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Spin Waves, Vortices, and the Structure of Equilibrium States in the Classical XY Model

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Abstract. We prove that, for spin systems with a continuous symmetry group on lattices of arbitrary dimension, the surface tension vanishes at all temperatures. For the classical XY model in zero magnetic field, this result is shown to imply absence of interfaces in the thermodynamic limit, at arbitrary temperature. We show that, at values of the temperature at which the free energy of that model is continuously differentiable, i.e. at all except possibly countably many temperatures, there is *either* a *unique translation-invariant equilibrium state*, *or all* such states are labelled by the elements of the symmetry group, SO(2). Moreover, there are *no non-translation-invariant, but periodic* equilibrium states. We also reconsider the representation of the XY model as a gas of spin waves and vortices and discuss the possibility that, in four or more dimensions, translation invariance may be broken by imposing boundary conditions which force an (open) vortex sheet through the system. Among our main tools are new correlation inequalities.

1. Introduction

In this paper we investigate the structure of the equilibrium states of the classical XY model in zero magnetic field.[1] It is well-known that there is only one translation invariant equilibrium state in two dimensions [1, 2]. There is however a phase transition (the Berezinskii-Kosterlitz-Thouless transition). A mathematical proof thereof has been given in [3]. In three or more dimensions the XY model exhibits spontaneous magnetization and symmetry breaking at sufficiently low temperatures [4, 5]. In this paper we give a complete description of all extremal, translation invariant equilibrium states, i.e. the pure phases, whenever the free energy is differentiable with respect to the temperature (Sect. 3.3): We prove that either the set of pure phases is in one-to-one correspondence with the internal symmetry group, or else there is only one translation invariant state. We use new

1 This model is of interest in connection with the theory of superfluid Helium and with superconductivity, for example

correlation inequalities to establish this result. Some of our results have been extended to a rather general class of models in [6]. We also investigate in detail the question whether the classical XY model admits non-translation invariant equilibrium states. We use our new correlation inequalities to prove that there are no equilibrium states which describe the coexistence of two pure phases, in the thermodynamic limit. Indeed we can show that the "Bloch wall" between two distinct phases has an infinite thickness in the thermodynamic limit: This is a direct manifestation of the continuous character of the internal symmetry group. The spins have the tendency of turning very slowly from one direction to a different one. This fact is responsible for the absence of spontaneous symmetry breaking in two dimensions [7–9]. In Sect. 3 we show that the same property prevents the existence of non-translation invariant states exhibiting an interface of the type considered by Dobrushin in the Ising model, *independently of the dimension of the system.* In the Ising model the "topologically stable" defects are the Peierls contours (Bloch walls). In three dimensions they are two-dimensional, and we can impose boundary conditions which force a contour through the entire system. Since this defect is stable at low temperatures, there are non-translation invariant states [10]. The results concerning the Ising model are briefly recapitulated in Sect. 2. In the XY model, the topologically stable defects are the *vortices* which have dimension $d-2$. We show in Sect. 4 that they might provide a *mechanism for the breakdown of translation invariance*, analogous to the one provided by Peierls contours in the Ising model. Therefore we conjecture that the XY model has non-translation invariant equilibrium states in dimension $\geqq 4$. (In four dimensions, vortices are two-dimensional sheets which are expected to undergo a roughening transition very similar to the one described by the solid-on-solid model [3]. In five or more dimensions, vortices presumably remain rigid up to the critical temperature. There are in general *no periodic states*, like "vortex crystals", for arbitrary d.) Some of our results have been announced and described in [11]. Generalizations and new applications of our methods appear in [6] and [12]. Among the results established in [12] are:

(1) Consider a classical, two-component, charge-symmetric Coulomb gas in dimension $d \geqq 2$, and suppose the charged particles are confined between two condensor plates of diameter L which carry a surface charge per unit "area" σ, $-\sigma$, respectively, and are separated by a distance $\propto L$, say. *Then the limiting state*, as $L \to \infty$ (and averaged over translations), is independent of σ, i.e. arbitrary surface charges can be screened, and there is no net electric field in the bulk. Our methods can also be applied to lattice gauge theory. For example:

(2) If the string tension in a pure, abelian lattice gauge theory (with Wilson action, to be specific) vanishes, then electric flux sheets are "rough", i.e. the theory has already passed the roughening transition. Thus, in such models

$$\beta_{\text{roughening}} \leqq \beta_{\text{deconfining}},$$

as expected. Here $\beta = e^{-2}$, and e is the gauge coupling constant.

(3) In the thermodynamic limit the state of an abelian lattice gauge theory, with Wilson action and with boundary conditions which preserve the positivity of the state as a measure, is *unique*, provided the vacuum energy density (or "free energy density") is continuously differentiable in β. Hence vacuum degeneracy can occur only at a point of a first order transition.

2. The Ising Model

In this section we briefly review the structure of equilibrium states in the Ising model, in order to introduce some of the main concepts which are discussed in subsequent sections. The reader may find a more detailed exposition of the subject in [13]. We consider the Ising model on the lattice

$$\mathbb{L} = (\mathbb{Z}^d)^* = \{x : x^i + \tfrac{1}{2} \in \mathbb{Z},\ i = 1, \ldots, d\}.$$

The spin at x takes the values $\sigma(x) = \pm 1$, and the Hamiltonian is

$$H = -\sum_{\langle xy \rangle} \sigma(x)\sigma(y),$$

where $\langle xy \rangle$ denotes, as usual, a pair of nearest neighbors of $\mathbb{L}$. Such a pair is called a *bond*. The pure phase with non-negative magnetization is constructed as the thermodynamic limit of finite volume Gibbs states with $+$ boundary conditions. We choose for example a sequence of boxes $\Lambda(L, T)$,

$$\Lambda(L, T) = \{x \in \mathbb{L} : |x^i| \leqq L,\ i \geqq 2,\ |x^1| \leqq T\},$$

and the value of the spins outside $\Lambda(L, T)$ is equal to $+1$. Then we let L and T tend to infinity. At low temperatures, the configurations of the model are naturally described by the so-called *Peierls contours.* These geometrical objects represent the "*topologically stable*" *defects* of the model. They specify all *frustrated* bonds of $\mathbb{L}$, i.e. all bonds $\langle xy \rangle$ in a configuration with the property that $\sigma(x)\sigma(y) = -1$. These contours are usually defined as subsets of the dual lattice, $\mathbb{L}^* \cong \mathbb{Z}^d$, and are made of all $(d-1)$-dimensional unit cells of $\mathbb{L}^*$, which are the dual cells of frustrated bonds. In the case of $+$ boundary conditions, all Peierls contours are $(d-1)$-dimensional, closed surfaces. We construct an equilibrium state, at low temperatures, which describes the coexistence of two phases with opposite magnetization, by modifying the boundary conditions: We reverse all spins outside $\Lambda(L, T)$ with $x^1 < 0$. This defines the so-called $\pm$ boundary conditions. At this point one usually takes the limit T going to infinity. One obtains in this way an equilibrium state $\langle (\cdot) \rangle_L^{\pm}$ in an infinitely high cylinder with finite cross-section. In this state the expectation value $\langle \sigma(x^1, 0, \ldots, 0) \rangle_L^{\pm}$ is positive for $x^1 > 0$ and, by symmetry, negative for $x^1 < 0$. Moreover the limit of $\langle \sigma(x^1, 0, \ldots, 0) \rangle_L^{\pm}$, when x^1 tends to infinity, is reached exponentially fast and is larger than $m^*(\beta)$, the spontaneous magnetization of the infinite volume system. In other words, this state describes a transition region between two domains with opposite magnetization. Such a transition region is called a *Bloch wall.* It is interesting to analyze the effect of the modification of the boundary conditions on the structure of configurations. The $\pm$ boundary condition enforces the presence of *one open* Peierls contour, whose boundary is given by the intersection of the plane $x^1 = 0$ with the boundary of $\Lambda(L) = \{x : |x^i| \leqq L,\ i \geqq 2\}$. All other Peierls contours are *closed*, as in the case of $+$ boundary conditions. At low temperature, one can show that the Bloch wall has a finite *intrinsic thickness*, which is essentially *independent* of L, *even in the two-dimensional* Ising model [14, 15]. A Bloch wall gives a contribution to the free energy of order $0(L^{d-1})$. Hence we define the specific free energy of the Bloch wall by

$$\tau = -\frac{1}{\beta} \lim_{L\to\infty} \frac{1}{(2L)^{d-1}} \lim_{T\to\infty} \log \frac{Z^{+-}_{L,T}}{Z^{+}_{L,T}}, \tag{2.1}$$

where $Z^{+-}_{L,T}, Z^{+}_{L,T}$ are the partition functions of the system in $\Lambda(L,T)$ with $\pm$ boundary conditions and $+$ boundary conditions, respectively. The quantity $\tau=\tau(\beta)$ is also called surface tension. One knows the following lower and upper bounds on τ, [16, 17]:

$$\tau(\beta) \leqq 2(m^*(\beta))^2, \tag{2.2}$$

and

$$\tau(\beta) \geqq \frac{2}{\beta} \int_0^\beta (m^*(\beta'))^2 d\beta'. \tag{2.3}$$

These bounds imply that the surface tension is nonzero if and only if the spontaneous magnetization is nonzero, i.e. if and only if the inverse temperature is greater than β_c, the inverse critical temperature. It is important to realize that a *nonzero surface tension* corresponds to a *finite, intrinsic thickness* of the Bloch wall, and that this property does *not* mean that the themodynamic limit $(L\to\infty)$ of $\langle(\cdot)\rangle^{\pm}_{L}$ gives a non-translation invariant state. Indeed, thermal fluctuations (surface waves) can delocalize the Bloch wall, and therefore the equilibrium state may be *translation invariant* in the thermodynamic limit, *even* if the surface tension is *positive*. This is precisely what happens in the two-dimensional Ising model [14]. By contrast, in the three-dimensional model, the Bloch wall has not only a finite thickness, but it is rigid, i.e. localized in space, at sufficiently low temperatures [10, 18].

As a consequence, the equilibrium state constructed with $\pm$ boundary conditions breaks the translation invariance of the "dynamics" (Hamilton function) of this model.

The s-o-s model [3] may be used to provide a simplified description of the large fluctuations of the Bloch wall, or *interface*, of the three-dimensional Ising model which one expects to be asymptotically exact, as the roughening transition is approached. In this model, the interface is described by a height function

$$h: x \in \Lambda \subset \mathbb{Z}^2 \mapsto h(x) \in \mathbb{Z},$$

with

$$h(x)=0, \quad \text{for} \quad x \notin \Lambda.$$

The statistical weight of the interface corresponding to a given height function h is given by

$$Z^{-1}_{\beta,\Lambda} \prod_{\langle xy\rangle \subset \Lambda} e^{-\beta|h(x)-h(y)|}. \tag{2.4}$$

Let $\langle(\cdot)\rangle_\beta$ denote the expectation in the state given by (2.4), in the limit $\Lambda \uparrow \mathbb{Z}^2$. It has been proven in [3] that $\langle(h(x)-h(y))^2\rangle_\beta \leqq \text{const}$, uniformly in x and y, if β is sufficiently large, but

$$c\log(|x-y|+1) \leqq \langle(h(x)-h(y))^2\rangle_\beta \leqq c' \log(|x-y|+1)$$

if $\beta<\beta_0$, for some finite, positive β_0.

Thus, one expects that, above the roughening temperature, the interfaces of models like the three-dimensional Ising model exhibit logarithmic fluctuations, and translation invariance is restored. But a rigorous analysis is still missing.

When $\beta < \beta_c$ (the critical temperature) the surface tension of the Ising model vanishes, and the interface becomes "fat". One of the results proven in the next section is that if the surface tension in an abelian spin system, like the Ising- or XY model, vanishes then the state with $\pm$ boundary conditions is translation invariant.

3. The Structure of the Pure Phases, and Absence of Interfaces in the XY Model

3.1. Specific Free Energy of a Bloch Wall. The spins $\mathbf{S}(x)$, $x \in \mathbb{L}$, in the XY model are random variables with values in S^1. We parametrize them by angles, $\Theta(x) \in [0, 2\pi)$, i.e. $\mathbf{S}(x) = (\cos\Theta(x), \sin\Theta(x))$. The Hamiltonian is formally given by

$$H = -\sum_{\langle xy \rangle} \cos(\Theta(x) - \Theta(y)). \tag{3.1}$$

The pure phases at low temperatures (i.e. the extremal translation invariant equilibrium states [19]) are obtained by taking as boundary conditions $\Theta(x) = \phi$, for all x outside $\Lambda(L, T)$, where $0 \leqq \phi < 2\pi$. One of the new results of this section is that *all* pure phases are constructed in this manner. Therefore, we speak of the pure phase ϕ. We first investigate the Bloch wall between the pure phases $\phi = 0$ and $\phi = \alpha$. We show that the Bloch wall has infinite thickness in the thermodynamic limit, since we prove that the specific free energy of the Bloch wall is zero. This result is independent of the dimension d of the lattice. We proceed as in the Ising model (see Sect. 2) and we define the specific free energy of a Bloch wall by

$$\tau = -\frac{1}{\beta} \lim_{L \to \infty} \frac{1}{(2L)^{d-1}} \lim_{T \to \infty} \log \frac{Z^{0,\alpha}_{L,T}}{Z^{0}_{L,T}}, \tag{3.2}$$

where $Z^{0,\alpha}_{L,T}$, $Z^{0}_{L,T}$ are the partition functions of the model in $\Lambda(L, T)$ with $(0, \alpha)$- and 0-boundary conditions, respectively. These two boundary conditions are the analogues of the $\pm$ and $+$ boundary conditions in the Ising model, and they are defined in the same way. In particular, the analogue of the state $\langle(\cdot)\rangle^{\pm}_{L}$, denoted by $\langle(\cdot)\rangle^{0,\alpha}_{L}$, describes the coexistence of the pure phases $\phi = 0$ and $\phi = \alpha$ in the infinitely high cylinder $\Lambda(L)$, (see Sect. 2). Let $T > L$ and

$$\pi(L, T) = \log \frac{Z^{0,\alpha}_{L,T}}{Z^{0}_{L,T}}. \tag{3.3}$$

The following estimation of $\pi(L, T)$ implies immediately that $\tau = 0$, in any dimension d, which will yield the desired results.

Lemma 3.1. *For the XY model and for $T > L$, $0 \leqq -\pi(L, T) \leqq O(L^{d-2}\log L)$.*

Proof. We consider $Z^{0,\alpha}_{L,T}$. Let $\Omega(L, T)$ be the set of points in $\Lambda(L, T)$ which are at distance one from $\mathbb{L} \backslash \Lambda(L, T)$. The Hamiltonian in the box $\Lambda(L, T)$ with $(0, \alpha)$-boundary condition is

$$H^{0,\alpha}_{L,T} = -\sum_{\langle xy \rangle \subset \Lambda(L,T)} \cos(\Theta(\mathrm{x}) - \Theta(\mathrm{y})) - \sum_{\substack{\langle xy \rangle \\ x \in \Omega(L,T) \\ y \notin \Lambda(L,T)}} \cos(\Theta(x) - \hat{\Theta}(y)),$$

where $\hat{\Theta}(y)=0$ for all y with $y^1>0$ and $\hat{\Theta}(y)=\alpha$ for all y with $y^1<0$. The partition function $Z^{0,\alpha}_{L,T}$ is

$$\int_{-\pi}^{\pi}\dots\int \prod_{x\in\Lambda(L,T)} d\Theta(x)\exp(-\beta H^{0,\alpha}_{L,T}).$$

We make a change of variables, in order to obtain 0-boundary conditions. Let $\Theta(x)=\phi(x)+\gamma(x)$ with $\gamma(x)=0$ if $x\in\Omega(L,T)$, $x^1>0$, and $\gamma(x)=\alpha$ if $x\in\Omega(L,T)$, $x^1<0$. After this change of variables we can write the quotient $Z^{0,\alpha}_{L,T}/Z^0_{L,T}$ as

$$\left\langle \prod_{\langle xy\rangle\subset\Lambda(L,T)} \exp\beta\{\cos(\phi(x)-\phi(y)+\gamma(x)-\gamma(y))-\cos(\phi(x)-\phi(y))\}\right\rangle^0_{L,T},$$

where $\langle(\cdot)\rangle^0_{L,T}$ is the expectation value in the state with 0-boundary conditions. Using Jensen's inequality we get

$$\pi(L,T)=\log\frac{Z^{0,\alpha}_{L,T}}{Z^0_{L,T}}\geqq\beta\sum_{\langle xy\rangle}\langle\cos(\phi(x)-\phi(y)+\gamma(x)-\gamma(y))-\cos(\phi(x)-\phi(y))\rangle^0_{L,T}.$$

Since $\langle\sin(\phi(x)-\phi(y))\rangle^0_{L,T}=0$, because of the symmetry $\phi(x)\to-\phi(x)$, we get, using the inequality $\cos x-1\geqq-\frac{1}{2}x^2$,

$$\pi(L,T)\geqq-\frac{\beta}{2}\sum_{\langle xy\rangle}(\gamma(x)-\gamma(y))^2. \tag{3.4}$$

We choose $\gamma(x)$ as follows: Let $\lambda=\lambda(y^2,\dots,y^d)$ be the line

$$\lambda=\{x:x^2=y^2,\dots,x^d=y^d\}.$$

Let $m(\lambda)=\max\{|y^2|,\dots,|y^d|\}$. On the line λ, $\gamma(x)$ is given by

$$\left.\begin{array}{ll}\gamma(x)=0, & \text{if}\quad x^1>L-m(\lambda);\\ \gamma(x)=\alpha, & \text{if}\quad x^1<-(L-m(\lambda));\\ \gamma(x)=\dfrac{\alpha}{2}\left(1-\dfrac{x^1}{L-m(\lambda)}\right), & \text{if}\quad |x^1|\leqq L-m(\lambda).\end{array}\right\} \tag{3.5}$$

[Of course $\gamma(x)$ is already fixed on $\Omega(L,T)$.] It is not difficult to estimate the quantity

$$\sum_{\langle xy\rangle}(\gamma(x)-\gamma(y))^2$$

and to show that it is $O(L^{d-2}\log L)$.

The positivity of $-\pi(L,T)$ follows from the fact that the function

$$\prod_{\langle xy\rangle}\exp\{\beta\cos(\Theta(x)-\Theta(y))\}$$

is of positive type (or, alternatively, from correlation inequalities). □

Remark. It is possible to show that, for a quantity closely related to $\pi(L,T)$, the estimate in Lemma 3.1 cannot be improved at low temperatures. The transformation $\Theta(x)=\phi(x)+\gamma(x)$, defined in (3.5), suggests that $-\pi(L,T)$ is related to the mean energy of a vortex (i.e. a "topologically stable" defect of the XY model, analogous to the Peierls contours in the Ising model) winding around

$\{x:x^1=0\}\cap\Omega(L,T)$. One can actually show that the mean energy of a vortex, located on $\{x:x^1=0\}$ at a distance $\approx\frac{L}{2}$ from $\Omega(L,T)$, is proportional to $L^{d-2}\log L$, at sufficiently low temperatures, while at large temperatures the same quantity behaves like L^{d-2}. These matters are studied in more detail in Sect. 4.

3.2. The State $\langle(\cdot)\rangle^{0,\alpha}$ is Translation Invariant. We now study the thermodynamic limit of the state $\langle(\cdot)\rangle_L^{0,\alpha}$ describing the coexistence of the phases $\phi=0$ and $\phi=\alpha$ in the infinitely high cylinder $\Lambda(L)$. We shall assume that $\langle(\cdot)\rangle^{0,\alpha}=\lim_{L\to\infty}\langle(\cdot)\rangle_L^{0,\alpha}$ is invariant under the translations $a=(0,a^2,\ldots,a^d)$. (This is most likely the case, and, for periodic boundary conditions in the 2-, ..., n-directions, it is plainly true.) Using the fact that the specific free energy of the Bloch wall between the phases $\phi=0$ and $\phi=\alpha$ vanishes in the thermodynamic limit, we prove that $\langle(\cdot)\rangle^{0,\alpha}$ is translation invariant. We wish to emphasize that the reason why $\langle(\cdot)\rangle^{0,\alpha}$ is translation invariant is very different from the reason why $\langle(\cdot)\rangle^{\pm}$ is translation invariant in the two-dimensional Ising model: In the former case, the reason is that the "Bloch wall" disappears, in the sense that its thickness, i.e. its transverse extension, diverges to $+\infty$. In the latter case, the translation invariance is restored by fluctuations (surface waves) on a scale of $O(\sqrt{L})$ of the Bloch wall.

Our proof of translation invariance of $\langle(\cdot)\rangle^{0,\alpha}$ is divided into three steps: We first show that

$$\langle\cos(\Theta(x)-\Theta(y))\rangle^0=\langle(\cos(\Theta(x)-\Theta(y))\rangle^{0,\alpha}, \tag{3.6}$$

for all $\langle xy\rangle\subset\mathbb{L}$. Here $\langle(\cdot)\rangle^0$ is the pure phase $\phi=0$. The next step is to prove that (3.6) implies the stronger result

$$\left\langle\cos\left(\sum_x m(x)\Theta(x)\right)\right\rangle^0=\left\langle\cos\left(\sum_x m(x)\Theta(x)\right)\right\rangle^{0,\alpha} \tag{3.7}$$

for all functions $m:\mathbb{L}\to\mathbb{Z}$ of finite support satisfying $\sum_x m(x)=0$. To prove (3.7) we use new correlation inequalities. The details of this step are presented in Sect. 3.3. The final step consists in proving that one finds only translation invariant states when one decomposes $\langle(\cdot)\rangle^{0,\alpha}$ into extremal states.

First Step. Using the correlation inequality (Proposition 1 in [2])

$$\langle\cos(\Theta(x)-\Theta(y))\rangle_\Lambda^0\geqq\langle\cos(\Theta(x)-\Theta(y))\rangle_\Lambda^{0,\alpha}, \tag{3.8}$$

which is valid for any region Λ, we can find a lower bound for $-\tau(L,T)$. Indeed, let K be any fixed positive number and let $T>K$. Then we obtain immediately the following lower bound, leaving out positive terms:

$$-\frac{d\tau(L,T)}{d\beta}\geqq\sum_{\substack{\langle xy\rangle\subset\Lambda(L,T)\\|x^1|\leqq K}}(\langle\cos(\Theta(x)-\Theta(y))\rangle_{L,T}^0-\langle\cos(\Theta(x)-\Theta(y))\rangle_{L,T}^{0,\alpha}).$$

Let

$$\begin{aligned}f_{L,T}(x)&=f_{L,T}(x^2,\ldots,x^d)\\&=\tfrac{1}{2}\sum_{|x^1|\leqq K}\ \sum_{y:|x-y|=1}(\langle\cos(\Theta(x)-\Theta(y))\rangle_{L,T}^0-\langle\cos(\Theta(x)-\Theta(y))\rangle_{L,T}^{0,\alpha}).\end{aligned}$$

Then using again (3.8) we get

$$-\frac{d\pi(L,T)}{d\beta} \geqq \sum_{\substack{|x^i| \leqq L/2 \\ i \geqq 2}} f_{L,T}(x^2, \ldots, x^d). \tag{3.9}$$

For any fixed $(x^2, \ldots, x^d)$ we have

$$0 \leqq \lim_{L\to\infty} \lim_{T\to\infty} f_{L,T}(x) = f(0).$$

[At this point we assume the invariance of the state

$$\langle(\cdot)\rangle^{0,\alpha} = \lim_{L\to\infty} \langle(\cdot)\rangle_L^{0,\alpha} = \lim_{L\to\infty} \lim_{T\to\infty} \langle(\cdot)\rangle_{L,T}^{0,\alpha}$$

with respect to the horizontal translations $a=(0, a^2, \ldots, a^d)$.] Therefore

$$\lim_{L\to\infty} \frac{1}{L^{d-1}} \lim_{T\to\infty} \sum_{\substack{|x^i| \leqq L/2 \\ i \geqq 2}} f_{L,T}(x) = f(0),$$

and by Lemma 3.1

$$0 = -\lim_{L\to\infty} \frac{1}{L^{d-1}} \lim_{T\to\infty} \int_0^\beta \frac{d\pi(L,T)}{d\beta} d\beta \geqq \int_0^\beta f(0) d\beta \geqq 0.$$

This implies that, for almost all β,

$$\langle \cos(\Theta(x) - \Theta(y)) \rangle^0 = \langle \cos(\Theta(x) - \Theta(y)) \rangle^{0,\alpha}, \tag{3.10}$$

for all $\langle xy \rangle$, since K is arbitrary.

Third Step. Using correlation inequalities we prove in the

Second Step (postponed to Sect. 3.3) that

$$\left\langle \cos\left(\sum_x m(x)\Theta(x)\right)\right\rangle^0 = \left\langle \cos\left(\sum_x m(x)\Theta(x)\right)\right\rangle^{0,\alpha}, \tag{3.11}$$

for all functions m of finite support and with $\sum_x m(x) = 0$. It is well known that the set of equilibrium states is convex, and that every equilibrium state has a *unique* representation as a convex superposition of extremal equilibrium states [19]. Therefore, in order to prove that $\langle(\cdot)\rangle^{0,\alpha}$ is translation invariant, it is sufficient to show that $\langle(\cdot)\rangle^{0,\alpha}$ is a convex superposition of translation invariant equilibrium states. We now show that this property follows from the equalities (3.11).

Let ϱ be any extremal equilibrium state which appears in the decomposition of $\langle\cdot\rangle^{0,\alpha}$. Let ϱ_ϕ be the extremal state obtained by a rotation, ϕ, of the state ϱ. We also introduce

$$\bar{\varrho} = \int_{S^1} d\phi \varrho_\phi. \tag{3.12}$$

By construction

$$\bar{\varrho}\left(\cos\left(\sum_x m(x)\Theta(x)\right)\right) = \bar{\varrho}\left(\sin\left(\sum_x m(x)\Theta(x)\right)\right) = 0$$

for all functions m such that $\sum_x m(x) \neq 0$. We use now the following correlation inequalities

$$\left\langle \cos\left(\sum_x m(x)\Theta(x)\right)\right\rangle^0 \geqq \left\langle \cos\left(\sum_x m(x)\Theta(x)+\psi\right)\right\rangle, \tag{3.13}$$

which are valid for any equilibrium state $\langle(\cdot)\rangle$, any function m and any ψ. Let $\sum_x m(x)=0$. Since (3.11) and (3.13) hold, we must have

$$\varrho\left(\cos\left(\sum_x m(x)\Theta(x)\right)\right) = \left\langle \cos\left(\sum_x m(x)\Theta(x)\right)\right\rangle^0, \tag{3.14}$$

for any ϱ which appears in the extremal decomposition of $\langle(\cdot)\rangle^{0,\alpha}$. The result (3.14) implies (Theorem 1 in [2]) that

$$\varrho\left(\sin\left(\sum_x m(x)\Theta(x)\right)\right) = 0. \tag{3.15}$$

Indeed, we can write using (3.13)

$$\begin{aligned}\varrho\left(\cos\left(\sum_x m(x)\Theta(x)\pm\psi\right)\right) &= \cos\psi\cdot\varrho\left(\cos\left(\sum_x m(x)\Theta(x)\right)\right)\\ &\quad\mp\sin\psi\cdot\varrho\left(\sin\left(\sum_x m(x)\Theta(x)\right)\right)\\ &=\cos\psi\left\langle\cos\left(\sum_x m(x)\Theta(x)\right)\right\rangle^0\\ &\quad\mp\sin\psi\cdot\varrho\left(\sin\left(\sum_x m(x)\Theta(x)\right)\right)\\ &\leqq\left\langle\cos\left(\sum_x m(x)\Theta(x)\right)\right\rangle^0.\end{aligned}$$

Let $0<\psi<\pi$. Then

$$\pm\varrho\left(\sin\left(\sum_x m(x)\Theta(x)\right)\right) \leqq \frac{1-\cos\psi}{\sin\psi}\cdot\left\langle\cos\left(\sum_x m(x)\Theta(x)\right)\right\rangle^0.$$

Letting ψ tend to zero we get (3.15). Therefore Eqs. (3.14) and (3.15) are also true for $\bar{\varrho}$, and this is equivalent to

$$\bar{\varrho}(\cdot) = \int_{S^1} d\phi\langle(\cdot)\rangle^\phi, \tag{3.16}$$

(where $\langle(\cdot)\rangle^\phi$ is obtained by a rotation by ϕ of $\langle(\cdot)\rangle^0 = \lim\langle(\cdot)\rangle^0_{L,T}$), since the two states, $\bar{\varrho}$ and $\int_{S^1} d\phi\langle(\cdot)\rangle^\phi$, coincide on all local observables $\cos\left(\sum_x m(x)\Theta(x)\right)$ and $\sin\left(\sum_x m(x)\Theta(x)\right)$.

However, (3.12) and (3.16) provide us with two extremal decompositions of the same state. Since the extremal decomposition is unique, we have $\varrho=\langle(\cdot)\rangle^\phi$, for some ϕ, and therefore ϱ is translation invariant.

3.3. New Correlation Inequalities, and the Structure of the Pure Phases. In this subsection, we prove new correlation inequalities and use them to prove (3.11) and to determine all pure phases of the classical XY model.

Let m be any function defined on $\mathbb{L}$ with values in $\mathbb{Z}$ and such that $m(x) \neq 0$ for a finite number of x only. We write

$$m\Theta = \sum_x m(x)\Theta(x).$$

Let $\langle(\cdot)\rangle_\Lambda^0$ be the Gibbs state in the finite volume Λ with 0-boundary conditions, and let $\langle(\cdot)\rangle'_\Lambda$ be a Gibbs state in Λ with some arbitrary, but fixed boundary conditions.

We take two copies of the system, form their product and consider the product state (measure)

$$\langle(\cdot)\rangle_\Lambda^0 \otimes \langle(\cdot)\rangle'_\Lambda \equiv \langle(\cdot)\rangle. \tag{3.17}$$

Let $\cos m\Theta$ be an observable for the first copy and $\cos m\Theta'$ the same observable for the second copy.

Lemma 3.2. *For any positive λ and arbitrary m and n (with supports in Λ)*

$$\langle(\cos m\Theta \pm \cos m\Theta')\exp(\pm\lambda \cos n\Theta \cdot \cos n\Theta')\rangle \geqq 0.$$

Proof. We use Ginibre's method [20] and write

$$\cos n\Theta \cdot \cos n\Theta' = (1/2)(\cos n(\Theta' + \Theta) + \cos n(\Theta' - \Theta)).$$

We make the usual change of variables

$$\phi(x) = (1/2)(\Theta'(x) + \Theta(x)), \qquad \phi'(x) = (1/2)(\Theta'(x) - \Theta(x)).$$

After this change of variables the exponential factorizes, and we can repeat the arguments of Ginibre. □

Remark. Since, in Lemma 3.2, Λ is arbitrary, we can take the thermodynamic limit and use Lemma 3.2 for the product measure $\langle(\cdot)\rangle = \langle(\cdot)\rangle^0 \otimes \langle(\cdot)\rangle'$, where $\langle(\cdot)\rangle'$ is an arbitrary equilibrium state.

Lemma 3.3. *For an arbitrary equilibrium state $\langle(\cdot)\rangle'$, if*

$$\langle \cos m\Theta\rangle^0 = \langle \cos m\Theta\rangle'$$

and

$$\langle \cos n\Theta\rangle^0 = \langle \cos n\Theta\rangle' > 0,$$

then

$$\langle \cos(m \pm n)\Theta\rangle^0 = \langle \cos(m \pm n)\Theta\rangle'.$$

Proof. We expand the exponential

$$\exp(\pm\lambda \cos n\Theta \cdot \cos n\Theta') = 1 \pm \lambda \cos n\Theta \cdot \cos n\Theta' + O(\lambda^2).$$

Therefore, using Lemma 3.2,

$$\begin{aligned}\langle \cos m\Theta\rangle^0 - \langle \cos m\Theta\rangle' \geqq \pm\lambda(&\langle \cos n\Theta \cdot \cos m\Theta\rangle^0 \langle \cos n\Theta\rangle' \\ &- \langle \cos n\Theta \cdot \cos m\Theta\rangle' \langle \cos n\Theta\rangle^0) + O(\lambda^2).\end{aligned}$$

But the left-hand side is zero, by hypothesis, and we can divide by λ. Letting λ tend to zero and using the positivity of $\langle\cos n\Theta\rangle^0$, we get

$$\langle\cos n\Theta\cdot\cos m\Theta\rangle^0=\langle\cos n\Theta\cdot\cos m\Theta\rangle'.$$

This last equality can be written as

$$\langle\cos(n+m)\Theta\rangle^0+\langle\cos(n-m)\Theta\rangle^0=\langle\cos(n+m)\Theta\rangle'+\langle\cos(n-m)\Theta\rangle'.$$

Using (3.13), we conclude that

$$\langle\cos(n\pm m)\Theta\rangle^0=\langle\cos(n\pm m)\Theta\rangle'.\ \square$$

It is now clear that (3.10) implies (3.11), since we can apply Lemma 3.3 inductively. (The positivity of $\langle\cos(\Theta(x)-\Theta(y))\rangle^0$ is a consequence of Ginibre inequalities [20].)

Using the results of Sect. 3.2 and Lemma 3.3, we can prove the following proposition on the structure of the pure phases of the model.

Proposition 3.4. *The following two assertions,* A) *and* B), *are equivalent:*

A) *The free energy of the XY model is differentiable with respect to β, at some value β_0 of β.*

B) *All pure phases of the XY model are given by $\{\langle(\cdot)\rangle^\phi, 0\leqq\phi<2\pi\}$, for $\beta=\beta_0$.*

Proof. The condition A) is equivalent to

$$\langle\cos(\Theta(x)-\Theta(y))\rangle^0=\langle\cos(\Theta(x)-\Theta(y))\rangle$$

for any translation invariant equilibrium state and any $\langle xy\rangle$. Therefore $\langle\cos m\Theta\rangle^0=\langle\cos m\Theta\rangle$, for all m with $\sum_x m(x)=0$, by Lemma 3.3. The "Third Step" in Sect. 3.2 then completes the proof of Proposition 3.4. $\square$

Remarks. 1) Generalizations of this Proposition for a large class of ferromagnetic models can be found in [6].

2) All results of Sect. 3 are valid for the Villain model.

3) With the results of [1], we have the following situation (if condition A) is satisfied): Either $\langle\cos\Theta\rangle_\beta^0=0$, and therefore *all* equilibrium states are rotation invariant and there is only *one* translation invariant state, or $\langle\cos\Theta\rangle_\beta^0>0$, and each ϕ, $0\leqq\phi<2\pi$, corresponds to a distinct pure phase.

We wish to conclude this section with a result on the absence of periodic states.

Proposition 3.5. *At temperatures at which the free energy of the classical XY model is continuously differentiable, there are no non-translation invariant, but periodic equilibrium states, in any dimension d.*

Proof. Since, for an arbitrary equilibrium state, ϱ, of the classical XY model,

$$\langle\cos(\Theta(x)-\Theta(y))\rangle^0\geqq\varrho(\cos(\Theta(x)-\Theta(y))),$$

and since for any *periodic* state, ϱ, with domain of periodicity $C\subset\mathbb{L}$, the derivative of the free energy with respect to the inverse temperature β is given by

$$(2|C|)^{-1}\sum_{\substack{x'\in C\\|x'-y'|=1}}\varrho(\cos(\Theta(x')-\Theta(y')))=d\langle\cos(\Theta(x)-\Theta(y))\rangle^0,$$

for arbitrary $\langle xy \rangle$, we conclude that

$$\varrho(\cos(\Theta(x)-\Theta(y)))=\langle\cos(\Theta(x)-\Theta(y))\rangle^0,$$

for all $\langle xy \rangle$. It now follows from Lemma 3.3 and the "Third Step" of Sect. 3.2 that

$$\varrho=\int_{S^1} d\mu(\phi)\langle(\cdot)\rangle^{\phi},$$

for some probability measure μ. In particular, ϱ is translation invariant. This completes the proof. □

Remark. This result shows (among other things) that, in the threedimensional, classical XY model there are *no* states describing periodic arrays of parallel vortex lines, provided the free energy is continuously differentiable in β. (For a discussion of vortices see Sect. 4.)

4. Non-translation Invariant Equilibrium States and Specific Free Energy of Vortices

4.1. Main Conjecture. In this section we show how one might go about constructing a non-translation invariant equilibrium state for the classical XY model. We have proven in the last section that such a state cannot be constructed in a way similar to the one by which Dobrushin constructed non-translation invariant equilibrium states for the three- or higher dimensional Ising model. The reason is that the Bloch walls are not *stable defects* of the XY model. Rather, the stable defects of the XY model are the *vortices*. The vortices are $(d-2)$-dimensional defects. For $d=3$, respectively $d=4$, we can force a line defect, respectively a planar defect, into the system which are the counterparts of the line defect, respectively planar defect, produced in the Ising model by the $\pm$ boundary condition when $d=2$ respectively $d=3$. (See Sect. 2.) We do not expect that a non-translation invariant state can be constructed for the three-dimensional XY model, because a line defect undergoes macroscopic fluctuations. For the four dimensional model, energy-entropy considerations on the simplest deformations of the planar vortex indicate that this defect is presumably stable at very low temperatures. Therefore we conjecture:

Conjecture. Translation invariance of the XY model can be broken if the dimension of the lattice is larger or equal to four.

In the next Subsections we discuss this conjecture in some detail for the Villain model[2], which describes the same physics as the XY model, but which has the advantage that the introduction of defects, the vortices, is particularly transparent [21]. The Villain model is a planar spin model. The spins, parametrized by angles $\Theta(x)$, $x\in\mathbb{L}$, are random variables with values in S^1. We consider the model in the finite box

$$\Lambda=\{x\in\mathbb{L}, |x^i|\leqq L, i=1,\dots,d\}. \tag{4.1}$$

A boundary condition, ϕ, is given by fixing the value of $\Theta(x)$ for $x\in\mathbb{L}\backslash\Lambda$, i.e. $\Theta(x)=\phi(x)$. The Boltzmann factor of the model with this boundary condition is

2 Our arguments extend to the XY model, but are less transparent in that case

$$\prod_{\substack{\langle xy\rangle \\ \langle xy\rangle \cap \Lambda \neq \emptyset}} g_\beta(\Theta(x)-\Theta(y)), \tag{4.2}$$

with

$$g_\beta(\Theta)=\sum_{n\in\mathbb{Z}} \exp\left(-\frac{\beta}{2}(\Theta+2\pi n)^2\right). \tag{4.3}$$

The corresponding partition function is obtained by integrating all angular variables $\Theta(x)$, $x\in\Lambda$, over S^1. Before we express the Villain model in terms of spin waves and vortices (Subsect. 4.4), we have to introduce some formalism, in Subsect. 4.2 and 4.3. The discussion of our main conjecture starts in Subsect. 4.5.

4.2. Cell Complexes. It is useful to use geometrical concepts in the description of the Villain model. This is fairly standard; see e.g. [21–24].

The lattice $\mathbb{L}$ is considered as a *cell complex*, which consists of the ν-dimensional unit cells of $\mathbb{L}$ (called hereafter ν-cells), $\nu=0, 1, \ldots, d$. Thus, the 0-cells are the lattice sites, the 1-cells the bonds and the 2-cells the plaquettes of $\mathbb{L}$. Each cell has two possible orientations. If c is a cell, then $\bar{c}$ is the same cell with opposite orientation. The orientation is the conventional one, and the incidence function, I, of $\mathbb{L}$ is defined as usual. Let c be a ν-cell and c' a $(\nu-1)$-cell. Then $I(c,c')=+1$, respectively -1, if c' is contained in ∂c, and the orientation induced on c' is equal, respectively opposite, to the orientation of c'. Otherwise $I(c,c')=0$. The main property of I is

$$\sum_{c'} I(c,c')I(c',c'')=0, \tag{4.4}$$

where c is a ν-cell, c'' a $(\nu-2)$-cell and c' are $(\nu-1)$-cells. A *ν-chain* is a real function f defined on the ν-cells, with finite support and such that $f(\bar{c})=-f(c)$. The *boundary operation* δ transforms a ν-chain into a $(\nu-1)$-chain:

$$\delta f(c)=\sum_{c'} f(c')I(c',c); \tag{4.5}$$

($\delta f=0$ if f is a 0-chain). Using (4.4) we see easily that $\delta^2=0$. The *coboundary operation* d transforms a ν-chain into a $(\nu+1)$-chain

$$df(c)=\sum_{c'} f(c')I(c,c'). \tag{4.6}$$

The operator δ is the adjoint of d with respect to the scalar product

$$(f,g)=\sum_c f(c)g(c), \tag{4.7}$$

where in (4.7) we sum only over positively oriented cells. Indeed, one verifies immediately that

$$(df,g)=(f,\delta g). \tag{4.8}$$

The *dual complex* $\mathbb{L}^*$ is $\mathbb{Z}^d$, considered as a cell complex. To every ν-cell c of $\mathbb{L}$, there corresponds exactly one $(d-\nu)$-cell c^* of $\mathbb{L}^*$, such that c and c^* have exactly one point in common and $I(c,c_1)=I(c_1^*,c^*)$. The star operation transforms a ν-chain f on $\mathbb{L}$ into a $(d-\nu)$-chain on $\mathbb{L}^*$, which we also denote by f, in such a way that $f(c^*)=f(c)$. If $\delta f=g$ on $\mathbb{L}$, then $df=g$ on $\mathbb{L}^*$, where d is now the coboundary operation on $\mathbb{L}^*$. We also consider, in the next subsections, subsets of $\mathbb{L}$, or of $\mathbb{L}^*$, which are closed. A subset of $\mathbb{L}$, $\bar{\Omega}$, is *closed* if it contains with every cell also the cells on its boundary. If we restrict the incidence function I to this subset, then the property (4.4) is still valid. Therefore we can interpret this subset as a *cell complex*, and it is possible to define the boundary and the coboundary operations, with respect to this cell complex, by (4.5) and (4.6). They do *not* coincide with the corresponding operations in $\mathbb{L}$. All the cell complexes, which we introduce later, have trivial homology. In particular, Poincaré's Lemma is true: If f is a $\mathbb{R}$-valued, respectively $\mathbb{Z}$-valued, v-chain such that $df=0$, then there exists a $\mathbb{R}$-valued, respectively $\mathbb{Z}$-valued, $(v-1)$-chain g, such that $f=dg$. A similar statement holds for chains f with the property that $\delta f=0$. We shall use the same notations, d and δ, for the coboundary and boundary operations of the cell complex $\bar{\Omega}$, since it will be clear from context which operator is meant.

4.3. Remarks on the Laplacian. We introduce several subsets of the cell complexes $\mathbb{L}$ and $\mathbb{L}^*$:

$$\Omega=\{c\in\mathbb{L}, c\cap\Lambda\neq\emptyset\}, \tag{4.9}$$

where the subset Λ of $\mathbb{L}$ has been defined in (4.1),

$$\Omega^*=\{c^*\in\mathbb{L}^*, c\in\Omega\}, \tag{4.10}$$

$$\bar{\Omega}=\text{the closure of } \Omega. \tag{4.11}$$

The last subset is obtained by adding to each element of Ω its boundary cells. The subsets $\Omega^*\subset\mathbb{L}^*$ and $\bar{\Omega}\subset\mathbb{L}$ are closed and can therefore be interpreted as cell complexes; (see Subsect. 4.2).

Let A be the operator

$$A=d\delta, \tag{4.12}$$

defined on the *cell complex* $\bar{\Omega}$. We collect here a few remarks on A, as an operator on the 2-chains of the cell complex $\bar{\Omega}$. First we suppose that the dimension of the underlying lattice is two. If we label each plaquette of $\bar{\Omega}$ by its center, it is easy to verify that the action of $-A$ on the 2-chains coincides with the action of the lattice Laplacian on functions supported in the box $\{x\in\mathbb{Z}^2:|x^i|\leqq L, i=1,2\}$, with *Dirichlet* boundary conditions. Therefore A^{-1} exists on the space of 2-chains of $\bar{\Omega}$. Let us suppose now that the dimension d of the underlying lattice is larger or equal to three. We study the action of A on those 2-chains, n, of $\bar{\Omega}$ for which $dn=0$. They form a linear subspace C^0 of the space of 2-chains, and from the identity $d^2=0$ we obtain immediately that A leaves this subspace invariant. The space C^0 contains $\frac{d(d-1)}{2}$ subspaces C^0_{ij}, $i<j$, i and $j=1,\dots,d$: The subspace C^0_{ij} consists of all 2-chains, n, of $\bar{\Omega}$ such that $dn=0$ and the support of n contains only plaquettes parallel to the 2-dimensional plane $\Sigma_{ij}=\{x:x^k=0, k\neq i,j\}$. Using the condition $dn=0$, one may verify that the operator A leaves the spaces C^0_{ij} invariant. If we label each plaquette p of $\bar{\Omega}$, which is parallel to the plane Σ_{ij}, by its center, then the action of $-A$ on C^0_{ij} is the same as the action of the lattice Laplacian in an appropriate box with *mixed* boundary conditions: We have *Neumann* boundary conditions in all but the directions i and j, where we have *Dirichlet* boundary

conditions. Therefore the restriction of A to C_{ij}^0 is invertible in the subspace C_{ij}^0.

On the cell complex Ω^* we define the operator

$$B = \delta d, \tag{4.13}$$

acting on the space of $(d-2)$-chains with the property that $\delta n = 0$. As above, we notice that this space contains $d(d-1)/2$ subspaces. The action of $-B$ on one of these subspaces is the same as the action of the lattice Laplacian, as above, but now Dirichlet boundary conditions are replaced by Neumann boundary conditions and vice-versa.

4.4. Spin Waves and Vortices in the Villain Model. We first rewrite the Boltzmann factor (4.2) of the Villain model, using the formalism of Sects. 4.2 and 4.3. A spin configuration in Λ defines a 0-chain Θ with values in S^1. It is extended to a 0-chain on $\bar{\Omega}$ by putting

$$\Theta(x) = \phi(x) \quad \text{if} \quad x \in \bar{\Omega} \backslash \Lambda, \tag{4.16}$$

where ϕ is a given boundary condition. The Boltzmann factor with boundary condition ϕ is then given by

$$\prod_{b \in \Omega} g_\beta(d\Theta(b)), \tag{4.17}$$

where in (4.17) we take the product only over the positively oriented 1-cells b. The corresponding partition function, Z^ϕ, is obtained by integrating, in (4.17), all spin variables $\Theta(x)$, $x \in \Lambda$, over S^1. It is convenient to introduce a generalized Boltzmann factor

$$\prod_{b \in \Omega} g_\beta(d\Theta(b) + \gamma(b)), \tag{4.18}$$

where we impose *0-boundary conditions*, and where γ is an *arbitrary 1-chain* on $\bar{\Omega}$. The corresponding partition function is denoted $Z(\gamma)$. From now on we study $Z(\gamma)$. On account of (4.3), the partition function $Z(\gamma)$ is given by

$$Z(\gamma) = \int_0^{2\pi} \cdots \int \prod_{b \in \Omega} \left\{ \sum_{m(b) \in \mathbb{Z}} f_\beta(d\Theta(b) + 2\pi m(b) + \gamma(b)) \right\}, \tag{4.19}$$

with

$$f_\beta(\Theta) = \exp\left[-\frac{\beta}{2} \Theta^2 \right]. \tag{4.20}$$

We shall henceforth omit writing the integration measure $\prod_x d\Theta(x)$.

We first consider the sum over the variables $m(b)$. The dual of Ω is Ω^* (see (4.10)), and Ω^* is a cell complex. Let m be the $(d-1)$-chain on Ω^* defined by

$$m(b^*) = m(b), \qquad b \in \Omega. \tag{4.21}$$

Since $m(b) \in \mathbb{Z}$ is arbitrary, we see that m is an arbitrary $\mathbb{Z}$-valued $(d-1)$-chain on Ω^*. We decompose such chains into equivalence classes: Two chains m_1 and m_2 belong to the same class if $\delta m_1 = \delta m_2$. The classes are labelled by $n = \delta m$, n being a

$(d-2)$-chain. Since Ω^* is a cell complex with trivial homology, the equation

$$\delta m = 0 \tag{4.22}$$

is easily solved, using Poincaré's lemma:

$$m = \delta k, \tag{4.23}$$

k being a $\mathbb{Z}$-valued d-chain on Ω^*. Moreover, the solution is unique, since $\delta k = 0$ implies $k = 0$ on Ω^*. From (4.23) we get

$$m_1 = m_2 + \delta k, \quad \text{if} \quad \delta m_1 = \delta m_2. \tag{4.24}$$

The set of $(d-2)$-chains, n, which label the equivalence classes, is exactly the set of all $(d-2)$-chains such that

$$\delta n = 0. \tag{4.25}$$

In each equivalence class, labelled by n, we choose one representative and denote it by m'. Therefore we may rewrite (4.19) as

$$\begin{aligned} Z(\gamma) &= \int_0^{2\pi} \dots \int \sum_{\substack{n: \\ \delta n = 0}} \sum_{\substack{m: \\ \delta m = n}} \prod_{b^* \in \Omega^*} f_\beta(\delta\Theta(b^*) + 2\pi m(b^*) + \gamma(b^*)) \\ &= \int_{-\infty}^{+\infty} \dots \int \sum_{\substack{n: \\ \delta n = 0}} \prod_{b^* \in \Omega^*} f_\beta(\delta\Phi(b^*) + 2\pi m'(b^*) + \gamma(b^*)), \end{aligned} \tag{4.26}$$

after the change of variables

$$\Phi(x^*) = \Theta(x^*) + 2\pi k(x^*). \tag{4.27}$$

Since $\delta n = 0$, we can define (see Subsect. 4.3)

$$\tilde{m}(b^*) = (dB^{-1}n)(b^*). \tag{4.28}$$

By definition we have

$$d\tilde{m} = 0, \qquad \delta\tilde{m} = n. \tag{4.29}$$

Therefore, by Poincaré's lemma, there exists a real-valued d-chain q on Ω^* such that

$$m' = \tilde{m} + \delta q. \tag{4.30}$$

Moreover, q is unique. Let

$$\phi(x^*) = \Phi(x^*) + 2\pi q(x^*). \tag{4.31}$$

Using (4.30) and (4.31), we get

$$Z(\gamma) = \sum_{\substack{n: \\ \delta n = 0}} \int_{-\infty}^{+\infty} \dots \int \prod_{b^* \in \Omega^*} f_\beta(\delta\phi(b^*) + 2\pi\tilde{m}(b^*) + \gamma(b^*)). \tag{4.32}$$

The product in (4.32) can be written as

$$\exp\left[-\frac{\beta}{2}(\delta\phi + 2\pi\tilde{m} + \gamma, \delta\phi + 2\pi\tilde{m} + \gamma)\right], \tag{4.33}$$

where $(\cdot, \cdot)$ is the scalar product introduced in Subsect. 4.2. From (4.29) and (4.28) we get

$$(\delta\phi, \tilde{m}) = (\tilde{m}, \delta\phi) = (d\tilde{m}, \phi) = 0\,, \tag{4.34}$$

and

$$(\tilde{m}, \tilde{m}) = (B^{-1}n, \delta d B^{-1}n) = (B^{-1}n, n)\,. \tag{4.35}$$

Therefore our final expression for the generalized partition function *on the dual lattice Ω^** is

$$\begin{aligned} Z(\gamma) = \exp\left(-\frac{\beta}{2}(\gamma, \gamma)\right) \int\limits_{-\infty}^{+\infty} \dots \int \exp\left[-\frac{\beta}{2}(\delta\phi, \delta\phi) - \beta(\delta\phi, \gamma)\right] \\ \cdot \left\{ \sum_{\substack{n: \\ \delta n = 0}} \exp[-\beta 2\pi^2 (n, B^{-1}n) - 2\pi\beta(\delta\gamma, B^{-1}n)] \right\}. \end{aligned} \tag{4.36}$$

In the special case where $\gamma = 0$, this is the partition function for the Villain model with 0-boundary conditions. This partition function, $Z(\gamma = 0) \equiv Z^0$, is the product of a partition function of a gas of spin waves (with 0-boundary conditions)

$$Z^0_{\mathrm{s.w.}} = \int\limits_{-\infty}^{+\infty} \dots \int \prod_{b \in \Omega} \exp\left[-\frac{\beta}{2}(d\phi(b))^2\right], \tag{4.37}$$

and a partition function of a vortex gas, expressed on the dual lattice,

$$Z_v = \sum_{\substack{n: \\ \delta n = 0}} \exp[-\beta 2\pi^2 (n, B^{-1}n)]\,. \tag{4.38}$$

It is easy to generalize the computation of $Z(\gamma)$, in order to deal with the expectation value of local observables, $\exp\left(i \sum_x a(x)\Theta(x)\right)$, $a(x) \in \mathbb{Z}$: We get

$$\begin{aligned} \left\langle \exp\left(i \sum_x a(x)\Theta(x)\right)\right\rangle^0 = \left\langle \exp\left(i \sum_x a(x)\phi(x)\right)\right\rangle^0_{\mathrm{s.w.}} \\ \cdot \left\langle \exp\left(-i2\pi \sum_{x^*} a(x^*) q(x^*)\right)\right\rangle_v\,, \end{aligned} \tag{4.39}$$

where q is defined by (4.30). Since the local observable is periodic, the final result does *not* depend on the particular choice of m'. We now discuss a special case: Let x and y be a pair of points in Λ, such that there exists a path of positively oriented bonds b, starting at x and ending at y. Let $f_{xy}(b) = 1$, if b belongs to the path and $f_{xy}(b) = 0$ otherwise. Since $\exp i(\Theta(y) - \Theta(x)) = \exp i(f_{xy}, d\Theta)$, we get

$$\begin{aligned} \langle \exp i(\Theta(y) - \Theta(x))\rangle^0 = \langle \exp i(\phi(y) - \phi(x))\rangle^0_{\mathrm{s.w.}} \\ \cdot \langle \exp i2\pi(n, B^{-1}\delta f_{xy})\rangle_v \end{aligned} \tag{4.40}$$

where, in the last expectation, f_{xy} is the $(d-1)$-chain dual to the 1-chain, also denoted f_{xy}, defined above.

4.5. Non-Translation Invariant States. The (topologically) stable defects of the classical XY model are the vortices, which are described by the $(d-2)$-chains, n, introduced in the last subsection. We recall that $\delta n = 0$. Thus, the vortices form $(d-2)$-dimensional, closed "networks." These vortices play a role analogous to the one played by the Peierls contours in the Ising model. Indeed, in the XY model, in $d \geqq 3$ dimensions one can prove the existence of spontaneous magnetization at low temperatures by means of a Peierls type argument [5]. In order to construct a non-translation invariant state, we try to find boundary conditions which force a line defect through the system, if $d=3$, and a 2-dimensional defect, if $d=4$. As we already mentioned, we expect that the resulting equilibrium state is translation invariant in the thermodynamic limit in three dimensions, due to fluctuations of that line. However, we give a simple argument, suggesting that vortex sheets in four dimensions are rigid and well localized if the temperature is sufficiently low. Therefore we expect that, by forcing a vortex sheet through the system, translation invariance may be broken at low temperatures.

We begin by considering the three-dimensional model, since this case is simpler to visualize. The generalization of our arguments to four or more dimensions is then easy. Let α be the 2-chain on $\bar{\Omega}$ defined by

$$\left.\begin{aligned} \alpha(p) &= 1, \quad \text{if } p^* \text{ is a bond of } \Omega^* \text{ with } x^1 = x^2 = 0 \\ &= 0, \quad \text{otherwise.} \end{aligned}\right\} \tag{4.41}$$

Since $d\alpha = 0$, on $\bar{\Omega}$, we can define $\Delta^{-1}\alpha$; (see Subsect. 4.3). The support of the 2-chain $\Delta^{-1}\alpha$ on $\bar{\Omega}$ contains only plaquettes p, which are orthogonal to the x^3-axis. The restriction of $\Delta^{-1}\alpha$ to the plaquettes p contained in a plane $x^3 = c$ is independent of c. Moreover, if we define a 0-chain ε on

$$\{(x^1, x^2) : x^i \in \mathbb{Z}, |x^i| \leqq L, i = 1, 2\}$$

by

$$\varepsilon(x^1, x^2) = \Delta^{-1}\alpha(p), \tag{4.42}$$

where (x^1, x^2, c) is the center of the plaquette p, then ε is the solution of

$$(-\Delta\varepsilon)(x^1, x^2) = \begin{cases} 1 & \text{if } x^1 = x^2 = 0 \\ 0, & \text{otherwise,} \end{cases} \tag{4.43}$$

where $-\Delta$ is the lattice Laplacian acting on functions defined on the subset introduced above, with Dirichlet boundary conditions. Let

$$\gamma = 2\pi \cdot \delta\Delta^{-1}\alpha. \tag{4.44}$$

By construction we have

$$\delta\gamma = 0 \quad \text{and} \quad d\gamma = 2\pi\alpha. \tag{4.45}$$

Lemma 4.1. *There exists a 0-chain χ on $\bar{\Omega}$ such that*

$$\gamma = d\chi \bmod 2\pi.^3$$

Proof. As for $\Delta^{-1}\alpha$ we verify easily that the support of the 1-chain γ contains only bonds of $\bar{\Omega}$, which are orthogonal to the x^3-axis. Moreover the restriction of γ to the bonds contained in a plane $x^3 = c$ is independent of c. Therefore it is sufficient to prove the lemma for the restriction of γ to such a plane. Let ℓ be the line

3 χ is analogous to the potential of the magnetic field generated by an infinitely long, conducting wire

$$\ell=\{(x^1,x^2,c):x^2=0,x^1\geqq 0\}. \tag{4.46}$$

We set

$$\chi(1/2,1/2,c)=0. \tag{4.47}$$

Let b_1 be the bond with starting point $(1/2,1/2,c)$ and endpoint $(-1/2,1/2,c)$. We define $\chi(-1/2,1/2,c)$ by

$$d\chi(b_1)=\gamma(b_1). \tag{4.48}$$

Let b_2 be the bond with starting point $(-1/2,1/2,c)$ and endpoint $(-1/2,-1/2,c)$. We define $\chi\,(-1/2,-1/2,c)$ by

$$d\chi(b_2)=\gamma(b_2). \tag{4.49}$$

In this way we can define, everywhere on $\bar{\Omega}$, a 0-chain χ, and, in that definition, only bonds are involved which do *not* cross the line ℓ. This is a consequence of Stokes theorem and property (4.45). Using again (4.45) it is immediate that, for each bond b crossing ℓ,

$$d\chi(b)+2\pi=\gamma(b). \quad \square \tag{4.50}$$

We introduce boundary conditions for the Villain model in the box Λ by setting

$$\phi(x)=\chi(x), \qquad x\in\bar{\Omega}, \qquad x\notin\Lambda. \tag{4.51}$$

This boundary condition produces a vortex line crossing the box Λ. To see this, we express Z^ϕ, the corresponding partition function, as in Subsect. 4.4: Z^ϕ is given by

$$\int_0^{2\pi}\dots\int\prod_{b\in\Omega}g_\beta(d\theta(b)), \tag{4.52}$$

where $\Theta(x)=\phi(x)$ if $x\in\bar{\Omega}\backslash\Lambda$. We change variables: We replace $\Theta(y)$ by $\Theta(y)+\chi(y)$, for $y\in\Lambda$. Therefore

$$Z^\phi=\int_0^{2\pi}\dots\int\prod_{b\in\Omega}g_\beta(d\Theta(b)+d\chi(b)). \tag{4.53}$$

Since $g_\beta(\Theta)$ is a *periodic* function we can write, using Lemma 4.1,

$$Z^\phi=\int_0^{2\pi}\dots\int\prod_{b\in\Omega}g_\beta(d\Theta(b)+\gamma(b)), \tag{4.54}$$

where γ is the 1-chain defined by (4.44). This last expression for Z^ϕ coincides with $Z(\gamma)$, as given by (4.19). The generalized partition function, $Z(\gamma)$, has been factorized in a spin wave – and a vortex contribution in (4.36). Since $\delta\gamma=0$, we have

$$(d\phi,\gamma)=(\phi,\delta\gamma)=0. \tag{4.55}$$

We have to compute

$$(\delta\gamma,B^{-1}n), \tag{4.56}$$

with n and γ defined on *.

In (4.56) γ is the dual chain of the 1-chain defined by (4.44) on Ω. Therefore, if $2\pi m \equiv \delta\gamma$ on Ω^*, we get

$$m(p^*) = \alpha(p^*), \tag{4.57}$$

for every $(d-2)$-cell p^* in Ω^* which is *not* on the boundary. If p^* is contained in the boundary of $\Omega^* m(p^*)$ is determined by the values which γ takes on 1-cells $b \in \bar{\Omega} \backslash \Omega$. Moreover we have $\delta m = 0$. We can write the partition function Z^{ϕ} as a product of the partition function $Z^0_{\text{s.w.}}$, (4.37), of the gas of spin waves, with 0-boundary contditions, and the partition function of the vortices, Z^m_v, given by

$$Z^m_v = \sum_{\substack{n: \\ \delta n = 0}} \exp[-\beta 2\pi^2 (n+m, B^{-1}(n+m))]. \tag{4.58}$$

The last equality is obtained by noticing that (4.45) implies $d\gamma = 0$ for the $(d-1)$-chain γ on Ω^*. Therefore there exists a $(d-2)$-chain η on Ω^* such that $d\eta = \gamma$. Since $2\pi m = \delta\gamma$, we have

$$2\pi B^{-1} m = B^{-1}\delta\gamma = B^{-1}\delta d\eta. \tag{4.59}$$

B^{-1} is the inverse of δd on the space of $(d-2)$-chains n *such that* $\delta n = 0$. Therefore $B^{-1}\delta d\eta = \lambda$ with $\delta\lambda = 0$, and $B^{-1}\delta d\eta - \eta$ is in the kernel of B. This means that

$$B^{-1}\delta d\eta - \eta = w, \quad \text{with} \quad dw = 0. \tag{4.60}$$

Therefore we get

$$(2\pi)^2 (m, B^{-1}m) = (\delta\gamma, B^{-1}\delta\gamma) = (\gamma, dB^{-1}\delta d\eta) = (\gamma, d(\eta + w)) = (\gamma, \gamma). \tag{4.61}$$

We have thus proved that the boundary condition ϕ given by (4.51) produces a line defect through the box Λ.

The generalization to the four-dimensional case is easy. On $\bar{\Omega}$ we introduce a 2-chain α such that

$$\begin{aligned} \alpha(p) &= 1, \quad \text{if } p^* \text{ is a plaquette of } \Omega^* \text{ with } x^1 = x^2 = 0 \\ &= 0, \quad \text{otherwise}. \end{aligned} \tag{4.62}$$

Again $d\alpha = 0$ on $\bar{\Omega}$ and we can define $A^{-1}\alpha$. The 2-chain $A^{-1}\alpha$ has the same structure as before. We define γ by (4.44) and by construction (4.45) holds. Lemma 4.1 can be proved in exactly the same way. Therefore we define the boundary condition ϕ by (4.51). The computation of Z^{ϕ} is the same as before, and the final result is again given by

$$Z^{\phi} = Z^0_{\text{s.w.}} \cdot Z^m_v, \tag{4.63}$$

where $Z^0_{\text{s.w.}}$ is defined in (4.37) and Z^m_v in (4.58). Thus the boundary condition ϕ produces a two-dimensional defect crossing the box Λ.

At very low temperatures, there are few vortices. The configuration of vortices $m+n$ can be decomposed into connected components. If m and n are disconnected, then the defect imposed by the boundary condition ϕ is the plane $x^1 = x^2 = 0$ on the dual lattice. But if m and n are not disconnected, this planar defect is slightly deformed. At low temperatures we expect that an approximate description of this defect, like the s-o-s description of the Ising interface, should be qualitatively correct. In such an approximate description, one only considers configurations, n, with the property that the connected component of $m+n$ only takes the values $\pm 1, 0$, and one only permits local deformations without overhang. Using the inequality

$$(n, B^{-1}n) \geqq \frac{1}{2d}(n, n) \tag{4.64}$$

and an explicit calculation, one may show by a standard energy-entropy argument, that these deformations can deform the vortex sheet in the $x^1 = x^2 = 0$ plane only *locally* and that the defect is therefore rigid if the temperature is small enough ($\beta \gg 1$). This is analogous to the proof of the rigidity of the interface in the s-o-s model at low temperature.

4.6. Specific Free Energy of Vortices. The surface tension τ in the Ising model is defined by (2.1). This thermodynamic quantity can be used to distinguish between the low temperature behaviour and the high temperature behaviour of the model. If the temperature T is below the critical temperature, then $\tau > 0$. Otherwise $\tau = 0$. [See (2.2) and (2.3).] Heuristically, the fact that τ is nonzero at low temperatures is a consequence of the Peierls contour, imposed by the $\pm$ boundary conditions, which produces a Bloch wall of finite thickness. It is thus natural to introduce a thermodynamic quantity $\hat{\tau}$ associated with vortices, which are forced into the system by the boundary condition ϕ [see (4.51)]. We define

$$\hat{\tau} = -\frac{1}{\beta} \lim_{L\to\infty} \frac{1}{L^{d-2}\log L} \log \frac{Z_L^\phi}{Z_L^0}. \tag{4.65}$$

Here Z_L^ϕ, respectively Z_L^0, are the partition functions of the system in the box Λ with boundary conditions ϕ, respectively 0. Using (4.38) and (4.58) we get

$$\log \frac{Z_L^\phi}{Z_L^0} \equiv F_L(m) = \log \left(\frac{\sum\limits_{n:\delta n=0} \exp(-\beta 2\pi^2(n+m, B^{-1}(n+m))}{\sum\limits_{n:\delta n=0} \exp(-\beta 2\pi^2(n, B^{-1}n))} \right) \geqq -\beta 2\pi^2(m, B^{-1}m). \tag{4.66}$$

where $2\pi m = \delta\gamma$ and γ is defined by (4.44). Instead of considering the quantity $\hat{\tau}$, we can introduce an analogous quantity $\tilde{\tau}_q$ as follows. Let $\mathscr{L}$ be the $(d-1)$-dimensional box in $\mathbb{L}^*$, given by

$$\mathscr{L} = \{x \in \mathbb{L}^*; |x^i| \leqq L', i = 1, \ldots, d-1, x^d = 0\} \tag{4.67}$$

with $L' < L$. Let $m_L{}'$ be either one of the two $(d-2)$-chains on $\mathbb{L}^*$, such that $\delta m_{L'} = 0$ and

$$\begin{aligned} m_{L'}(c) &= 1, \quad \text{if } c \text{ is a } (d-2)\text{-cell in the boundary of } \mathscr{L}, \\ m_{L'}(c) &= 0, \quad \text{otherwise}. \end{aligned} \tag{4.68}$$

We replace m in (4.66) by $q \cdot m_{L'}$, and we define

$$\tilde{\tau}_q = -\frac{1}{\beta} \lim_{L'\to\infty} \frac{1}{(L')^{d-2}\log L'} \lim_{L\to\infty} F_L(qm_{L'}). \tag{4.69}$$

Both quantities $\tilde{\tau}_q$ and $\hat{\tau}$ have, most likely, the same quantitative behaviour as functions of β. At low temperatures they are nonzero and at high temperatures they vanish. One can therefore use them to distinguish between the low-temperature and the high-temperature regimes of the model in every dimension $d \geqq 2$. (If $d=2$, the boundary of $\mathscr{L}$ consists of two points and the condition $\delta m_{L'}=0$ is replaced by the usual neutrality condition.) Finally we notice that $\tilde{\tau}_q$ is also related to the quantity τ defined by (3.2). (The difference between $\tilde{\tau}_q$ and τ is similar to the difference between the short long-range order and the long long-range order [25].) The next proposition is essentially contained in [26, 3].

Proposition 4.2. *If q is not an integer and for $d \geqq 2$, $\tilde{\tau}_q > 0$ if β is large enough and $\tilde{\tau}_q = 0$ if β is small enough.*

Proof. We define on Ω^*

$$\gamma_{L'} = 2\pi q d B^{-1} m_{L'}. \tag{4.65}$$

Therefore $d\gamma_{L'}=0$ and $\delta\gamma_{L'}=2\pi q m_{L'}$. (If $d=2$ we impose the usual neutrality condition. Then $B^{-1}m_{L'}$ exists.) Using the results of Sect. 4.4, we get

$$\tilde{\tau}_q = -\frac{1}{\beta} \lim_{L'\to\infty} \frac{1}{(L')^2 \log L'} \lim_{L\to\infty} \frac{Z_L(\gamma_{L'})}{Z_L^0}. \tag{4.66}$$

In (4.66), the partition functions are defined on $\bar{\Omega}$, and therefore $\gamma_{L'}$ is a 1-chain on $\bar{\Omega}$, and its support is contained in Ω. In particular

$$Z_L(\gamma_{L'}) = \int_0^{2\pi} \dots \int \prod_{b\in\Omega} g_\beta(d\Theta(b) + \gamma_{L'}(b)). \tag{4.67}$$

We perform a duality transformation. The Fourier series of $g_\beta(\Theta + \gamma_{L'})$ is

$$g_\beta(\Theta + \gamma_{L'}) = \sum_{m\in\mathbb{Z}} \hat{g}_\beta(m) e^{im\Theta} e^{im\gamma_{L'}}, \tag{4.68}$$

with

$$\hat{g}_\beta(m) = \frac{1}{\sqrt{2\pi\beta}} \exp\left(-\frac{m^2}{2\beta}\right). \tag{4.69}$$

Inserting (4.68) in (4.67) and integrating the variables Θ, we get

$$Z_L(\gamma_{L'}) \propto \sum_{\substack{m \\ \delta m = 0}} \prod_{b\in\Omega} \hat{g}_\beta(m(b)) \exp(i m(b) \gamma_{L'}(b)), \tag{4.70}$$

where we sum over all 1-chains m with supports in Ω. On Ω^* the same quantity is written as

$$Z_L(\gamma_{L'}) \propto \sum_{\substack{m: \\ dm=0}} \exp\left(-\frac{1}{2\beta}(m,m)\right) \exp i(m, \gamma_{L'}), \tag{4.71}$$

where m is now a $(d-1)$-chain. Since $dm=0$, there exists a $\mathbb{Z}$-valued $(d-2)$-chain α on Ω^*, such that

$$m = d\alpha. \tag{4.72}$$

Therefore

$$Z_L(\gamma_{L'}) \propto \sum_{[\alpha]} \exp\left(-\frac{1}{2\beta}(d\alpha, d\alpha)\right) \exp i(\alpha, \delta\gamma_{L'}), \tag{4.73}$$

where $\sum_{[\alpha]}$ ranges over all equivalence classes of $(d-2)$-chains, α, labelled by $d\alpha$, and

$$\frac{Z_L(\gamma_{L'})}{Z_L^0} = \int d\mu_L(\alpha) \exp i(\alpha, \delta\gamma_{L'}), \tag{4.74}$$

where $d\mu_L(\alpha)$ is the probability measure given by

$$(Z_L^0)^{-1} \exp\left[-\frac{1}{2\beta}(d\alpha, d\alpha)\right]. \tag{4.75}$$

(The measure $d\mu_L$ is actually defined on the equivalence classes $[\alpha]$.) In the two-dimensional case, $d=2$, we obtain for $\tilde{\tau}_q$ exactly the fractional charge correlation, since $\delta\gamma_{L'} = 2\pi q m_{L'}$. In this case, the Proposition has been proven in [3]. Thus, let $d \geqq 3$. We modify the probability measure $d\mu_L(\alpha)$ as follows: We multiply the density of $d\mu_L$ by

$$\prod_{p^*}{}' \exp\left[-\frac{M^2}{2}(\alpha(p^*))^2\right], \tag{4.76}$$

where the product in (4.76) is taken over all $(d-2)$-cells of Ω^*, which are *not* perpendicular to the two-dimensional plane $x^1 = \ldots = x^{d-2} = 0$. We normalize this new measure and denote the resulting probability measure by $d\mu_{L,M^2}$. Using inequalities related to ones proven by Park [27], we get

$$\int d\mu_L(\alpha) \exp i(\alpha, \delta\gamma_{L'}) \leqq \int d\mu_{L,M^2}(\alpha) \exp i(\alpha, \delta\gamma_{L'}). \tag{4.77}$$

In the limit $M^2 \to \infty$, the probability measure $d\mu_{L,\infty}$ is concentrated on the $(d-2)$-chains α with $\alpha(p^*) = 0$, if p^* is not perpendicular to the plane $x^1 = \ldots = x^{d-2} = 0$. Therefore the measure factorizes in L^{d-2} independent factors. Each of these measures is concentrated on the $(d-2)$-chains α, the supports of which contain only $(d-2)$-cells p^*, whose centers have *fixed* $(x^1, \ldots, x^{d-2})$-coordinates, and which are of course perpendicular to the plane $x^1 = \ldots = x^{d-2} = 0$. Therefore we have obtained the following lower bound for $\tilde{\tau}_q$:

$$\tilde{\tau}_q(d-\dim) \geqq \tilde{\tau}_q(2-\dim), \tag{4.78}$$

which proves that $\tilde{\tau}_q$ (d-dim) is positive at sufficiently large values of β, by [3].

Using a standard high-temperature expansion one can prove that

$$\frac{Z_L(\gamma_{L'})}{Z_L^0} = \exp O((L')^{d-2}), \tag{4.79}$$

and therefore $\tilde{\tau}_q = 0$, if β is small enough. This proof is carried out conveniently by studying the quotient $Z_L(\gamma_{L'})/Z_L^0$ in the original spin representation (in terms of angular variables). It is then given by a convergent high temperature expansion, for small enough β.

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