \psi^4(\vec{r}) + \vec{h} \vec{\psi}(\vec{r}) \right] \tag{2.70}$$

and parametrises the field by its modulus and angle,

$$\vec{\psi}(\vec{r}) = |\phi_0(\vec{r})| (\cos \phi(\vec{r}), \sin \phi(\vec{r})) \qquad (\text{or } \ \vec{\psi}(\vec{r}) = |\phi_0(\vec{r})| e^{i\phi(\vec{r})}) \ . \tag{2.71}$$

Figure 9.2. A 'Mexican hat' potential.

Figure 2.13: A Mexican hat potential, figure taken from [8].

to rewrite the Landau free-energy of a generic configuration in the absence of the external field $\vec{h}$ as

$$F[\phi_0,\phi] = \int d^dr \left[\frac{1}{2}(\vec{\nabla}\phi_0(\vec{r}))^2 + \frac{T-T_c}{T_c}\phi_0^2(\vec{r}) + \frac{\lambda}{4!}\phi_0^4(\vec{r})\right] \tag{2.72}$$

$$+\frac{\phi_0^2}{2}\int d^dr\,[\vec{\nabla}\phi(\vec{r})]^2\,. \tag{2.73}$$

The first term is just similar to the Landau free-energy of a *massive scalar field* configuration in the Ising model. The second-term quantifies the free-energy of the spin-wave configurations (in higher dimensions topological defects also exist, for example, in $d=3$ this model has vortex lines with linear singularities). The local angle is simply a *massless scalar field* in d dimensional space. The correlation functions of the ϕ field behave as

$$\langle\,\phi(\vec{r})\phi(\vec{r}')\,\rangle \sim (2-d)^{-1}|\vec{r}-\vec{r}'|^{2-d} \tag{2.74}$$

in the large $|\vec{r}-\vec{r}'|$ limit for $d=1,2$. The behaviour is logarithmic in $d=2$ (the $2d$ XY model). The correlation reaches a constant in $d>2$.

Let us now focus on the generic *d dimensional $O(n)$ model*. The free-energy à la Landau is the one in Eq. (2.69)

$$F[\vec{\psi}] = \int d^dr \left[\frac{1}{2}(\vec{\nabla}\vec{\psi}(\vec{r}))^2 + \frac{T-T_c}{T_c}\psi^2(\vec{r}) + \frac{\lambda}{4!}\psi^4(\vec{r}) + \vec{h}\vec{\psi}(\vec{r})\right] \tag{2.75}$$

where $\psi^2 \equiv \sum_{a=1}^N \psi_a^2$ is the result of a sum over n components. The potential $V(\psi^2)$ has the Mexican hat form sketched in Fig. 2.13 (credit to A. M. Tsvelik), with extrema at

$$\vec{\psi}=\vec{0} \qquad \text{or} \qquad \psi^2 = -\frac{4!}{2\lambda}\frac{T-T_c}{T_c} \tag{2.76}$$

Clearly, the latter exists only if $T<T_c$ and we focus on this range of temperatures. It is clear that the condition on ψ^2 admits an infinite number of solutions, in other words,

there is a *ground state manifold*, corresponding to the circular bottom of the valley in the Mexican hat potential. The pinning field $\vec{h}$ can then be used to force the system to choose one among all these degenerate directions in the n dimensional space, in which the field "condenses". Let us suppose that this is the nth direction that we therefore call *longitudinal*. The rotation symmetry in the remaining *transverse* $n-1$ directions remains unbroken and the symmetry is therefore spontaneously broken to $O(n-1)$. The expected values of such a configuration is then

$$\langle \psi_a(\vec{r}) \rangle = \psi \delta_{an} \tag{2.77}$$

while the fluctuations are

$$\begin{aligned} \psi_n(\vec{r}) &= \langle \psi_n(\vec{r}) \rangle + \delta\psi_n(\vec{r}) \\ \psi_{a\neq n}(\vec{r}) &= \delta\psi_{a\neq n} \end{aligned} \tag{2.78}$$

(think of the case $n = 3$, choosing the n direction to be the z vertical one and the rotations around this axis). Replacing these forms in the Landau free-energy one finds that the longitudinal mode is massive while the transverse ones are massless (just decoupled Gaussian fields).

The correlation functions, $C_{ab}(\vec{r}) = \langle \psi_a(\vec{r}) \psi_b(\vec{0}) \rangle$, can be written as

$$C_{ab}(\vec{r}) = \delta_{ab} \left[C_L(r) \delta_{an} + C_T(r)(1 - \delta_{an}) \right] . \tag{2.79}$$

We recall that a and b label the components in the n-dimensional space. C_L is the *longitudinal* correlation (parallel to an infinitesimal applied field that selects the ordering direction, $\vec{h} = h\hat{e}_n$) and C_T is the *transverse* (orthogonal to the applied field) one. A simple calculation shows that the longitudinal component behaves just as the correlation in the Ising model. It is a massive scalar field. The transverse directions, instead, are massless: there is no restoring force to the tilt of the full system. These components behave just as the angle in the XY model, $C_T(\vec{r}) \sim r^{2-d}$ (the power law decay becomes a logarithm in $d = 2$). These are called *Goldstone modes* or *soft modes*.

2.4.10 The Higgs mechanism

A particular feature of models with continuous symmetry breaking in *gauge theories* is that gauge fields acquire a mass through the process of spontaneous symmetry breaking. Take the classical Abelian field theory

$$\mathcal{L}[A_\mu, \phi] = \int d^d r \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + (D_\mu \phi)^* (D^\mu \phi) + V(\phi) \right] \tag{2.80}$$

with $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, $D_\mu = \partial_\mu + ieA_\mu$ and ϕ a complex field. The potential is

$$V(\phi) = \mu(\phi^* \phi) + \lambda(\phi^* \phi)^2 \tag{2.81}$$

with $\mu < 0$ and $\lambda > 0$. The ϕ configuration that renders V minimum is such that $\phi_0^*\phi_0 = -2\mu/\lambda$. Without loss of generality one can choose ϕ_0 to be real through a uniform rotation over all space. It is easy to verify that replacing ϕ by $(\phi_0 + \delta\phi) + i\phi_2$ where ϕ_2 is an imaginary part (playing the role of the transverse components in the analysis of the $O(n)$ model) one finds that the quadratic Lagrangian does not have a ϕ^2 term (massless field) but instead a quadratic term in A appears. The gauge field acquired a mass (there is also a $A_\mu\partial^\mu\phi_2$ term that can be eliminated with a change of variables).

This phenomenon has been discovered in the study of superconductors by P. W. Anderson. Indeed, one can find a short account of the historic development in Wikipedia: *The mechanism was proposed in 1962 by Philip W. Anderson, who discussed its consequences for particle physics but did not work out an explicit relativistic model. The relativistic model was developed in 1964 by three independent groups Robert Brout and François Englert, Peter Higgs and Gerald Guralnik, Carl Richard Hagen, and Tom Kibble. Slightly later, in 1965, but independently from the other publications the mechanism was also proposed by Alexander Migdal and Alexander Polyakov at that time Soviet undergraduate students. However, the paper was delayed by the Editorial Office of JETP, and was published only in 1966.* The Nobel Prize was given to F. Englert and P. Higgs in 2013 *"for the theoretical discovery of a mechanism that contributes to our understanding of the origin of mass of subatomic particles, and which recently was confirmed through the discovery of the predicted fundamental particle, by the ATLAS and CMS experiments at CERN's Large Hadron Collider"*.

2.5 2d Melting

Consider a sufficiently dense system so that it should be a solid, possibly in a crystalline phase and evaluate the effect of thermal fluctuations. Does the solid melt? Which are the mechanisms leading to melting? Which is the order of the phase transition taking the solid into a liquid?

These questions received an answer that draw consensus around the fact that the transition is of first order in $d = 3$. However, the situation is trickier in $d = 2$. We discuss this case below.

2.5.1 Positional vs. orientational order

In the 30s [33] and Landau [31, 32] argued that it is not possible to find long-range positional order in low dimensional systems with short-range interactions.

Peierls used the simplest possible model for a solid, one of beads placed on a d-dimensional lattice, with Hookean couplings between nearest-neighbours, in canonical equilibrium, that is to say, a *harmonic solid*. The question he asked was whether such a system could sustain periodic order over long distances under thermal fluctuations, and he concluded that this is not possible in $d \leq 2$, while it is in $d \geq 3$. Landau based his

arguments instead on his theory of phase transitions and reached the same conclusion. In the 60s, the numerical simulations of [35] pointed towards a first order phase transition between solid and liquid. A more general proof of absence of crystalline order in $2d$, that does not rely on the harmonic approximation but uses a classical limit of Bogoliubov's inequality [36], was given later by [37].

An equilibrium amorphous state has a uniform averaged density $\langle\rho\rangle = \rho_0$, while a zero temperature crystalline state has a periodic one

$$\rho(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{R}_i) \tag{2.82}$$

with i a label that identifies the particles or lattice sites, and $\mathbf{R}_i$ the position of the ith vertex of the lattice. At zero temperature a perfectly ordered state, with periodic density is allowed for all $d \geq 1$. However, thermal fluctuations make the atoms vibrate around their putative lattice sites, and the instantaneous position of the ith atom becomes

$$\mathbf{r}_i = \mathbf{R}_i + \mathbf{u}_i = \mathbf{R}_i + \mathbf{u}(\mathbf{R}_i) \tag{2.83}$$

with $\mathbf{u}_i = \mathbf{u}(\mathbf{R}_i)$ its displacement from $\mathbf{R}_i$. A simple way to see the lack of positional order in low dimensions (and the existence of it in higher dimensions) is to compute the mean-square displacement of the atoms assuming thermal equilibrium. Take a generic pair-wise potential

$$U_{\rm tot} = \frac{1}{2}\sum_{ij} U(\mathbf{r}_i - \mathbf{r}_j) = \frac{1}{2}\sum_{ij} U(\mathbf{R}_i - \mathbf{R}_j + \mathbf{u}_i - \mathbf{u}_j)\ . \tag{2.84}$$

Indeed, the total harmonic potential energy is [34]

$$\begin{aligned} U_{\rm tot} &= U_{\rm gs} + \frac{1}{2}\sum_{ij}\sum_{\mu\nu}(u_i^\mu - u_j^\mu)\,\frac{\partial^2 U}{\partial_{r_i^\mu}\partial_{r_j^\nu}}(\mathbf{R}_i - \mathbf{R}_j)\,(u_i^\nu - u_j^\nu) \\ &= U_{\rm gs} + \frac{1}{2}\sum_{ij}\sum_{\mu\nu} u_i^\mu D_{\mu\nu}(\mathbf{R}_i - \mathbf{R}_j) u_j^\nu \end{aligned} \tag{2.85}$$

where $U_{\rm gs} = \frac{1}{2}\sum_{i\neq j} U(\mathbf{R}_i - \mathbf{R}_j)$, and in the second term μ, ν run from 1 to d, $D_{ij}^{\mu\nu} \equiv D_{\mu\nu}(\mathbf{R}_i - \mathbf{R}_j) = \delta_{ij}\sum_k \phi_{ik}^{\mu\nu} - \phi_{ij}^{\mu\nu}$ and $\phi_{ik}^{\mu\nu} = \partial^2 U(\mathbf{r})/\partial r_i^\mu \partial r_k^\nu$. Three symmetries of the couplings follow immediately $D_{ij}^{\mu\nu} = D_{ji}^{\nu\mu}$, $D_{ij}^{\mu\nu} = D_{ji}^{\mu\nu}$ (from the inversion symmetry of a Bravais lattice), and $\sum_i D_{ij}^{\mu\nu} = 0$ (from the uniform translation invariance of the full lattice). After a Fourier transform $U_{\rm tot}$ becomes

$$U_{\rm tot} = U_{\rm gs} + \frac{1}{2}\sum_{\mathbf{k}}\sum_{\mu\nu} \tilde{u}_\mu^*(\mathbf{k})\tilde{D}_{\mu\nu}(\mathbf{k})\tilde{u}_\nu(\mathbf{k})\ , \tag{2.86}$$

where $\tilde{u}_\mu(\mathbf{k}) = \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i}\mathbf{u}_i$ and $\tilde{u}_\mu^*(\mathbf{k}) = \tilde{u}_\mu(-\mathbf{k})$ since $\mathbf{u}_i$ is real. Next one needs to estimate the $\mathbf{k}$ dependence of $\tilde{D}_{\mu\nu}(\mathbf{k})$. Using the symmetries of $D_{ij}^{\mu\nu}$, its Fourier transform $\tilde{D}_{\mu\nu}(\mathbf{k})$

can be recast as

$$\tilde{D}_{\mu\nu}(\mathbf{k}) = -2\sum_{\mathbf{R}} D_{\mu\nu}(\mathbf{R})\sin^2(\mathbf{k}\cdot\mathbf{R}/2) \approx -2\sum_{\mathbf{R}} D_{\mu\nu}(\mathbf{R})(\mathbf{k}\cdot\mathbf{R}/2)^2 \ , \tag{2.87}$$

after a small $\mathbf{k}$ approximation. It is now possible to further assume

$$\tilde{D}_{\mu\nu}(\mathbf{k}) \mapsto k^2 A_{\mu\nu} \tag{2.88}$$

where the important k^2 dependence has been extracted. $U_{\rm tot}$ thus becomes the energy of an ensemble of harmonic oscillators. The equipartition of quadratic degrees of freedom in canonical equilibrium yields

$$\langle \tilde{u}^*_\mu(\mathbf{k})\tilde{u}_\nu(\mathbf{k})\rangle = \frac{k_B T}{k^2}\ A^{-1}_{\mu\nu} \tag{2.89}$$

and a logarithmic divergence of the displacement mean-square displacement

$$\Delta u^2 \equiv \langle |\mathbf{u}(\mathbf{r}) - \mathbf{u}(\mathbf{r}')|^2\rangle \sim k_B T \ln|\mathbf{r}-\mathbf{r}'| \qquad \text{in } \ d=2 \tag{2.90}$$

follows as a consequence of the logarithmic divergence of the integral $\int d^2k\ k^{-2}$.

An even simpler derivation of the same result goes as follows. Take the harmonic Hamiltonian $H = \frac{c}{2}\int d^d\mathbf{r}\ (\nabla\mathbf{u})^2$ as a starting point. The excitation of a spin-wave with wavelength L (wave vector $2\pi/L$) then requires an energy $E \approx L^d(2\pi/L)^2 \propto L^{d-2}$ that diverges with L for $d=3$, is independent of L for $d=2$ (marginal case) and decreases as L^{-1} for $d=1$.

The divergence of the mean-square displacement in Eqn. (2.89) implies that any atom displaces a long distance from each other and hence no long-range order is possible in $d=2$. This weird effect is due to the dimensionality of space. In three dimensions, the mean square fluctuation is finite.

A more general proof of the lack of positional order in $d \le 2$ that goes beyond the harmonic approximation was by Mermin [37]. In this paper, he first proposed the following criterium for crystallinity:

$$\begin{array}{lcll} \tilde{\rho}(\mathbf{k}) & = & 0 & \text{for } \mathbf{k} \text{ not a reciprocal lattice vector ,} \\ \tilde{\rho}(\mathbf{k}) & \neq & 0 & \text{for at least one non-zero reciprocal lattice vector ,} \end{array} \tag{2.91}$$

with $\tilde{\rho}(\mathbf{k})$ the Fourier transform of $\rho(\mathbf{r})$, in the thermodynamic limit, that is

$$\tilde{\rho}(\mathbf{k}) = \frac{1}{N}\sum_{i=1}^{N} e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i} \ . \tag{2.92}$$

Using Bogolyubov's identity, Mermin showed that the condition (2.90) cannot be satisfied in $d \le 2$ since in thermal equilibrium at non-vanishing temperature, for all $\mathbf{k}$, $\langle\tilde{\rho}(\mathbf{k})\rangle$ is bounded form above by a quantity that vanishes in the thermodynamic limit.

The possibility of a two-dimensional system with constant density (all Fourier modes vanish) being, however, anisotropic over long distances was left open by Peierls and Landau. The actual definition of the orientational order was also given by Mermin in his 1968 paper. Within the harmonic solid model he simply noticed that

$$\langle [\mathbf{r}(\mathbf{R}+\mathbf{a}_1)-\mathbf{r}(\mathbf{R})]\cdot[\mathbf{r}(\mathbf{R}'+\mathbf{a}_1)-\mathbf{r}(\mathbf{R}')]\rangle \tag{2.93}$$

approaches a_1^2 at long distances $|\mathbf{R}-\mathbf{R}'|\to\infty$, implying that the orientation of the local order is maintained all along the sample. The status of the studies of orientational order in two dimensional systems in the 90s is summarised in [38].

Because the symmetry group of both phases is the same in the thermodynamic limit (QLRO does not result in a macroscopic broken symmetry), it seems that a phase transition is not necessary. However, as we have seen, the loss of order in the low temperature phase is very weak, and samples of macroscopic but finite size are expected to exhibit broken symmetry, so that for all practical purposes there is a symmetry difference between the two phases, and we would expect a phase transition.

2.5.2 Melting scenarii

In $d\geq 3$ melting is a first order phase transition between crystal and liquid (although the details of how this transition occurs are still not fully understood and may depend on the material). In $d=2$, instead, there is no full consensus yet as to which are the mechanisms for melting and how the passage from solid (with quasi-long-range positional and long-range orientational order) to liquid (with both short-range positional and orientational order) occurs. In the late 70s Halperin & Nelson [39] and Young [40] suggested that the transition can occur in two steps, with an intermediate anisotropic *hexatic phase* with short-range positional and quasi-long-range orientational order. Both transitions, between solid and hexatic on the one hand, and hexatic and liquid on the other, were proposed to be driven by the dissociation of *topological defects*, and therefore be of BKT type:

- In the first stage, at the melting transition T_m, dislocation pairs unbind to form a bond orientationally ordered hexatic liquid.
- In the second stage, at T_i, the disclination pairs which make up the dislocations unbind to form an isotropic liquid.

What are these topological defects? In two dimensions, an isolated *dislocation* is formed by inserting an extra half row of particles into a triangular lattice. Similarly, an isolated *disclination* is formed by inserting (removing) a 60^o wedge of material into (from) a triangular lattice, to form a $+1(-1)$ disclination. A $+1$ disclination corresponds to a point having sevenfold symmetry, while a -1 disclination corresponds to a point of fivefold symmetry. Dislocations and disclinations are considered topological defects because they cannot be eliminated from the lattice without a global rearrangement of particles (inserting or removing a half-row or a 60^o wedge of particles).

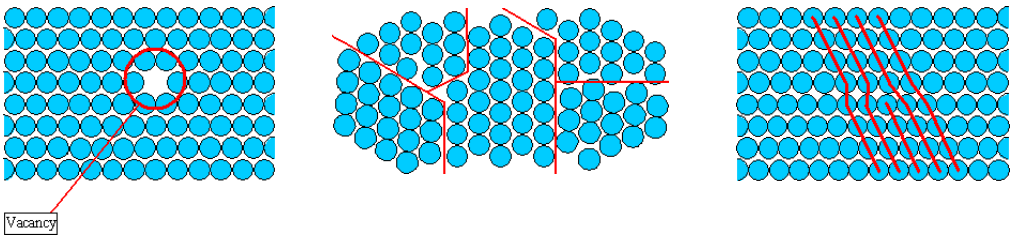

Figure 2.14: A vacancy, a grain boundary between regions with different order and a dislocation in a triangular lattice.

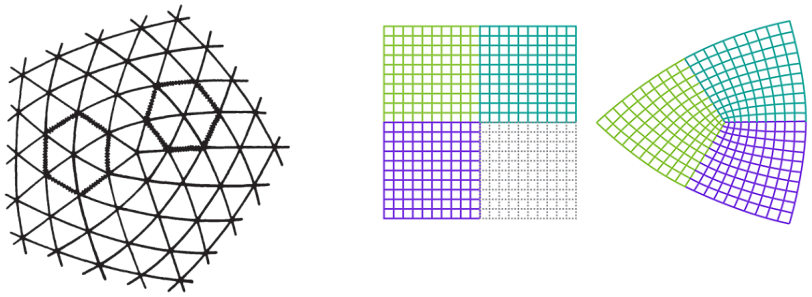

Figure 2.15: Disclination in a triangular and a square lattice.

Moreover, within the KTHNY theory, the *finite size scaling* of the order parameters is expected to be as follows. In the solid phase the translational order parameter should decay with system size as $N^{-\eta}$ with $\eta \leq 1/3$. In the hexatic phase the hexatic order parameter should decay with system size as $N^{-\eta_6}$ with $\eta_6 \to 0$ at the transition with the solid and, according to Nelson & Halperin, $\eta_6 \to 1/4$ at the transition with the liquid. All these conclusions were derived from an RG analysis of the continuous elastic model of a solid separated into the contribution of the smooth displacements and the one of the defects.

A large number of numerical and experimental attempts to confirm (or not) this picture followed. A summary of the situation at the beginning of the 90s can be found in [38] and close to ten years ago in [41]. Early numerics and experiments faced some difficulty in establishing the existence of the hexatic phase, and suggested instead coexistence between solid and liquid as expected in a single first order phase transition scenario. However, by the turn of the century the existence of the hexatic phase was settled and quite widely accepted (see the references by Maret *et al.* cited below) although evidence for both transitions being of BKT kind remained still elusive.

More recently, Krauth and collaborators [43, 44, 45] came back to this problem with powerful numerical techniques and they suggested that, for sufficiently hard repulsive interactions between disks, the transition between the hexatic and liquid phases is of first order. A phenomenon similar to the one put forward by Domany, Schick and Swendsen [29]

with a numerical study, and later shown rigorously by van Enter and Shlosman [30] for the $2d$ XY model with a different potential, would then be at work. Namely, that the BKT transition derived with renormalisation group techniques would be preempted by a first order one. This new scenario allows for co-existence of the liquid and hexatic phases in a finite region of the phase diagram. The mechanisms for the transitions could then be the following.

- In the first stage, at T_m, dislocation pairs unbind to form a bond orientationally ordered hexatic phase.
- In the second stage, at T_i, grain boundaries made of strings of alternating five and seven fold defects would percolate across the sample and liquify it.

While real time video microscopy on superparamagnetic colloids interacting via a *soft* r^{-3} *potential* tend to confirm the KTHNY scenario experimental evidence for the new scenario in a colloidal *hard disks* system was recently given. It seems plausible that the mechanism for melting in $2d$ be non-universal and depend on the interaction potential and other specificities of the systems. Indeed, the numerical simulations prove that for sufficiently soft potential the first order transition is replaced by the conventional BKT one [45]. Moreover, a choice between the two is also made by the *form* of the particles: a dependence of the order of the transition with the number of sides of the constituent polygons was claimed in this paper.

The nature of the second transition, at T_i, remains, therefore, to be understood.

2.6 Summary

This Section contains a (very) rapid summary of what we discussed

2.6.1 First order phase transitions

In a first-order phase transition a state that is stable on one side of the transition, becomes metastable on the other side of it. The order parameter jumps at the transition, for example, from zero in the disordered phase to a non-vanishing value in the ordered one. The correlation length, that is extracted from the correlations of the fluctuations of the order parameter with respect to its average, is always finite.

In common discussions of this kind of transition, the interplay between only two states is considered, each one being the preferred one on the two sides of the transition. But this is not necessarily the case and a competition between various equivalent stable states can also arise. The dynamics of first order phase transitions is driven by nucleation of the new stable phase within the metastable one in which the system is placed initially. During a long period of time the system attempts to nucleate one or more bubbles of the stable phase until some of them reach the critical size and then quickly grow. In the multi-nucleation problem, two possibilities then arise: either one of them rapidly conquers the

full sample or many of them touch, get stuck, and a new coarsening process establishes. The latter case is the one that will be of interest in the hexatic-liquid transition, as we will argue below.

2.6.2 Second order phase transitions

In a second-order phase transition a state that is stable on one side of the transition, becomes unstable on the other side of it and, typically, divides continuously into an even number of different stable points, related in pairs by symmetry. The order parameter is continuous at the transition and, for example, it grows from zero in the ordered phase. The correlation length, also extracted from the correlations of the fluctuations of the order parameter with respect to its average, diverges algebraically on both sides of the transition.

When the parameters are taken across the critical value, the system needs to accommodate to the new conditions and it does progressively, by locally ordering domains of each of the possible and equivalent new equilibrium states. The latter process is called coarsening or domain growth and, although it is a very general phenomenon, its details depend on some characteristics of the problem as the conservation laws and the dimension of the order parameter. The symmetry breaking process, whereby one of the equivalent equilibrium states conquers the full sample, is achieved late after the system is taken across the phase transition. Indeed, equilibration takes a time that scales with the system size and diverges in the thermodynamic limit.

2.6.3 Infinite order phase transitions

Berezinskii-Kosterlitz-Thouless (BKT) phase transitions lack an order parameter taking a non-vanishing value on one side of the transition (in the thermodynamic limit) and are not related to spontaneous symmetry breaking. They are transitions of a different kind, driven by the unbinding of topological defects when a critical value of a control parameter (typically temperature over an energy scale) is reached. In the disordered phase the density of free topological defects is finite and the correlation function of the would-be order parameter decays exponentially, with a correlation length that is proportional to the distance between unbound defects. This length diverges exponentially at the transition and remains infinite in the full quasi-long-range ordered phase. Topological defects exist in the ordered phase but they bound in pairs and such localised in space. The divergence of the correlation length implies that the correlations of the would-be order parameter decay algebraically beyond the transition, that the system has quasi long range order and that this full phase behaves as a critical point. In terms of the associated susceptibility, it is finite in the disordered phase and it diverges in the full subcritical phase. Even more so, the transition is characterised by essential singularities in all thermodynamic functions. The reason for this behaviour are (spin or density) wave excitations with a linear dispersion relation at long wave-lengths. The dynamics of such phase transitions is characterised by the growth of the quasi-long-range order and the annihilation of topological

defects.

Appendices

2.A Polar coordinate system

The polar coordinate system is such that

$$\begin{aligned} \hat{e}_r &= \cos\varphi\hat{e}_x + \sin\varphi\hat{e}_y \\ \hat{e}_\varphi &= -\sin\varphi\hat{e}_x + \cos\varphi\hat{e}_y \end{aligned} \tag{2.A.1}$$

and

$$\hat{e}_\varphi = \hat{e}_z \times \hat{e}_r \ . \tag{2.A.2}$$

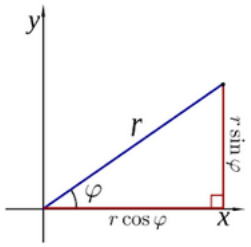

Figure 2.16: Polar coordinates notation convention.

2.B Fourier transform

We define the Fourier transform (FT) of a function $f(\vec{x})$ defined in a volume V as

$$\tilde{f}_{\vec{k}} = V^{-1}\int_V d^d x\ f(\vec{x})\, e^{i\vec{k}\vec{x}} \tag{2.B.1}$$

This implies

$$f(\vec{x}) = \sum_{\vec{k}} \tilde{f}_{\vec{k}}\, e^{-i\vec{k}\vec{x}} \tag{2.B.2}$$

where the sum runs over all $\vec{k}$ with components k_i satisfying $k_i = 2\pi n_i/L$ with n_i an integer and L the linear size of the volume V.

In the large V limit these equations become

$$\tilde{f}(\vec{k}) = V^{-1} \int_V d^d x \; f(\vec{x})\, e^{-i\vec{k}\vec{x}} \tag{2.B.3}$$

$$\tilde{f}(\vec{x}) = \int_V \frac{d^d k}{(2\pi)^d} \; f(\vec{k})\, e^{i\vec{k}\vec{x}} \tag{2.B.4}$$

The Fourier transform of a real function $f(\vec{x})$ satisfies $\tilde{f}^*(\vec{k}) = \tilde{f}(-\vec{k})$.

2.C The angle correlation

In terms of the Fourier components, the canonical measure is a Gaussian, with a weight that is just a sum over independent modes,

$$P[\{\phi_{\vec{k}}\}] \propto e^{-\frac{K}{V}\sum_{\vec{k}} k^2 |\phi_{\vec{k}}|^2} = e^{-\frac{K}{V}\sum_{\vec{k}} k^2 \phi_{\vec{k}}\phi_{-\vec{k}}} \tag{2.C.1}$$

where we collected in K all the parameters in the Hamiltonian times the inverse temperature β of the Boltzmann weight. We avoid using tilde to distinguish the Fourier transformed from the original fields as the interpretation should be obvious. Each mode is an independent random variable with a Gaussian distribution of zero mean and correlations

$$\langle \phi_{\vec{k}} \phi_{\vec{k}'} \rangle = \frac{V}{K k^2} \; \delta_{\vec{k},-\vec{k}'} \; . \tag{2.C.2}$$

From this expression one can easily compute the averages and correlations in real space. First, $\langle \phi(\vec{r}) \rangle = 0$. Next,

$$\langle \phi(\vec{r})\phi(\vec{r}') \rangle = \frac{1}{V^2} \sum_{\vec{k}} \sum_{\vec{k}'} e^{\mathrm{i}\vec{k}\cdot\vec{r}} e^{\mathrm{i}\vec{k}'\cdot\vec{r}'} \langle \phi_{\vec{k}} \phi_{\vec{k}'} \rangle = \frac{1}{VK} \sum_{\vec{k}} \frac{e^{\mathrm{i}\vec{k}\cdot(\vec{r}-\vec{r}')}}{k^2} \; . \tag{2.C.3}$$

In the continuum limit the sum over modes can be replaced by an integral, $\frac{1}{V}\sum_{\vec{k}} \cdots \mapsto \int \frac{d^d k}{(2\pi)^d} \cdots$ and

$$\langle \phi(\vec{r})\phi(\vec{r}') \rangle = \frac{1}{K} \int \frac{d^d k}{(2\pi)^d} \frac{e^{\mathrm{i}\vec{k}\cdot(\vec{r}-\vec{r}')}}{k^2} = -\frac{1}{K} C_d(\vec{r}-\vec{r}') \; . \tag{2.C.4}$$

The right-hand-side is the Coulomb potential due to a unit charge at the origin in a d-dimensional space, since it is the solution to

$$\nabla^2 C_d(\vec{r}) = \delta^d(\vec{r}) \; . \tag{2.C.5}$$

This equation is solved using Gauss' theorem

$$\int_V d^d r \; \nabla^2 C_d(\vec{r}) = \int_S d\vec{S} \cdot \vec{\nabla} C_d(\vec{r}) = 1 \; . \tag{2.C.6}$$

For a spherically symmetric solution $C_d(\vec{r}) = C_d(r)$ and $\vec{\nabla} C_d(\vec{r}) = dC_d(r)/dr\, \hat{e}_r$, and the equation becomes

$$1 = S_d r^{d-1} \frac{dC_d(r)}{dr} \qquad \text{with} \qquad S_d = \frac{2\pi^{d/2}}{(d/2-1)!} \tag{2.C.7}$$

the area of a d dimensional sphere with unit radius. From this equation one deduces the long distance behaviour

$$\lim_{r \gg a} C_d(r) = \begin{cases} c_0 & d > 2 \\ \frac{\ln r}{2\pi} & d = 2 \\ \frac{r^{2-d}}{(2-d)S_d} & d < 2 \end{cases} \tag{2.C.8}$$

and, therefore, the phase fluctuations

$$\langle [\phi(\vec{r}) - \phi(\vec{0})]^2 \rangle = \frac{2[r^{2-d} - a^{2-d}]}{K(2-d)S_d} \tag{2.C.9}$$

(the subtracted constant has been fixed so that this quantity vanishes at zero distance) one finds that while they are finite for $d > 2$, they diverge for $d \leq 2$, and order is thus destroyed by the spin-waves at sufficiently low dimensions.

References

[1] H. E. Stanley, *Introduction to phase transitions and critical phenomena* (Oxford University Press, New York, 1971).

[2] N. Goldenfeld, *Lectures on phase transitions and the renormalization group* (Addison-Wesley, 1992).

[3] J. Cardy, *Scaling and renormalization in Statistical Physics*, Cambridge Lecture notes in physics (Cambridge University Press, 1996).

[4] D. J. Amit, *Field theory, the renormalization group and critical phenomena* (World Scientific, Singapore, 1984).

[5] G. Parisi, *Statistical field theory* (Addison-Wesley, 1988).

[6] B. Simon, *Phase Transitions and Collective Phenomena* (Cambridge University Press, 1997).

[7] I. Herbut, *A modern approach to critical phenomena* (Cambridge University Press, 2006).

[8] A. M. Tsvelik, *Quantum field theory in condensed matter*, 2nd ed. (Cambridge University Press, 2007).

[9] M. Kardar, *Statistical Physics of Fields*, (Cambridge University Press, 2007).

[10] N. D. Mermin, *Absence of Ordering in Certain Classical Systems*, J. Math. Phys. **8**, 1061 (1967).

[11] N. D. Mermin and H. Wagner, *Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models*, Phys. Rev. Lett. **17**, 1133 (1966).

[12] S. Coleman and E. J. Weinberg, *Radiative corrections as the origin of spontaneous symmetry breaking*, Phys. Rev. D **8**, 1888 (1973).

[13] P. C. Hohenberg, *Existence of long-range order in one and two dimensions*, Phys. Rev. **158**, 383 (1967).

[14] P. Archambault, S. T. Bramwell, J.-Y. Fortin, P. W. C. Holdsworth, S. Peysson, J.-F. Pinton, *Universal magnetic fluctuations in the two-dimensional XY model*, J. App. Phys. **83**, 7234 (1998)
S. T. Bramwell, P. W. C. Holdsworth, and J.-F. Pinton, *Universality of rare fluctuations in turbulence and critical phenomena*, Nature **396**, 552 (1998).
S. T. Bramwell, K. Christensen, J.-Y. Fortin, P. C. W. Holdsworth, H. J. Jensen, S. Lise, J. López, M. Nicodemi, J.-F. Pinton, and M. Sellitto, *Universal Fluctuations in Correlated Systems*, Phys. Rev. Lett. **84**, 3744 (2000).

[15] H. E. Stanley and T. A. Kaplan, *Possibility of a Phase Transition for the Two-Dimensional Heisenberg Model*, Phys. Rev. Left. **17**, 913 (1966).

[16] M. A. Moore, *Additional Evidence for a Phase Transition in the Plane-Rotator and Classical Heisenberg Models for Two-Dimensional Lattices*, Phys. Rev. Lett. **23**, 861 (1969).

[17] D. Mukamel, *Statistical mechanics of systems with long range interactions*, in *Long range interacting systems* Les Houches IX,T. Dauxois, S. Ruffo and L. F. Cugliandolo eds., (Oxford University Press, 2010).

[18] J. M. Kosterlitz and D. J. Thouless, *Long range order and metastability in two dimensional solids and superfluids*, J. Phys. C: Solid State Phys. **5**, L124 (1972).

[19] J. M. Kosterlitz and D. J. Thouless, *Ordering, metastability and phase transitions in two-dimensional systems*, J. Phys. C: Solid State Phys. **6**, 1181 (1973).

[20] J. M. Kosterlitz, *The critical properties of the two-dimensional XY model*, J. Phys. C: Solid State Phys. **7**, 1046 (1974).

[21] Very nice computer program demonstrations can be found here: `https://quantumtheory.physik.unibas.ch/people/bruder/Semesterprojekte2007/p6/index.html#x1-30002`, A. Käser, T. Maier, and T. Rautenkranz (2007).

[22] Several animation in YouTube show the dynamics of the $2d$ XY model; see *e.g.* `https://www.youtube.com/watch?v=VpRBfOnc-pg` by S. Burton.

[23] R. E. Peierls, *Uber die statistischen Grundlagen der Elektronentheorie der Metalle*, Helv. Phys. Acta **7**, 24 (1934).

[24] R. E. Peierls, *Surprises in Theoretical Physics* (Princeton University Press, 1979) and refs. therein.

[25] P. Chaikin and T. Lubensky, *Principles of Condensed Matter Physics*, (Cambridge University Press, 1995).

[26] Y. Komura and Y. Okabe, *Large-Scale Monte Carlo Simulation of Two-Dimensional Classical XY Model Using Multiple GPUs*, J. Phys. Soc. Japan **81**, 113001 (2012).

[27] M. Hasenbusch, *The Binder Cumulant at the Kosterlitz-Thouless Transition*, J. Stat. Mech P08003 (2008)

[28] G. M. Wysin, A. R. Pereira, I. A. Marques, S. A. Leonel and P. Z. Coura, *Extinction of BKT transition by nonmagnetic disorder in planar-symmetry spin models*, Phys. Rev. B **72**, 094418 (2005).

[29] E. Domany, M. Schick and Swendsen, *First-order transition in an XY model with nearest-neighbor interactions*, Phys. Rev. Lett. **52**, 1535 (1984).

[30] A. C. D. Van Enter and S. B. Shlosman, *First-order transitions for n-vector models in two and more dimensions: Rigorous proof*, Phys. Rev. Lett. **89**, 285702 (2002).

[31] L. D. Landau, *On the theory of phase transitions i.*, Phys. Z. Sowjet **11**, 26 (1937).

[32] L. D. Landau, *On the theory of phase transitions ii.*, Phys. Z. Sowjet **11**, 545 (1937).

[33] R. E. Peierls, *Bemerkungen über umwandlungstemperaturen*, Helv. Phys. Acta Supp. II, **7**, 91 (1934).

[34] N. W. Ashcroft and N. D. Mermin *Solid State Physics*, Ch. 22, Classical Theory of the Harmonic Crystal (Harcourt College Publisher, Forth Worth., 1976).

[35] B. J. Alder and T. E. Wainwright, *Phase Transition in Elastic Disks*, Phys. Rev. **127**, 359 (1962).

[36] N. N. Bogoliubov, Phys. Abhandl. S. U **6**, 113 (1962).

[37] N. D. Mermin, *Crystalline order in two dimensions*, Phys. Rev. **176**, 250 (1968).

[38] *Bond-Orientational Order in Condensed Matter Systems*, K. J. Strandburg ed. (Springer-Verlag, Heidelberg, 1992).

[39] D. R. Nelson and B. I. Halperin, *Dislocation-mediated melting in two dimensions*, Phys. Rev. B **19**, 2457 (1979).

[40] A. P. Young, *Melting and the vector Coulomb gas in two dimensions*, Phys. Rev. B **19**, 1855 (1979).

[41] U. Gasser, *Crystallization in three- and two-dimensional colloidal suspensions*, J. Phys.: Cond. Matt. **21**, 203101 (2009).

[42] E. Bernard and W. Krauth and D. B. Wilson, *Event-chain Monte Carlo algorithms for hard-sphere systems*, Phys. Rev. E **80**, 056704, (2009).

[43] E. Bernard and W. Krauth, *Two-Step Melting in Two Dimensions: First-Order Liquid-Hexatic Transition*, Phys. Rev. Lett. **107**, 155704, (2011).

[44] M. Engel, J. A. Anderson, S. C. Glotzer, M. Isobe, E. P. Bernard and W. Krauth, *Hard-disk equation of state: First-order liquid-hexatic transition in two dimensions with three simulation methods*, Phys. Rev. E **87**, 042134 (2013).

[45] S. Kapfer and W. Krauth, *Two-Dimensional Melting: From Liquid-Hexatic Coexistence to Continuous Transitions*, Phys. Rev. Lett. **114**, 035702 (2015).