Spontaneous breaking of rotational symmetry in the presence of defects

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Abstract

We prove a strong form of spontaneous breaking of rotational symmetry for a simple model of two-dimensional crystals with random defects in thermal equilibrium at low temperature. The defects consist of isolated missing atoms.

1 Introduction

1.1 Motivation

Solid state physics is about crystals. In spite of the tremendous achievements and numerous applications of solid state physics, existence of crystals is mathematically not rigorously understood. In particular, understanding the melting transition from crystals to liquids seems out of reach for mathematicians. The unfortunate situation is illustrated by the following quote from Le Bris and Lions from 2005 [7, Section 6.1]: *"Can one have some mathematical insight on the reason why matter at zero temperature arranges in periodic crystals? This so-called* crystal problem *is a cornerstone of physics. Unfortunately, nothing or almost nothing is known at the theoretical level. [. . .] The mathematical literature is really poor on the subject, whatever the model chosen."* Due to recent work of Theil [11] and Flatley and Theil [3], crystallization at temperature zero is mathematically much better understood by now. However, rigorous results for positive temperature are still scarce.

For a mathematical approach towards crystallization at positive temperature, the breaking of continuous symmetries appears a useful tool for recognizing crystals. There are different approaches to spontaneous symmetry breaking, of which we shall explain

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two. The first approach concerns Gibbs measures in infinite volume. A symmetry group of the local specifications of Gibbs measures is spontaneously broken if there exists a Gibbs measure which is not invariant under all operations in this symmetry group. The second approach concerns the infinite volume limit of finite volume Gibbs measures with boundary conditions. As before, we assume that the local specifications are left invariant by some symmetry group. However the boundary conditions are assumed to violate some of these symmetries. The symmetry group is spontaneously broken if even in the infinite volume limit, the random configuration does not exhibit all the symmetries of the local specifications. Typical examples of such symmetries are internal symmetries like spin flips and spatial translations and rotations. Intuitively speaking, spontaneous symmetry breaking in a particle system may be interpreted as long-range order.

Preservation of translational symmetry is well understood in two dimensions, see for example Richthammer [10]. Among the more recent results on translational symmetry breaking in crystalline systems, we mention Aizenman, Jansen, and Jung [1].

Hardly any mathematical results in realistic models are known in three dimensions. A possible mathematical picture for the melting phenomenon in three dimensions is the following: For low temperature, below the melting point, spatial symmetries like translations and rotations might be spontaneously broken. Above the melting point, the symmetries are preserved (i.e., not spontaneously broken). Proving this picture for any realistic interaction potential is a major challenge for mathematical physics.

For very high temperature, however, we are in a gas phase and the Gibbs measure is therefore unique (Dobrushin uniqueness arguments, e.g. [6]). The mathematical notion of spontaneous breaking of the full translational symmetry group $\mathbb{R}^3$ down to some lattice symmetry is related to the experimental observation of sharp Bragg peaks in X-ray diffraction patterns at low temperatures up to the melting point. Crystallographers even define crystals via the occurrence of such Bragg peaks [9].

Merkl and Rolles [8] prove spontaneous breaking of rotational symmetry for a toy model of a crystal without defects. However, crystals at positive temperature exhibit defects. These can be all kinds of local defects (e.g. missing atoms) and various non-local defects. In this work, we consider a variant of the model from [8] which allows the simplest type of local defects, isolated missing single atoms. Our approach can be generalized in a straightforward way to isolated islands of missing atoms as long as the islands are of bounded size. The model forbids non-local defects like crystal boundaries and dislocation lines by definition. Furthermore, to make the presentation as simple as possible, we work in two dimensions although the methods work as well in higher dimensions. Roughly speaking, the higher the dimension, the easier symmetries are spontaneously broken. For this reason, we consider dimension two the most interesting for rotational symmetry breaking. We see the current work as one step towards a better mathematical understanding of rotational symmetry breaking in crystals.

A first step towards more general defects in dimension $d \geq 2$ is recently done by Aumann [2]. Gaál [5] treats the case of hard spheres.

The presence of defects makes a Fourier analysis technique inappropriate for our model. It is replaced by a geometric rigidity result from Friesecke, James, and Müller [4]. On a macroscopic scale, geometric rigidity is well understood. This starts with a result of Liouville. Consider a continuously differentiable map such that the derivative at any point is a rotation. By Liouville's result it is indeed globally a rotation. Friesecke, James, and Müller [4] prove a powerful approximate version of Liouville's result.

1.2 The model

We formulate our results in terms of a random point configuration described by a random function ω defined on the triangular lattice. Values of ω describe either the

location of an atom in the complex plane $\mathbb{C}$ or signalize the absence of an atom. (Quasi-) Periodic boundary conditions are imposed on ω; cf. (1.1). The probability distribution of ω is described by Boltzmann weights in terms of a Hamiltonian coming from rotationally invariant local interactions, which favor the standard configuration, where particles are located on a triangular lattice.

Assumptions. Throughout, we fix

(a) a real-valued potential function V defined in an open interval containing 1. We assume that V is twice continuously differentiable with $V'' > 0$ and $V'(1) = 0$.

(b) $\alpha \in (0, 1)$ sufficiently small, depending on V. (More specifically, α needs to be so small that V is defined on $[1 - \alpha, 1 + \alpha]$ and Corollary 2.4 below holds.)

(c) $l \in (1 - \alpha/2, 1 + \alpha/2)$. This parameter equals the distance of neighboring particles in the standard configuration defined in (1.10) below. Thus, it is a control parameter for the "pressure" of the system.

Let $(\mathcal{A}_2, E)$ denote the triangular lattice, viewed as an undirected graph: $\mathcal{A}_2 = \mathbb{Z} + \tau\mathbb{Z}$ with $\tau = e^{\pi i/3}$ and $E = \{\{x, y\} : x, y \in \mathcal{A}_2, |x - y| = 1\}$; here $|z|$ denotes the Euclidean length of $z \in \mathbb{C}$. We write $x \sim y$ if $\{x, y\} \in E$.

Let $N \in \mathbb{N}$. We define the set $\Omega^*_{l,N}$ of configurations ω with periodic boundary conditions to consist of all $\omega \in (\mathbb{C} \cup \{\circ\})^{\mathcal{A}_2}$ such that

$$\omega(x + Nz) = \omega(x) + lNz \text{ for all } x, z \in \mathcal{A}_2 \text{ with } \omega(x) \neq \circ, \tag{1.1}$$

and $\omega(x + Nz) = \circ$ for $x, z \in \mathcal{A}_2$ with $\omega(x) = \circ$. This condition is sometimes called quasi-periodicity; though this must not be confused with quasicrystals. For $x \in \mathcal{A}_2$, $\omega(x) \in \mathbb{C}$ is interpreted as the location of the particle with index x. If $\omega(x) = \circ$, then there is a *hole* or a *defect* associated with x. Using quasi-periodicity, any $\omega \in \Omega^*_{l,N}$ is uniquely determined by its restriction to the set of representatives

$$I_N := \{x + \tau^2 y : x, y \in \{0, \dots, N - 1\}\} \tag{1.2}$$

of $\mathcal{A}_2/N\mathcal{A}_2$. This allows us to identify $\Omega^*_{l,N}$ with $(\mathbb{C} \cup \{\circ\})^{I_N}$.

Informally speaking, shifts of the index lattice by the box size N may be ignored. Formally, two configurations $\omega, \omega' \in \Omega^*_{l,N}$ are identified if there exists $z \in \mathcal{A}_2$ such that for all $x \in \mathcal{A}_2$ one has $\omega(x) = \omega'(x + Nz)$. Let $\underline{\Omega}_{l,N}$ be the quotient space with respect to the equivalence relation given by this identification. One may identify $\underline{\Omega}_{l,N}$ with a measurable set of representatives $\underline{\Omega}_{l,N} \subset \Omega^*_{l,N}$.

We introduce the set

$$\Lambda_{lN} := [0, lN) + \tau^2[0, lN) \tag{1.3}$$

of representatives for $\mathbb{C}/lN\mathcal{A}_2$. Although the precise choice of the set of representatives for $\underline{\Omega}_{l,N}$ in $\Omega^*_{l,N}$ is irrelevant, a possible choice is $\omega(x) \in \Lambda_{lN}$ for the lexicographically smallest $x \in I_N$ with $\omega(x) \neq \circ$ if ω is not the constant configuration with value $\circ$.

Let

$$\text{defects}(\omega) := \omega^{-1}(\{\circ\}) \cap I_N \tag{1.4}$$

denote the set of defects in the configuration ω. For $x \in I_N$ and $z \in \{1, \tau\}$, let

$$\Delta_{x,z} := \{x + sz + t\tau z : s, t > 0, s + t < 1\} \tag{1.5}$$

denote the open triangle with corner points x, $x + z$, and $x + \tau z$. Let

$$\mathcal{T}_N := \{\Delta_{x,z} : x \in I_N, z \in \{1, \tau\}\} \quad \text{and} \quad \mathcal{T} := \{\Delta_{x,z} : x \in \mathcal{A}_2, z \in \{1, \tau\}\}. \tag{1.6}$$

Note that the closures of the triangles in $\mathcal{T}_N$ cover Λ_{1N}. Let

$$\mathcal{N} := \{\tau^j : j \in \mathbb{Z}\} \tag{1.7}$$

denote the set of neighbors of 0 in $\mathcal{A}_2$.

The space $\Omega_{l,N}$ of *allowed* configurations consists of all $\omega \in \underline{\Omega}_{l,N}$ satisfying the following properties (Ω1)–(Ω4):

(Ω1) *Hard-core restriction:* $|\omega(x) - \omega(y)| \in (1 - \alpha, 1 + \alpha)$ for all $x, y \in \mathcal{A}_2$ with $x \sim y$, $\omega(x) \neq \circ$, and $\omega(y) \neq \circ$.

(Ω2) *Defects are isolated:* For all $x, y \in \mathcal{A}_2$, one can have $\omega(x) = \circ$ and $\omega(y) = \circ$ only if $x = y$ or $|x - y| > 2$. This means that nearest and next-nearest neighbors of defects are present.

For $x \in \mathcal{A}_2$, let

$$\hat{\omega}(x) := \begin{cases} \omega(x) & \text{if } \omega(x) \neq \circ, \\ \frac{1}{6} \sum_{z \in \mathcal{N}} \omega(x + z) & \text{if } \omega(x) = \circ. \end{cases} \tag{1.8}$$

Extend $\hat{\omega}$ piecewise affine linearly to a map $\hat{\omega} \colon \mathbb{C} \to \mathbb{C}$ requiring that $\hat{\omega}$ is affine linear on the closure of every triangle in $\mathcal{T}$.

The map $\hat{\omega}$ is onto as can be seen from the following topological fact. Consider a lattice $\Gamma \subset \mathbb{R}^2$ of rank 2. Then, every continuous map $f \colon \mathbb{R}^2 \to \mathbb{R}^2$ with $f(x+y) = f(x)+y$ for all $x \in \mathbb{R}^2$ and $y \in \Gamma$ is onto. Indeed, $f - \mathrm{Id}$ is bounded, and thus the restriction of f to a large circle centered at any given $z \in \mathbb{R}^2$ has winding number 1 around z. Deforming the large circle to a point, it follows that $z \in \mathrm{range}(f)$.

We require:

(Ω3) *Excluded volume:* $\hat{\omega} \colon \mathbb{C} \to \mathbb{C}$ is one-to-one (and thus bijective).

(Ω4) *Orientation preservation:* For all $x \in \mathcal{A}_2$ and all $z \in \mathcal{N}$, one has

$$\mathrm{Im} \left(\frac{\hat{\omega}(x + \tau z) - \hat{\omega}(x)}{\hat{\omega}(x + z) - \hat{\omega}(x)} \right) > 0. \tag{1.9}$$

We remark that we could drop condition (Ω4) because it follows from the other conditions (Ω1)–(Ω3). Since the proof of this fact is more analytic than stochastic and is not needed in the current paper, we skip it. Condition (Ω3) is a very natural physical condition. For sufficiently small α, it is presumably possible to skip also this condition. Thus (Ω1) and (Ω2) are the relevant restrictions for our analysis while (Ω3) and (Ω4) are technically convenient.

Note that the *standard configuration*

$$\omega_l \colon \mathcal{A}_2 \to \mathbb{C}, v \mapsto lv \tag{1.10}$$

is an allowed configuration. Thus, $\Omega_{l,N} \neq \emptyset$.

Let $m \in \mathbb{R}$; m has the interpretation of a *chemical potential*. It parametrizes the energetic cost of a defect. Define the Hamiltonian

$$H_{m,N}(\omega) := \frac{1}{2} \sum_{x \in I_N} \sum_{y \in \mathcal{A}_2 : y \sim x} 1_{\{\omega(x) \neq \circ, \omega(y) \neq \circ\}} V(|\omega(x) - \omega(y)|) + m \sum_{x \in I_N} 1_{\{\omega(x) = \circ\}} \tag{1.11}$$
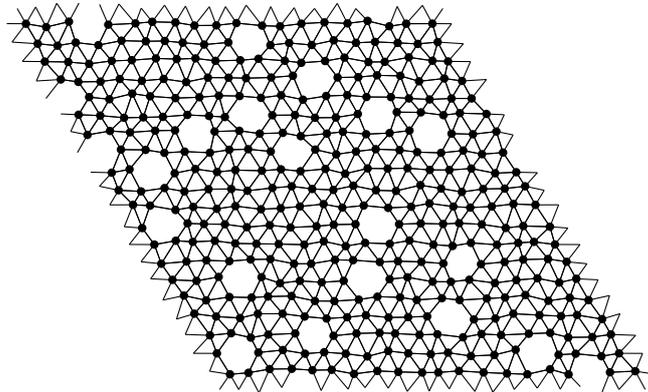
Figure 1: An illustration of an allowed configuration on I_N.

for $\omega \in \Omega_{l,N}$.

Let λ denote the Lebesgue measure on $\mathbb{C}$. We endow $(\mathbb{C} \cup \{\circ\})^{I_N}$ with the reference measure $(\lambda + \delta_{\circ})^{I_N}$. This yields a reference measure on $\Omega_{l,N}^*$. Restricting this reference measure to $\underline{\Omega}_{l,N}$ and using the above identification, this defines in turn a reference measure μ_N on $\underline{\Omega}_{l,N}$. Note that $\mu_N(\Omega_{l,N}) < \infty$ as a consequence of $(\Omega 1)$.

For $\beta > 0$, we define the Boltzmann measure $P_{\beta,m,N}$ on $\Omega_{l,N}$ by

$$P_{\beta,m,N}(d\omega) := \frac{1}{Z_{\beta,m,N}} e^{-\beta H_{m,N}(\omega)} \mu_N(d\omega) \tag{1.12}$$

with partition sum

$$Z_{\beta,m,N} := \int_{\Omega_{l,N}} e^{-\beta H_{m,N}(\omega)} \mu_N(d\omega). \tag{1.13}$$

Clearly, $P_{\beta,m,N}$ and $Z_{\beta,m,N}$ depend also on α, l, and V. Usually, we suppress these parameters in the notation. Since V is bounded on $[1 - \alpha, 1 + \alpha]$ and $\mu_N(\Omega_{l,N}) < \infty$, it follows that $Z_{\beta,m,N} < \infty$. Lemma 3.1 below shows that $Z_{\beta,m,N} > 0$ holds as well.

1.3 Results

We remark that under the assumptions stated at the beginning of Section 1.2, for all $\beta > 0$, $m \in \mathbb{R}$, $N \in \mathbb{N}$ with $N \geq 4$, $x \in \mathcal{A}_2$, and $z \in \mathcal{N}$, one has

$$E_{P_{\beta,m,N}}[\hat{\omega}(x + z) - \hat{\omega}(x)] = lz. \tag{1.14}$$

This follows from (1.1) together with the translational invariance of $P_{\beta,m,N}$. In particular, under $P_{\beta,m,N}$, the distribution of $\hat{\omega}(x + z) - \hat{\omega}(x)$ is not rotationally invariant. Note that $|\hat{\omega}(x + z) - \hat{\omega}(x)|$ is bounded uniformly in N, and thus, equation (1.14) remains true when one takes subsequential weak limits as $N \to \infty$. As a consequence, any infinite volume Gibbs measure obtained as such a subsequential limit is not rotationally invariant. However, this soft result contains no quantitative information on the long-range order. In particular, it does not answer how close directions between neighboring particles are to the corresponding directions in the standard triangular lattice.

Therefore, we prove a much stronger form of breaking of rotational symmetry. For sufficiently low temperature and for sufficiently large chemical potential m, uniformly in

the system size N, the directions between neighboring particles are typically arbitrarily close to the corresponding directions in the standard triangular lattice. In this sense, we have strong long-range directional order for low temperature.

Theorem 1.1. *Under the assumptions stated at the beginning of Section 1.2, there is a constant $m_0 = m_0(V)$, such that the following holds:*

$$\lim_{\beta \to \infty} \sup_{N \geq 4} \sup_{m \geq m_0} \sup_{x \in \mathcal{A}_2} \sup_{z \in \mathcal{N}} E_{P_{\beta,m,N}}[|\hat{\omega}(x + z) - \hat{\omega}(x) - lz|^2] = 0. \tag{1.15}$$

Corollary 1.2. *Under the assumptions of Theorem 1.1,*

$$\lim_{\beta \to \infty} \sup_{N \geq 4} \sup_{m \geq m_0} \sup_{x \in \mathcal{A}_2} \sup_{z \in \mathcal{N}} E_{P_{\beta,m,N}}[|\omega(x + z) - \omega(x) - lz|^2 1_{\{\omega(x+z) \neq \bigcirc, \omega(x) \neq \bigcirc\}}] = 0. \tag{1.16}$$

A technically more convenient though equivalent way to express (1.15) is the following theorem. For every triangle $\Delta \in \mathcal{T}$, $\hat{\omega}$ is affine linear on Δ. Hence, its Jacobian $\nabla \hat{\omega}$ is constant on Δ; we denote by $\nabla \hat{\omega}(\Delta)$ this constant value.

Theorem 1.3. *Under the assumptions of Theorem 1.1,*

$$\lim_{\beta \to \infty} \sup_{N \geq 4} \sup_{m \geq m_0} \sup_{\Delta \in \mathcal{T}_N} E_{P_{\beta,m,N}}[|\nabla \hat{\omega}(\Delta) - l\mathrm{Id}|^2] = 0. \tag{1.17}$$

The excluded cases $N < 4$ are somehow uninteresting and pathological; cf. Figure 2.

Finally, a remark on infinite volume limits. Since the above results are uniform in the size N of the underlying lattice, the finite-volume results carry over to infinite-volume Gibbs measures obtained as subsequential limits as $N \to \infty$.

Organization. In our proof of these results, we proceed as follows. In Section 2, we compare the Hamiltonian of a configuration $\omega \in \Omega_{l,N}$ with the Hamiltonian of the *standard configuration* ω_l. Subsequently, in Section 3, we use these estimates to bound the partition sum from below and the internal energy from above. Our proofs rely crucially on the following rigidity estimate. We use it both locally (in Lemma 2.6), and globally (in Lemma 3.2).

Theorem 1.4 (Friesecke, James, and Müller [4, Theorem 3.1]). *Let U be a bounded Lipschitz domain in $\mathbb{R}^n$, $n \geq 2$. There exists a constant $C(U)$ with the following property: For each $v \in W^{1,2}(U, \mathbb{R}^n)$ there is an associated rotation $R \in \mathrm{SO}(n)$ such that*

$$\|\nabla v - R\|_{L^2(U)} \leq C(U)\|\mathrm{dist}(\nabla v, \mathrm{SO}(n))\|_{L^2(U)}. \tag{1.18}$$

We are interested in bounded domains $U \subset \mathbb{R}^2$ which are bounded by finitely many pieces of straight lines and in continuous functions $v \colon U \to \mathbb{R}^2$ that are piecewise affine linear with respect to a triangulation of U. Note that these functions belong to $W^{1,2}(U, \mathbb{R}^2)$.

Remark 1.5. The constant $C(U)$ in Theorem 1.4 is invariant under scaling: $C(\gamma U) = C(U)$ for all $\gamma > 0$. Indeed, setting $v_\gamma(\gamma x) = \gamma v(x)$ for $x \in U$, we have $\nabla v_\gamma(\gamma x) = \nabla v(x)$ and hence $\|\nabla v_\gamma - R\|_{L^2(\gamma U)} = \gamma^{n/2}\|\nabla v - R\|_{L^2(U)}$ and $\|\mathrm{dist}(\nabla v_\gamma, \mathrm{SO}(n))\|_{L^2(\gamma U)} = \gamma^{n/2}\|\mathrm{dist}(\nabla v, \mathrm{SO}(n))\|_{L^2(U)}$. This implies that for the interior U_N of Λ_{1N}, one can choose the constant $C(U_N)$ in Theorem 1.4 as a constant c_1 independent of N.

2 An estimate for the Hamiltonian

We identify $\mathbb{C}$ with $\mathbb{R}^2$. In this section, we prove the following.

Lemma 2.1. *There exist constants $c_2 = c_2(V) > 0$ and $m_1 = m_1(V) > 0$ such that for all $N \geq 4$ and $\omega \in \Omega_{l,N}$, one has*

$$H_{m,N}(\omega) - H_{m,N}(\omega_l) \geq c_2 \sum_{\Delta \in \mathcal{T}_N} \text{dist}(l^{-1}\nabla\hat{\omega}(\Delta), \text{SO}(2))^2 + (m - m_1)|\,\text{defects}(\omega)|. \quad (2.1)$$

In particular, for $m \geq m_1$, one has $H_{m,N}(\omega) \geq H_{m,N}(\omega_l)$ for all $\omega \in \Omega_{l,N}$.

In this sense, ω_l is a ground state for the Hamiltonian. A key ingredient for the proof is the fact that deforming all triangles does not change the total area covered, cf. (2.30), where we use (Ω3).

Here and in the rest of the paper, the distance is taken with respect to an arbitrary norm $\|\cdot\|$ on 2×2-matrices (except for Lemma 3.2, where the Frobenius norm is convenient).

First, we estimate the contribution of the Hamiltonian for single triangles. Then, we show that the defects are negligible.

2.1 Estimates for individual triangles

Let Δ be a triangle in $\mathbb{R}^2$ with corner points A_1, A_2, A_3, i.e. the interior of the convex hull of $\{A_1, A_2, A_3\}$. Let further $\omega \colon \mathbb{R}^2 \to \mathbb{R}^2$ be the affine linear map that maps $0, 1, \tau$ to A_1, A_2, A_3, respectively. We assume that (A_1, A_2, A_3) is positively oriented, i.e. $\det \nabla\omega > 0$. We introduce the sides of the triangle:

$$\begin{aligned}
\vec{a}_1 &:= A_3 - A_2, \qquad \vec{a}_2 := A_1 - A_3, \qquad \vec{a}_3 := A_2 - A_1, \\
a_j &:= |\vec{a}_j|.
\end{aligned} \quad (2.2)$$

Recall from (1.5) that $l\Delta_{0,1}$ is an equilateral triangle with side length l.

Throughout, we write $T \asymp S$ for terms $T \geq 0$ and $S \geq 0$ if there are uniform constants $c, C > 0$ such that $cT \leq S \leq CT$ holds. If the constants depend on the fixed potential V, we write $T \asymp_V S$.

Lemma 2.2. *Let $p(l) := 2\sqrt{3}V'(l)/l$. For sufficiently small $\alpha > 0$ and side lengths $a_1, a_2, a_3 \in (1 - \alpha, 1 + \alpha)$, one has*

$$\sum_{j=1}^{3} V(a_j) - 3V(l) - p(l)(\lambda(\Delta) - \lambda(l\Delta_{0,1})) \asymp_V \sum_{j=1}^{3}(a_j - l)^2. \quad (2.3)$$

Proof. Heron's formula gives the area of the triangle Δ with side length a_1, a_2, and a_3 as

$$\begin{aligned}
\lambda(\Delta) &= \frac{1}{4}\sqrt{(a_1 + a_2 - a_3)(a_2 + a_3 - a_1)(a_3 + a_1 - a_2)(a_1 + a_2 + a_3)} \\
&=: A(a_1, a_2, a_3).
\end{aligned} \quad (2.4)$$

The function A is twice continuously differentiable with

$$\frac{\partial A}{\partial a_j}(l, l, l) = \frac{l}{2\sqrt{3}} \quad \text{for } j \in \{1, 2, 3\}. \quad (2.5)$$

All second derivatives of $A(a_1, a_2, a_3)$ are bounded for $a_1, a_2, a_3 \in (1 - \alpha, 1 + \alpha)$, with $\alpha > 0$ small enough. Consequently,

$$\lambda(\Delta) - \lambda(l\Delta_{0,1}) = \frac{l}{2\sqrt{3}}\Big(\sum_{j=1}^{3} a_j - 3l\Big) + \sum_{j=1}^{3} O((a_j - l)^2) \quad \text{as } a_j \to l. \quad (2.6)$$

Since V is twice differentiable, we get using the last equation

$$\sum_{j=1}^{3} V(a_j) - 3V(l) = V'(l)\Big(\sum_{j=1}^{3} a_j - 3l\Big) + \frac{1}{2}V''(l)\sum_{j=1}^{3}(a_j - l)^2 + \sum_{j=1}^{3} o_V((a_j - l)^2)$$

$$= \frac{2\sqrt{3}V'(l)}{l}(\lambda(\Delta) - \lambda(l\Delta_{0,1})) + V'(l)\sum_{j=1}^{3} O((a_j - l)^2)$$

$$+ \frac{1}{2}V''(l)\sum_{j=1}^{3}(a_j - l)^2 + \sum_{j=1}^{3} o_V((a_j - l)^2) \quad \text{as } a_j \to l. \tag{2.7}$$

By assumption, $\inf_{1-\frac{\alpha}{2}\leq l\leq 1+\frac{\alpha}{2}} V''(l) > 0$. Clearly $V'(1) = 0$ implies

$$\sup_{1-\frac{\alpha}{2}\leq l\leq 1+\frac{\alpha}{2}} |V'(l)| \leq \frac{\alpha}{2} \sup_{1-\frac{\alpha}{2}\leq \xi\leq 1+\frac{\alpha}{2}} |V''(\xi)| = O_V(\alpha).$$

The claim follows for α small enough. $\qquad\square$

Lemma 2.3. *For sufficiently small $\tilde{\alpha} > 0$ and side lengths $a_1, a_2, a_3 \in (1 - \tilde{\alpha}, 1 + \tilde{\alpha})$, one has*

$$\sum_{j=1}^{3}(a_j - 1)^2 \asymp \text{dist}(\nabla\omega, \text{SO}(2))^2 \tag{2.8}$$

with ω defined before (2.2).

Proof. Let $E_1 = 0$, $E_2 = 1$, $E_3 = \tau$ denote the corner points of the standard equilateral triangle. Set $M := \nabla\omega$; M is constant since ω is affine linear. Consequently, for any cyclic permutation (i, j, k) of $(1, 2, 3)$, one has

$$a_i = |\omega(E_j) - \omega(E_k)| = |M(E_j - E_k)| = |Mv_i|, \tag{2.9}$$

where we set $v_i := E_j - E_k$. Clearly, $|v_i| = 1$. Now $a_i - 1 \asymp (a_i - 1)(a_i + 1) = a_i^2 - 1$ because $a_i \in (1 - \tilde{\alpha}, 1 + \tilde{\alpha})$ and $\tilde{\alpha}$ is small enough. Using (2.9), we obtain

$$a_i - 1 \asymp a_i^2 - 1 = \langle v_i, M^*Mv_i \rangle - |v_i|^2 = \langle v_i, (M^*M - \text{Id})v_i \rangle. \tag{2.10}$$

For $Q \in \mathbb{R}^{2\times 2}_{\text{sym}}$, the set of symmetric 2×2 matrices, set $\|Q\|_v := (\sum_{j=1}^{3}\langle v_j, Qv_j \rangle^2)^{1/2}$. Clearly, $\|\cdot\|_v$ is a seminorm on $\mathbb{R}^{2\times 2}_{\text{sym}}$. To see that it is a norm, assume that $\|Q\|_v = 0$, i.e. $\langle v_j, Qv_j \rangle = 0$ for $j = 1, 2, 3$. Using $v_1 + v_2 + v_3 = 0$ and the symmetry of Q, it follows that $\langle v_j, Qv_k \rangle = 0$ for all $j, k \in \{1, 2, 3\}$. Since v_1, v_2, v_3 span $\mathbb{R}^2$, we conclude $Q = 0$. Since all norms on $\mathbb{R}^{2\times 2}_{\text{sym}}$ are equivalent, we have shown

$$\sum_{j=1}^{3}(a_j - 1)^2 \asymp \|M^*M - \text{Id}\|^2 \tag{2.11}$$

for any norm $\|\cdot\|$.

We use now the following fact: Assume that S is a compact submanifold of $\mathbb{R}^d$, given as a set of zeros

$$S = \{x \in U : f(x) = 0\} \tag{2.12}$$

for some open set $U \subseteq \mathbb{R}^d$ and some smooth function $f \colon U \to \mathbb{R}^m$, $m \leq d$. Assume further that ∇f has rank m on S. Then, there is a neighborhood $U' \subseteq U$ of S such that for all $x \in U'$,

$$\text{dist}(x, S) \asymp \|f(x)\|. \tag{2.13}$$

We apply this fact to $S = SO(2)$, $U = \{Q \in \mathbb{R}^{2\times 2} : \det Q > 0\}$, and $f : U \to \mathbb{R}^{2\times 2}_{\mathrm{sym}}$, $f(Q) = Q^*Q - \mathrm{Id}$; its derivative has full rank on S. For $\tilde{\alpha} > 0$ sufficiently small and $|a_j - 1| < \tilde{\alpha}$, $j = 1, 2, 3$, $M = \nabla\omega$ is close to $SO(2)$; recall that $\det M = \det \nabla\omega > 0$ by our assumption on ω. Consequently,

$$\|M^*M - \mathrm{Id}\| \asymp \mathrm{dist}(M, SO(2)). \tag{2.14}$$

Together with (2.11), this implies the claim. □

Combining Lemmas 2.2 and 2.3 and scaling with l, which is close to 1, yields the following.

Corollary 2.4. *For sufficiently small $\alpha > 0$ and side lengths $a_1, a_2, a_3 \in (1 - \alpha, 1 + \alpha)$, and $1 - \alpha/2 < l < 1 + \alpha/2$, one has*

$$\sum_{j=1}^{3} V(a_j) - 3V(l) - p(l)(\lambda(\Delta) - \lambda(l\Delta_{0,1})) \asymp_V \mathrm{dist}(l^{-1}\nabla\omega, SO(2))^2 \tag{2.15}$$

with ω defined before (2.2).

2.2 Contributions from defects

Definition 2.5. *For $x \in \mathcal{A}_2$, let $U_0(x) := \{\Delta \in \mathcal{T} : x \in \mathrm{closure}(\Delta)\}$ denote the set of all triangles in $\mathcal{T}$ incident to x. Let*

$$U_1(x) := \{\Delta \in \mathcal{T} : \text{ all corner points of } \Delta \text{ are contained in } x + \mathcal{N} + \mathcal{N}\} \setminus U_0(x) \tag{2.16}$$

denote the "second layer" of triangles around x. In the special case $x = 0$, we abbreviate $U_0 := U_0(0)$ and $U_1 := U_1(0)$ (see Figure 2).
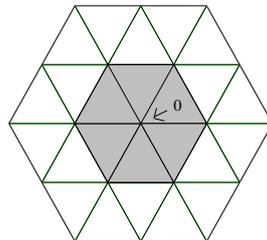
Figure 2: The gray area illustrates U_0 and the white area U_1 for $N \geq 4$. For $N < 4$, which is excluded, some of the triangles would coincide.

Lemma 2.6. *There exists a constant $c_3 > 0$ such that for all $N \geq 4$ and $\omega \in \Omega_{l,N}$ with $\omega(0) = \bigcirc$, one has*

$$\sum_{\Delta \in U_0} \mathrm{dist}(\nabla\hat{\omega}(\Delta), SO(2))^2 \leq c_3 \sum_{\Delta \in U_1} \mathrm{dist}(\nabla\hat{\omega}(\Delta), SO(2))^2. \tag{2.17}$$

Proof. We apply the theorem by Friesecke et al. (Theorem 1.4) to the interior U of $\bigcup_{\Delta \in U_1} \mathrm{closure}(\Delta)$, using

$$\lambda(\Delta_{0,1}) \sum_{\Delta \in U_1} \mathrm{dist}(\nabla\hat{\omega}(\Delta), SO(2))^2 = \|\mathrm{dist}(\nabla\hat{\omega}, SO(2))\|^2_{L^2(U)}. \tag{2.18}$$

Hence there exists a rotation $R \in SO(2)$ with

$$\sum_{\Delta \in U_1} \|\nabla\hat{\omega}(\Delta) - R\|^2 \leq C(U) \sum_{\Delta \in U_1} \mathrm{dist}(\nabla\hat{\omega}(\Delta), SO(2))^2. \tag{2.19}$$

We introduce the piecewise affine linear map $\sigma \colon \operatorname{conv hull}(\mathcal{N} + \mathcal{N}) \to \mathbb{R}^2$, $\sigma(x) = \hat{\omega}(x) - \hat{\omega}(0) - Rx$. The map σ belongs to the finite-dimensional vector space W of all continuous piecewise affine linear maps $\sigma' \colon \operatorname{conv hull}(\mathcal{N} + \mathcal{N}) \to \mathbb{R}^2$ which are affine linear on the closure of every Δ and satisfy $\sigma'(0) = 0 = \frac{1}{6}\sum_{\tau \in \mathcal{N}} \sigma'(\tau)$. By definition of σ, one has

$$\sum_{\Delta \in U_1} \|\nabla \hat{\omega}(\Delta) - R\|^2 = \sum_{\Delta \in U_1} \|\nabla \sigma(\Delta)\|^2. \tag{2.20}$$

If $Q(\sigma') := \sum_{\Delta \in U_1} \|\nabla \sigma'(\Delta)\|^2 = 0$ for some $\sigma' \in W$, then $\sigma' = 0$. Indeed, we obtain first that σ' is constant on all triangles in U_1. The value $\sigma'(0) = 0$ is the average of this constant; hence the constant vanishes. Consequently, the quadratic form $Q \colon W \to \mathbb{R}$ is positive definite. Since W is finite-dimensional, any quadratic form on W is bounded from above by a constant multiple of Q. In particular, for some constant $c_4 > 0$ and any $\sigma' \in W$,

$$\sum_{\Delta \in U_0} \|\nabla \sigma'(\Delta)\|^2 \leq c_4 \sum_{\Delta \in U_1} \|\nabla \sigma'(\Delta)\|^2. \tag{2.21}$$

For the special case $\sigma' = \sigma$ this yields

$$\sum_{\Delta \in U_0} \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2 \leq \sum_{\Delta \in U_0} \|\nabla \hat{\omega}(\Delta) - R\|^2 = \sum_{\Delta \in U_0} \|\nabla \sigma(\Delta)\|^2$$

$$\leq c_4 \sum_{\Delta \in U_1} \|\nabla \sigma(\Delta)\|^2 \leq c_4 C(U) \sum_{\Delta \in U_1} \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2. \tag{2.22}$$

$\square$

We call the triangle $\Delta_{x,z} \in \mathcal{T}_N$ *present* in the configuration $\omega \in \Omega_{l,N}$ if $\omega(x) \neq \circ$, $\omega(x + z) \neq \circ$, and $\omega(x + \tau z) \neq \circ$. Let

$$\mathcal{T}_N^{\operatorname{pres}}(\omega) := \{\Delta \in \mathcal{T}_N : \Delta \text{ is present in } \omega\}. \tag{2.23}$$

If there is a defect at x, then by assumption $(\Omega 2)$, all triangles in the second layer $U_1(x)$ are present.

Lemma 2.7. *For all $N \geq 4$ and $\omega \in \Omega_{l,N}$, one has*

$$\sum_{\Delta \in \mathcal{T}_N} \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2 \asymp \sum_{\Delta \in \mathcal{T}_N^{\operatorname{pres}}(\omega)} \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2, \tag{2.24}$$

where the constants for $\asymp$ can be chosen independently of ω.

Proof. The bound "$\geq$" holds trivially. For the upper bound, we proceed by splitting the sum as follows

$$\sum_{\Delta \in \mathcal{T}_N} \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2 = \sum_{\Delta \in \mathcal{T}_N^{\operatorname{pres}}(\omega)} \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2$$

$$+ \sum_{x \in \operatorname{defects}(\omega)} \sum_{\Delta \in U_0(x)} \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2. \tag{2.25}$$

By Lemma 2.6,

$$\sum_{x \in \operatorname{defects}(\omega)} \sum_{\Delta \in U_0(x)} \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2 \leq c_3 \sum_{x \in \operatorname{defects}(\omega)} \sum_{\Delta \in U_1(x)} \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2$$

$$= c_3 \sum_{\Delta \in \mathcal{T}_N^{\operatorname{pres}}(\omega)} \sum_{x \in \operatorname{defects}(\omega)} 1_{U_1(x)}(\Delta) \operatorname{dist}(\nabla \hat{\omega}(\Delta), \operatorname{SO}(2))^2. \tag{2.26}$$

Now, $\sum_{x \in \operatorname{defects}(\omega)} 1_{U_1(x)}(\Delta) \leq 9$ for all $\omega \in \Omega_{l,N}$ and $\Delta \in \mathcal{T}_N$. The claim follows. $\square$

2.3 Proof of Lemma 2.1

Let $\omega \in \Omega_{l,N}$. For $x \in I_N$ and $y \in \mathcal{A}_2$ with $x \sim y$, $\omega(x) \neq \circ$ and $\omega(y) \neq \circ$, we call the undirected edge $\{x, y\}$

- a *boundary edge* with respect to ω if there exists $z \in \mathcal{A}_2$ with $z \sim x$, $z \sim y$, and $\omega(z) = \circ$;
- an *inner edge* with respect to ω otherwise.

We denote the set of boundary and inner edges with respect to ω by $\partial E_N(\omega)$ and $E_N^\circ(\omega)$, respectively.

Proof of Lemma 2.1. For all $x \in I_N$ and $y \in I_{N+1}$ with $x \sim y$, one has $|\omega_l(x) - \omega_l(y)| = l$ for the standard configuration ω_l. Thus, any edge $\{x, y\}$ contributes the amount $V(l)$ to $H_{m,N}(\omega_l)$.

Let $\omega \in \Omega_{l,N}$. For $\Delta \in \mathcal{T}_N^{\mathrm{pres}}(\omega)$, let $a_j(\Delta)$, $j = 1, 2, 3$, denote the side lengths of the triangle $\hat{\omega}(\Delta)$. For any $x \in I_N$ with $\omega(x) = \circ$, there are 6 edges incident to x which are neither boundary edges nor inner edges with respect to ω. Consequently, we obtain

$$
\begin{aligned}
&H_{m,N}(\omega) - H_{m,N}(\omega_l) + (6V(l) - m)|\operatorname{defects}(\omega)| \\
&= \sum_{\{x,y\} \in \partial E_N(\omega) \cup E_N^\circ(\omega)} [V(|\omega(x) - \omega(y)|) - V(l)] \\
&= \frac{1}{2} \sum_{\Delta \in \mathcal{T}_N^{\mathrm{pres}}(\omega)} \left(\sum_{j=1}^{3} V(a_j(\Delta)) - 3V(l) \right) + \frac{1}{2} \sum_{\{x,y\} \in \partial E_N(\omega)} [V(|\omega(x) - \omega(y)|) - V(l)]. \quad (2.27)
\end{aligned}
$$

For the last equation, note that the first term counts only half of the contribution from boundary edges, although their contribution needs to be fully counted.

Since $|V|$ is bounded on $(1 - \alpha, 1 + \alpha)$ by some constant $c_5(V)$, we get the following estimate for the last sum in (2.27):

$$
\sum_{\{x,y\} \in \partial E_N(\omega)} [V(|\omega(x) - \omega(y)|) - V(l)] \geq -2c_5(V)|\partial E_N(\omega)|
$$

$$
= -12c_5(V)|\operatorname{defects}(\omega)|. \quad (2.28)
$$

We now estimate the first sum on the right hand side of (2.27). By (Ω1), one has $a_j(\Delta) \in (1 - \alpha, 1 + \alpha)$ and, by (Ω4), $\det \nabla \hat{\omega}(\Delta) > 0$ for all $\Delta \in \mathcal{T}_N^{\mathrm{pres}}(\omega)$. Thus, Corollary 2.4 and Lemma 2.7 yield

$$
\begin{aligned}
&\sum_{\Delta \in \mathcal{T}_N^{\mathrm{pres}}(\omega)} \left(\sum_{j=1}^{3} V(a_j(\Delta)) - 3V(l) - p(l)(\lambda(\hat{\omega}(\Delta)) - \lambda(l\Delta_{0,1})) \right) \\
&\asymp_V \sum_{\Delta \in \mathcal{T}_N^{\mathrm{pres}}(\omega)} \operatorname{dist}(l^{-1} \nabla \hat{\omega}(\Delta), \mathrm{SO}(2))^2 \\
&\asymp_V \sum_{\Delta \in \mathcal{T}_N} \operatorname{dist}(l^{-1} \nabla \hat{\omega}(\Delta), \mathrm{SO}(2))^2. \quad (2.29)
\end{aligned}
$$

Note that by (Ω3) and periodicity (1.1), $\hat{\omega}$ maps any measurable set of representatives of $\mathbb{C}$ modulo $N\mathcal{A}_2$ onto a set having the Lebesgue measure $\lambda(\Lambda_{lN})$. Consequently,

$$
\sum_{\Delta \in \mathcal{T}_N} (\lambda(\hat{\omega}(\Delta)) - \lambda(l\Delta_{0,1})) = \lambda(\Lambda_{lN}) - \lambda(l\Lambda_{1N}) = 0. \quad (2.30)
$$

Hence, since for $x \in \operatorname{defects}(\omega)$ the area of the image of the hexagon $U_0(x)$ under $\hat{\omega}$ is uniformly bounded by $(\Omega 1)$ and $(\Omega 2)$, we find

$$\left| \sum_{\Delta \in \mathcal{T}_N^{\mathrm{pres}}(\omega)} (\lambda(\hat{\omega}(\Delta)) - \lambda(l\Delta_{0,1})) \right| = \left| \sum_{\Delta \in \mathcal{T}_N \setminus \mathcal{T}_N^{\mathrm{pres}}(\omega)} (\lambda(\hat{\omega}(\Delta)) - \lambda(l\Delta_{0,1})) \right|$$
$$\leq c_6 | \operatorname{defects}(\omega)| \tag{2.31}$$

with a uniform constant $c_6 > 0$. Combining this with (2.29), we obtain

$$\sum_{\Delta \in \mathcal{T}_N^{\mathrm{pres}}(\omega)} \Big(\sum_{j=1}^{3} V(a_j(\Delta)) - 3V(l) \Big)$$
$$\geq c_7 \sum_{\Delta \in \mathcal{T}_N} \operatorname{dist}(l^{-1}\nabla\hat{\omega}(\Delta), \mathrm{SO}(2))^2 - c_6 |p(l)| \cdot | \operatorname{defects}(\omega)| \tag{2.32}$$

with a constant $c_7 > 0$.

Note that $p(l) = 2\sqrt{3}V'(l)/l$ as defined in Lemma 2.2 is bounded for $l \in (1 - \alpha/2, 1 + \alpha/2)$. Combining (2.27), (2.28), and (2.32) yields the claim. $\qquad\square$

3 Uniform finite-volume estimates

3.1 Lower bound for the partition sum

Lemma 3.1. *For all $\varepsilon > 0$, there exists $r = r(\varepsilon) > 0$ such that for all $\beta > 0$, m, N, one has*

$$Z_{\beta,m,N} \geq \frac{\lambda(\Lambda_{lN})}{\pi r^2} e^{-|I_N|(3\beta\varepsilon - \log(\pi r^2))} e^{-\beta H_{m,N}(\omega_l)}. \tag{3.1}$$

Proof. For $r > 0$, we consider the set of configurations which are, up to translations, sufficiently close to the standard configuration and have no defects

$$S_{r,l,N} := \{\omega \in \underline{\Omega}_{l,N} : \omega(x) \neq \circ \text{ and } |\omega(x) - \omega(0) - \omega_l(x)| < r \text{ for all } x \in \mathcal{A}_2\}. \tag{3.2}$$

Let $\varepsilon > 0$. Since V is continuous, for all sufficiently small $r > 0$, for all N, for all $\omega \in S_{r,l,N}$ and all $x, y \in \mathcal{A}_2$ with $x \sim y$, one has $|V(|\omega(x)-\omega(y)|) - V(l)| < \varepsilon$. Consequently, $|H_{m,N}(\omega) - H_{m,N}(\omega_l)| \leq 3|I_N|\varepsilon$ for all $\omega \in S_{r,l,N}$ and we conclude for all $\beta > 0$ that

$$Z_{\beta,m,N} \geq \int_{S_{r,l,N} \cap \Omega_{l,N}} e^{-\beta H_{m,N}(\omega)} \mu_N(d\omega) \geq e^{-3\beta|I_N|\varepsilon} e^{-\beta H_{m,N}(\omega_l)} \mu_N(S_{r,l,N} \cap \Omega_{l,N}). \tag{3.3}$$

We now argue that $S_{r,l,N} \subseteq \Omega_{l,N}$ for sufficiently small $r \in (0, \alpha/4)$. Using $|l - 1| < \alpha/2$, we get for all $\omega \in S_{r,l,N}$ and $x, y \in \mathcal{A}_2$ with $x \sim y$,

$$\big| |\omega(x) - \omega(y)| - 1 \big| \leq \big| |\omega(x) - \omega(y)| - l \big| + |l - 1|$$
$$< \big| |\omega(x) - \omega(y)| - |\omega_l(x) - \omega_l(y)| \big| + \alpha/2$$
$$< 2r + \alpha/2 \leq \alpha. \tag{3.4}$$

Hence, condition $(\Omega 1)$ is satisfied. Condition $(\Omega 2)$ is satisfied by absence of defects in $S_{r,l,N}$.

To see that $\hat{\omega}$ is one-to-one, note that for sufficiently small r and $\omega \in S_{r,l,N}$, the Jacobi matrix $\nabla\hat{\omega}$ is close to l times the identity matrix and hence $\langle v, \nabla\hat{\omega}(x)v \rangle > 0$ for all $v \in \mathbb{R}^2 \setminus \{0\}$ and all $x \in \mathbb{R}^2$ for which $\hat{\omega}$ is differentiable at x. This shows that condition $(\Omega 3)$ is fulfilled.

Condition $(\Omega 4)$ is satisfied for ω_l and translations of it, and consequently also for $\omega \in S_{r,l,N}$ for r sufficiently small. We conclude $S_{r,l,N} \subseteq \Omega_{l,N}$. Thus, $\mu_N(S_{r,l,N}) = (\pi r^2)^{|I_N|-1}\lambda(\Lambda_{lN})$ by the definition of μ_N, since integration over $\omega(x)$ for all $x \neq 0$ given $\omega(0)$ yields the factor πr^2 and integration over $\omega(0)$ yields the volume $\lambda(\Lambda_{lN})$. Consequently, we get the assertion (3.1) of the lemma. $\qquad\square$

3.2 Upper bound for the internal energy

For $\omega \in \Omega_{l,N}$, we abbreviate

$$A_{m,l,N}(\omega) := H_{m,N}(\omega) - H_{m,N}(\omega_l). \tag{3.5}$$

Recall from Remark 1.5 that $U_N = (0,N) + \tau^2(0,N)$.

Lemma 3.2. *There exists a constant $c_8 > 0$ such that for all $\beta > 0$, $m \in \mathbb{R}$, $N \geq 4$, and $\omega \in \Omega_{l,N}$, one has*

$$A_{m,l,N}(\omega) - (m - m_1)|\operatorname{defects}(\omega)| \geq c_8 \|l^{-1}\nabla\hat{\omega} - \operatorname{Id}\|^2_{L^2(U_N)} \tag{3.6}$$

with m_1 the constant from Lemma 2.1.

Proof. For this proof, it is convenient to work with the Frobenius norm on $2 \times 2-$matrices and its corresponding inner product. Recall that all triangles in $\mathcal{T}_N$ have the same Lebesgue measure. Using this and Lemma 2.1, we get

$$\begin{aligned} A_{m,l,N}(\omega) - (m - m_1)|\operatorname{defects}(\omega)| \geq & c_2 \sum_{\Delta \in \mathcal{T}_N} \operatorname{dist}(l^{-1}\nabla\hat{\omega}(\Delta), \operatorname{SO}(2))^2 \\ = & c_2 \lambda(\Delta_{0,1})^{-1} \sum_{\Delta \in \mathcal{T}_N} \lambda(\Delta)\operatorname{dist}(l^{-1}\nabla\hat{\omega}(\Delta), \operatorname{SO}(2))^2 \\ = & c_2 \lambda(\Delta_{0,1})^{-1} \|\operatorname{dist}(l^{-1}\nabla\hat{\omega}, \operatorname{SO}(2))\|^2_{L^2(U_N)}. \end{aligned} \tag{3.7}$$

By Theorem 1.4 and Remark 1.5 there exists a random rotation $R_N(\omega) \in \operatorname{SO}(2)$ such that one has

$$\|\operatorname{dist}(l^{-1}\nabla\hat{\omega}, \operatorname{SO}(2))\|^2_{L^2(U_N)} \geq c_1^{-1}\|l^{-1}\nabla\hat{\omega} - R_N(\omega)\|^2_{L^2(U_N)}. \tag{3.8}$$

Combining (3.7) and (3.8) yields

$$\begin{aligned} A_{m,l,N}(\omega) - (m - m_1)&|\operatorname{defects}(\omega)| \geq c_8\|l^{-1}\nabla\hat{\omega} - R_N(\omega)\|^2_{L^2(U_N)} \\ = c_8 & \left(\|l^{-1}\nabla\hat{\omega} - \operatorname{Id}\|^2_{L^2(U_N)} + 2\langle l^{-1}\nabla\hat{\omega} - \operatorname{Id}, \operatorname{Id} - R_N(\omega)\rangle_{L^2(U_N)} + \|\operatorname{Id} - R_N(\omega)\|^2_{L^2(U_N)} \right) \\ \geq c_8 & \left(\|l^{-1}\nabla\hat{\omega} - \operatorname{Id}\|^2_{L^2(U_N)} + 2\langle l^{-1}\nabla\hat{\omega} - \operatorname{Id}, \operatorname{Id} - R_N(\omega)\rangle_{L^2(U_N)} \right) \end{aligned}$$
$$\tag{3.9}$$

with a constant $c_8 > 0$. We introduce the periodic function $\sigma_\omega(x) := l^{-1}\hat{\omega}(x) - x$ for $x \in \mathbb{C}$. Its derivative equals $\nabla\sigma_\omega = l^{-1}\nabla\hat{\omega} - \operatorname{Id}$. By the fundamental theorem of calculus, derivatives of periodic functions are orthogonal in L^2 to any constant function. Thus, the scalar product on the right-hand side in (3.9) vanishes, and we get the claim. $\square$

Lemma 3.3. *There exists a uniform constant c_9 such that the following holds: For all $\delta > 0$, there exist $c_{10} > 0$ and $c_{11} \in \mathbb{R}$ such that for any $\beta \geq c_9$, $m \geq m_0 := m_1 + 1$ (with m_1 as in Lemma 2.1) and any $N \geq 4$, one has*

$$\frac{1}{|\mathcal{T}_N|}E_{P_{\beta,m,N}}[A_{m,l,N}] \leq \frac{\delta}{2} + c_{10}\exp\left\{ |I_N|\left(-\frac{\beta\delta}{8} - \log\beta + c_{11} \right) \right\}. \tag{3.10}$$

As a consequence,

$$\limsup_{\beta \to \infty}\sup_{N \geq 4}\sup_{m \geq m_0}\frac{1}{|\mathcal{T}_N|}E_{P_{\beta,m,N}}[A_{m,l,N}(\omega)] \leq 0. \tag{3.11}$$

Proof. Let $\delta > 0$. We calculate

$$Z_{\beta,m,N} E_{P_{\beta,m,N}}[A_{m,l,N}(\omega)] = \int_{\Omega_{l,N}} A_{m,l,N}(\omega) e^{-\beta H_{m,N}(\omega)} \mu_N(d\omega)$$

$$= e^{-\beta H_{m,N}(\omega_l)} \int_{\Omega_{l,N}} A_{m,l,N}(\omega) e^{-\beta A_{m,l,N}(\omega)} \mu_N(d\omega). \tag{3.12}$$

Next, we split the domain of integration into

$$\Omega_{l,N}^{>\delta} := \{\omega \in \Omega_{l,N} : A_{m,l,N}(\omega) > \delta|I_N|\} \quad \text{and} \quad \Omega_{l,N}^{\leq\delta} := \Omega_{l,N} \setminus \Omega_{l,N}^{>\delta}. \tag{3.13}$$

For the latter domain, we estimate

$$\int_{\Omega_{l,N}^{\leq\delta}} A_{m,l,N}(\omega) e^{-\beta A_{m,l,N}(\omega)} \mu_N(d\omega) \leq \delta|I_N| Z_{\beta,m,N} e^{\beta H_{m,N}(\omega_l)}$$

$$= \frac{\delta}{2}|\mathcal{T}_N| Z_{\beta,m,N} e^{\beta H_{m,N}(\omega_l)}. \tag{3.14}$$

For the remaining part, we first apply the inequality $xe^{-x} \leq e^{-x/2}$ with $x = \beta A_{m,l,N}$, then we use the exponential Chebyshev inequality. This yields

$$\int_{\Omega_{l,N}^{>\delta}} A_{m,l,N}(\omega) e^{-\beta A_{m,l,N}(\omega)} \mu_N(d\omega) \leq \frac{1}{\beta} \int_{\Omega_{l,N}^{>\delta}} e^{-\beta A_{m,l,N}(\omega)/2} \mu_N(d\omega)$$

$$\leq \frac{1}{\beta} \int_{\Omega_{l,N}} e^{\beta(A_{m,l,N}(\omega) - \delta|I_N|)/4} e^{-\beta A_{m,l,N}(\omega)/2} \mu_N(d\omega)$$

$$= \frac{e^{-\beta\delta|I_N|/4}}{\beta} \int_{\Omega_{l,N}} e^{-\beta A_{m,l,N}(\omega)/4} \mu_N(d\omega). \tag{3.15}$$

Lemma 3.2 implies

$$\int_{\Omega_{l,N}} e^{-\beta A_{m,l,N}(\omega)/4} \mu_N(d\omega)$$

$$\leq \int_{\Omega_{l,N}} \exp\left\{-\beta\frac{c_8}{4}\|l^{-1}\nabla\hat{\omega} - \mathrm{Id}\|_{L^2(U_N)}^2 - \frac{\beta}{4}(m - m_1)|\mathrm{defects}(\omega)|\right\} \mu_N(d\omega). \tag{3.16}$$

We use again the notation $\sigma_\omega(x) := l^{-1}\hat{\omega}(x) - x$ for $x \in \mathbb{C}$:

$$\|l^{-1}\nabla\hat{\omega} - \mathrm{Id}\|_{L^2(U_N)}^2 = \|\nabla\sigma_\omega\|_{L^2(U_N)}^2$$

$$= \sum_{\Delta \in \mathcal{T}_N} \|\nabla\sigma_\omega\|_{L^2(\Delta)}^2 = \lambda(\Delta_{0,1}) \sum_{\Delta \in \mathcal{T}_N} \|\nabla\sigma_\omega(\Delta)\|^2. \tag{3.17}$$

Take an equilateral triangle $\Delta \in \mathcal{T}_N$ with corner points A, B, and C. We claim that

$$\|\nabla\sigma_\omega(\Delta)\|^2 \geq c_{12} \left(\|\sigma_\omega(A) - \sigma_\omega(B)\|^2 + \|\sigma_\omega(B) - \sigma_\omega(C)\|^2 + \|\sigma_\omega(C) - \sigma_\omega(A)\|^2\right) \tag{3.18}$$

with a constant $c_{12} > 0$ not depending on the choice of Δ. Since σ_ω is affine linear on Δ, the claim reduces to showing for any matrix $M \in \mathbb{R}^{2 \times 2}$

$$\|M\|^2 \geq c_{12} \left(\|MA - MB\|^2 + \|MB - MC\|^2 + \|MC - MA\|^2\right). \tag{3.19}$$

Note that translating Δ does not change the claim. Thus, we can reduce the claim further to the special cases $\Delta = \Delta_{0,1}$ and $\Delta = \tau\Delta_{0,1}$. Since both sides in (3.19) are a square of a matrix norm on 2×2-matrices, and all such norms are equivalent, the claim (3.18) follows.

We bound (3.16) further from above using (3.17) and (3.18) to obtain the upper bound

$$\int_{\Omega_{l,N}} \exp\Big\{ -\beta c_{13} \sum_{\substack{x\in I_N,\, y\in\mathcal{A}_2 \\ x\sim y}} \|\sigma_\omega(x) - \sigma_\omega(y)\|^2 - \frac{\beta}{4}(m-m_1)|\operatorname{defects}(\omega)| \Big\} \mu_N(d\omega) \quad (3.20)$$

with a uniform constant $c_{13} > 0$. By partitioning $\Omega_{l,N}$ according to the set $D \subset I_N$ of defects, (3.20) is equal to

$$\sum_{D\subset I_N} e^{-\beta(m-m_1)|D|/4} \int_{\{\operatorname{defects}(\omega)=D\}} \exp\Big\{ -\beta c_{13} \sum_{\substack{x\in I_N,\, y\in\mathcal{A}_2 \\ x\sim y}} \|\sigma_\omega(x) - \sigma_\omega(y)\|^2 \Big\} \mu_N(d\omega).$$
$$(3.21)$$

By $(\Omega 2)$, defects are isolated in I_N. Whence, for each set D of defects, we can choose a spanning tree $\mathcal{S}$ of $I_N \setminus \operatorname{defects}(\omega)$. We bound (3.21) from above by restricting the sum of pairs $x \sim y$ to edges $\{x, y\}$ of $\mathcal{S}$,

$$\int_{\Omega_{l,N}} e^{-\beta A_{m,l,N}(\omega)/4} \mu_N(d\omega)$$
$$\leq \sum_{D\subset I_N} e^{-\beta(m-m_1)|D|/4} \int_{\{\omega\in\Omega_{l,N}:\operatorname{defects}(\omega)=D\}} \exp\Big\{ -\beta c_{13} \sum_{\{x,y\}\in\mathcal{S}} \|\sigma_\omega(x) - \sigma_\omega(y)\|^2 \Big\} \mu_N(d\omega)$$
$$\leq \sum_{D\subset I_N} e^{-\beta(m-m_1)|D|/4} \left(\int_{\mathbb{R}^2} e^{-\beta c_{13} l^{-2}\|u\|^2} \lambda(du) \right)^{|I_N|-|D|-1} \lambda(\Lambda_{lN}), \quad (3.22)$$

where the factor $\lambda(\Lambda_{lN})$ stems from integrating the root of $\mathcal{S}$ over the set of representatives Λ_{lN} of $\mathbb{C}/lN\mathcal{A}_2$; a Gaussian integral arises for each of the $|I_N| - |D| - 1$ edges of $\mathcal{S}$. In the last sum, we allow all subsets D of I_N regardless whether they occur as a set of defects of an allowed configuration. There exists a uniform constant $c_{14} > 0$ such that

$$\int_{\mathbb{R}^2} e^{-\beta c_{13} l^{-2}\|u\|^2} \lambda(du) \leq \frac{c_{14}}{2\beta}, \quad (3.23)$$

and hence

$$\int_{\Omega_{l,N}} e^{-\beta A_{m,l,N}(\omega)/4} \mu_N(d\omega)$$
$$\leq \left(\frac{c_{14}}{2\beta}\right)^{|I_N|-1} \lambda(\Lambda_{lN}) \sum_{D\subset I_N} \exp\Big\{ -\Big(\frac{\beta}{4}(m-m_1) + \log\Big(\frac{c_{14}}{2\beta}\Big)\Big)|D| \Big\}. \quad (3.24)$$

Take a uniform constant c_9 so large that for all $\beta \geq c_9$ and $m \geq m_0 = m_1 + 1$ one has

$$\frac{\beta}{4}(m-m_1) + \log\Big(\frac{c_{14}}{2\beta}\Big) \geq 0. \quad (3.25)$$

For these β and m, we get

$$\sum_{D\subset I_N} \exp\Big\{ -\Big(\frac{\beta}{4}(m-m_1) + \log\Big(\frac{c_{14}}{2\beta}\Big)\Big)|D| \Big\}$$
$$= \Big(1 + \exp\Big\{ -\frac{\beta}{4}(m-m_1) - \log\Big(\frac{c_{14}}{2\beta}\Big) \Big\}\Big)^{|I_N|} \leq 2^{|I_N|}. \quad (3.26)$$

Thus,

$$\int_{\Omega_{l,N}} e^{-\beta A_{m,l,N}(\omega)/4} \mu_N(d\omega) \leq 2\Big(\frac{c_{14}}{\beta}\Big)^{|I_N|-1} \lambda(\Lambda_{lN}). \quad (3.27)$$

We combine (3.12) with (3.14), (3.15), and (3.27) to obtain

$$E_{P_{\beta,m,N}}[A_{m,l,N}(\omega)] \leq \frac{\delta}{2}|\mathcal{T}_N| + \frac{2}{c_{14}} \frac{e^{-\beta\delta|I_N|/4}}{Z_{\beta,m,N}} \left(\frac{c_{14}}{\beta}\right)^{|I_N|} \lambda(\Lambda_{lN})e^{-\beta H_{m,N}(\omega_l)}. \qquad (3.28)$$

Next, we insert the lower bound for the partition sum from Lemma 3.1 with $\varepsilon := \delta/24$ and $r = r(\varepsilon)$. Using also $|\mathcal{T}_N| \geq 1$, we obtain

$$\begin{aligned} E_{P_{\beta,m,N}}[A_{m,l,N}(\omega)] &\leq \frac{\delta}{2}|\mathcal{T}_N| + \frac{2}{c_{14}} \frac{e^{-\beta\delta|I_N|/4}}{\pi^{-1}r^{-2}e^{-|I_N|(3\beta\varepsilon-\log(\pi r^2))}} \left(\frac{c_{14}}{\beta}\right)^{|I_N|} \\ &\leq \frac{\delta}{2}|\mathcal{T}_N| + c_{10}|\mathcal{T}_N| \exp\left\{|I_N|\left(-\frac{\beta\delta}{8} - \log\beta + c_{11}\right)\right\} \end{aligned} \qquad (3.29)$$

with constants $c_{10} > 0$ and $c_{11} \in \mathbb{R}$ depending on δ. This yields Claim (3.10).

For any given $\delta > 0$, $-\beta\delta/8 - \log\beta + c_{11}(\delta) \to -\infty$ as $\beta \to \infty$. Consequently, Claim (3.11) follows. □

3.3 Proof of the main results

Proof of Theorem 1.3. The claim follows if we show

$$\lim_{\beta\to\infty} \sup_{N\geq 4} \sup_{m\geq m_0} \frac{1}{|\mathcal{T}_N|} \sum_{\Delta\in\mathcal{T}_N} E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\Delta) - l\mathrm{Id}|^2] = 0. \qquad (3.30)$$

This can be seen as follows: For $x \in \mathcal{A}_2$, let $\theta_x \colon \Omega_{l,N} \to \Omega_{l,N}$, $\theta_x\omega(y) = \omega(y-x)$ for $y \in \mathcal{A}_2$, denote the shift operator. For any $x \in \mathcal{A}_2$, $P_{\beta,m,N}$ is invariant under θ_x. Consequently, for any $\tilde{\Delta} \in \mathcal{T}_N$ and $x \in I_N$, we get

$$E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\tilde{\Delta} + x) - l\mathrm{Id}|^2] = E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\tilde{\Delta}) - l\mathrm{Id}|^2]. \qquad (3.31)$$

For any $\Delta_1 \in \mathcal{T}_N$, the set $\left\{\Delta = \tilde{\Delta} + x : \tilde{\Delta} \in \{\Delta_1, \tau\Delta_1\}, x \in I_N\right\}$ modulo translations by elements of $N\mathcal{A}_2$ runs over all elements of $\mathcal{T}_N$. Using this first and then using (3.31) yields

$$\begin{aligned} \sum_{\Delta\in\mathcal{T}_N} E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\Delta) - l\mathrm{Id}|^2] &= \sum_{\tilde{\Delta}\in\{\Delta_1,\tau\Delta_1\}} \sum_{x\in I_N} E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\tilde{\Delta} + x) - l\mathrm{Id}|^2] \\ &= \sum_{\tilde{\Delta}\in\{\Delta_1,\tau\Delta_1\}} \sum_{x\in I_N} E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\tilde{\Delta}) - l\mathrm{Id}|^2] \\ &\geq \sum_{x\in I_N} E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\Delta_1) - l\mathrm{Id}|^2] \\ &= |I_N| E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\Delta_1) - l\mathrm{Id}|^2]. \end{aligned} \qquad (3.32)$$

Since $2|I_N| = |\mathcal{T}_N|$, (3.30) implies Claim (1.17).

To prove (3.30), we consider

$$\begin{aligned} l^{-2} \sum_{\Delta\in\mathcal{T}_N} \lambda(\Delta) E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\Delta) - l\mathrm{Id}|^2] &= \sum_{\Delta\in\mathcal{T}_N} \lambda(\Delta) E_{P_{\beta,m,N}}[|l^{-1}\nabla\hat{\omega}(\Delta) - \mathrm{Id}|^2] \\ &= E_{P_{\beta,m,N}}[\|l^{-1}\nabla\hat{\omega} - \mathrm{Id}\|^2_{L^2(U_N)}]. \end{aligned} \qquad (3.33)$$

Lemma 3.2 implies

$$0 \leq l^{-2} \sum_{\Delta\in\mathcal{T}_N} \lambda(\Delta) E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\Delta) - l\mathrm{Id}|^2] \leq c_8^{-1} E_{P_{\beta,m,N}}[A_{m,l,N}(\omega)] \qquad (3.34)$$

for $m \geq m_0 = m_1 + 1$. Note that the middle term in (3.34) equals up to a constant $\sum_{\Delta\in\mathcal{T}_N} E_{P_{\beta,m,N}}[|\nabla\hat{\omega}(\Delta) - l\mathrm{Id}|^2]$ because $\lambda(\Delta)$ is constant for $\Delta \in \mathcal{T}_N$. The claim follows from Lemma 3.3. □

Proof of Theorem 1.1. For any equilateral triangle with side length 1 having corner points $A_1, A_2, A_3 \in \mathbb{R}^2$, the map

$$\mathbb{R}^{2 \times 2} \ni M \mapsto \max\{\|M(A_2 - A_1)\|, \|M(A_3 - A_2)\|, \|M(A_1 - A_3)\|\} \qquad (3.35)$$

is a matrix norm and hence equivalent to any other matrix norm on $\mathbb{R}^{2 \times 2}$. Thus Theorem 1.1 follows from Theorem 1.3. $\qquad \square$

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