TWO GEOMETRIC LEMMATA FOR $S^{N-1}$-VALUED MAPS AND AN APPLICATION TO THE HOMOGENIZATION OF SPIN SYSTEMS∗

ANDREA BRAIDES** AND VALERIO VALLOCCHIA

Abstract. We prove two geometric lemmas for $S^{N-1}$-valued functions that allow to modify sequences of lattice spin functions on a small percentage of nodes during a discrete-to-continuum process so as to have a fixed average. This is used to simplify known formulas for the homogenization of spin systems.

Mathematics Subject Classification. 35B27, 74Q05, 49J45.

Received October 27, 2020. Accepted January 9, 2021.

Dedicated to Enrique Zuazua on the occasion of his 60th birthday.

1. Introduction

A motivation for the analysis in the present work has been the study of molecular models where particles are interacting through a potential including both orientation and position variables. In particular we have in mind potentials of Gay-Berne type in models of Liquid Crystals [5, 6, 17, 19, 20]. In that context a molecule of a liquid crystal is thought of as an ellipsoid with a preferred axis, whose position is identified with a vector $w \in \mathbb{R}^3$ and whose orientation is a vector $u \in S^2$. Given $\alpha$ and $\beta$ two such particles, the interaction energy will depend on their orientations $u_\alpha$, $u_\beta$ and the distance vector $\zeta_{\alpha \beta} = w_\beta - w_\alpha$. We will concentrate on some properties on the dependence of the energy on $u$ due to the geometry of $S^2$ (more in general, of $S^{N-1}$).

We restrict to a lattice model where all particles are considered as occupying the sites of a regular (cubic) lattice in the reference configuration. Note that in this assumption $\zeta_{\alpha \beta} = \beta - \alpha$ can be considered as an additional parameter and not a variable. Otherwise, in general the dependence on $\zeta_{\alpha \beta}$ is thought to be of Lennard-Jones type (for the treatment of such energies, still widely incomplete, we refer to [8, 10, 12]).

We introduce an energy density $G : \mathbb{Z}^m \times \mathbb{Z}^m \times S^{N-1} \times S^{N-1} \to \mathbb{R} \cup \{+\infty\}$, so that

$$G^\xi(\alpha, u, v) = G(\alpha, \alpha + \xi, u, v)$$

represents the free energy of two molecules oriented as $u$ and $v$, occupying the sites $\alpha$ and $\beta = \alpha + \xi$ in the reference lattice. Note that we have included a dependence on $\alpha$ to allow for a microstructure at the lattice level, but the energy density is meaningful also in the homogeneous case, with $G^\xi$ independent of $\alpha$. Such energies

∗The authors acknowledge the MIUR Excellence Department Project awarded to the Department of Mathematics, University of Rome Tor Vergata, CUP E83C18000100006.

Keywords and phrases: Spin systems, maps with values on the sphere, lattice energies, discrete-to-continuum, homogenization.

Dipartimento di Matematica Università di Roma “Tor Vergata”, via della ricerca scientifica 1, 00133 Rome, Italy.

** Corresponding author: braides@mat.uniroma2.it
are the basis for the variational analysis of complex multi-scale behaviours of spin systems (see, e.g., [9] for the
derivation of energies for liquid crystals, [2] for a study of the XY-model, [14] for a very refined study of the
N-clock model, [15, 16] for chirality effects).

In order to understand the collective behaviour of a spin system, we introduce a small scaling parameter
\( \varepsilon > 0 \), so that the description of such a behaviour can be formalized as a limit as \( \varepsilon \to 0 \). For each Lipschitz set
\( \Omega \) the discrete set \( \mathbb{Z}_\varepsilon(\Omega) := \{ \alpha \in \varepsilon \mathbb{Z}^m : (\alpha + [0, \varepsilon)^m) \cap \Omega \neq \emptyset \} \) represents a ‘discretization’ of the set \( \Omega \) at scale
\( \varepsilon \). We also let \( R > 0 \) define a cut-off parameter representing the relevant range of the interactions (which we
assume to be finite).

We define the family of scaled functionals

\[
E_\varepsilon(u) = \sum_{\xi \in \mathbb{Z}^m} \sum_{|\xi| \leq R} \varepsilon^m G^\varepsilon \left( \frac{\alpha}{\varepsilon}, u(\alpha), u(\alpha + \varepsilon \xi) \right)
\]

with domain functions \( u : \mathbb{Z}_\varepsilon(\Omega) \to S^{N-1} \), where \( R^\varepsilon(\Omega) := \{ \alpha \in \mathbb{Z}_\varepsilon(\Omega) : \alpha, \alpha + \varepsilon \xi \in \Omega \} \).

Extending functions defined on \( \mathbb{Z}_\varepsilon(\Omega) \) to piecewise-constant interpolations, we may define a discrete-to-
continuum convergence of \( u_\varepsilon \) to \( u \). The assumptions on \( G \) ensure that \( u \) takes values in the unit ball. We can then perform an asymptotic analysis using the notation of \( \Gamma \)-convergence (see e.g. [7, 8, 13]). Energies as \( E_\varepsilon \),
but with \( u \) taking values in general compact sets \( K \) have been previously studied by Alicandro, Cicalese and
Gloria (2008) [3], who describe the limit with a two-scale homogenization formula. In the case of \( S^{N-1} \)-valued
functions we simplify the homogenization formula reducing to test functions \( u \) satisfying a constraint on the
average. This is a non-trivial fact since this constraint is non-convex, and its proof is the main technical point
of the work.

The key observation is that we can modify the sequences \( u_\varepsilon \) so that they satisfy an exact condition on their
average. We formalize this fact in two geometrical lemmas. The first one is a simple observation that each point
in the unit ball in \( \varepsilon \mathbb{R}^N \) with \( N > 1 \) can be written exactly as the average of \( k \) vectors in \( S^{N-1} \) for all \( k \geq 2 \),
while the second one allows to modify sequences \( u_\varepsilon \) satisfying an asymptotic condition on the discrete average
of \( u_\varepsilon \) with a sequence \( \tilde{u}_\varepsilon \) satisfying a sharp one and with the same energy \( E_\varepsilon \) up to a negligible error. This can be
done if the asymptotic average of \( u_\varepsilon \) has modulus strictly less than one. In this case, most of the values of
\( u_\varepsilon \) are not aligned; this allows to use a small percentage of these values to correct the asymptotic average to a
sharp one by using the first lemma.

Optimizing on all the functions satisfying the same average condition satisfied by their limit we show that
the \( \Gamma \)-limit of the sequence \( E_\varepsilon \), for functions \( u \in L^\infty(\Omega, B_1^N) \) is a continuum functional

\[
E_0(u) = \int_\Omega G_{\text{hom}}(u) \, dx,
\]

and the function \( G_{\text{hom}} \) satisfies a homogenization formula

\[
G_{\text{hom}}(z) = \lim_{T \to \infty} \frac{1}{T^m} \inf_{T \to \infty} \left\{ \mathcal{E}_T(u) : \frac{1}{T^m} \sum_{\alpha \in \mathbb{Z}(Q_T)} u(\alpha) = z \right\},
\]

where \( Q_T = (0, T)^m \) and

\[
\mathcal{E}_T(u) = \sum_{\xi \in \mathbb{Z}^m} \sum_{|\xi| \leq R} G^\varepsilon(\beta, u(\beta), u(\beta + \xi)).
\]

Note that the constraint in the homogenization formula involves the values of \( u(\alpha) \), which belong to the non-
convex set \( S^{N-1} \). This is an improvement with respect to Theorem 5.3 in [3], where the integrand of the limit
is characterized imposing a weaker constraint on the average of $u$; namely it is shown that it equals

$$
\overline{G}_{\text{hom}}(z) = \lim_{\eta \to 0^+} \lim_{T \to \infty} \frac{1}{T^m} \inf \left\{ \mathcal{E}_T(u) : \left| \frac{1}{T^m} \sum_{\alpha \in Q_T} u(\alpha) - z \right| \leq \eta \right\},
$$

(1.1)

A formula with a sharp constraint may be useful in higher-order developments, which characterize microstructure, interfaces and singularities.

The plan of the paper is as follows. In Section 2 we introduce the notation for discrete-to-continuum homogenization. In Section 3 we state and prove the geometric lemmas on $S^{N-1}$-valued functions. In Section 4 we prove the homogenization formula, and finally in Section 5 we give a proof of the homogenization theorem.

2. Notation and setting

Let $m, n \geq 1$, $N \geq 2$ be fixed. We denote by $\{e_1, \ldots, e_m\}$ the standard basis of $\mathbb{R}^m$. Given two vectors $v_1, v_2 \in \mathbb{R}^n$, by $(v_1, v_2)$ we denote their scalar product. If $v \in \mathbb{R}^m$, we use $|v|$ for the usual euclidean norm. $S^{N-1}$ is the standard unit sphere of $\mathbb{R}^N$ and $B_N^1$ the closed unit ball of $\mathbb{R}^N$. If $x \in \mathbb{R}$, its integer part is denoted by $\lfloor x \rfloor$. We also set $Q_T = (0, T)^m$ and $B(\Omega)$ as the family of all open subsets of $\Omega$. If $A$ is an open bounded set, given a function $u : A \to \mathbb{R}^N$ we denote its average over $A$ as

$$
\langle u \rangle_A = \frac{1}{|A|} \int_A u(x) \, dx.
$$

2.1. Discrete functions

Let $\Omega \subset \mathbb{R}^m$ be an open bounded domain with Lipschitz boundary, and let $\varepsilon > 0$ be the spacing parameter of the cubic lattice $\varepsilon \mathbb{Z}^m$. We define the set

$$
Z_\varepsilon(\Omega) := \{ \alpha \in \varepsilon \mathbb{Z}^m : (\alpha + [0, \varepsilon)^m) \cap \Omega \neq \emptyset \}
$$

and we will consider discrete functions $u : Z_\varepsilon(\Omega) \to S^{N-1}$ defined on the lattice. For $\xi \in \mathbb{Z}^m$, we define

$$
R_\varepsilon^\xi(\Omega) := \{ \alpha \in Z_\varepsilon(\Omega) : \alpha, \alpha + \varepsilon \xi \in \Omega \},
$$

while the “discrete” average of a function $v : Z_\varepsilon(\Omega) \to S^{N-1}$ over an open bounded domain $A$ will be denoted by

$$
\langle v \rangle_{d,\varepsilon}^A = \frac{1}{\#(Z_\varepsilon(A))} \sum_{\alpha \in Z_\varepsilon(A)} v(\alpha).
$$

2.2. Discrete energies

We assume that the Borel function $G : \mathbb{R}^m \times \mathbb{R}^m \times S^{N-1} \times S^{N-1} \to \mathbb{R}$ satisfies the following conditions

(boundedness) $\sup \{ |G(\alpha, \beta, u, v)| : \alpha, \beta \in \mathbb{R}^m, u, v \in S^{N-1} \} < \infty$; \hspace{1cm} (2.1)
(periodicity) there exists $l \in \mathbb{N}$ such that $G(\cdot, \cdot, u, v)$ is $Q_l$ periodic; \hspace{1cm} (2.2)
(lower semicontinuity) $G$ is lower semicontinuous. \hspace{1cm} (2.3)

Given $\xi \in \mathbb{R}^m$, we use the notation

$$
G^\xi(\alpha, u, v) = G(\alpha, \alpha + \varepsilon \xi, u, v),
$$

(2.4)
and define the functionals

$$
\sum_{\xi \in \mathbb{Z}^m} \sum_{|\xi| \leq R} \varepsilon^m G^\xi \left( \frac{\Omega}{\varepsilon}, u(\alpha), u(\alpha + \xi \varepsilon) \right)
$$

(2.5)

for $u : \mathcal{Z}_\varepsilon(\Omega) \to \mathcal{S}^{N-1}$.

2.3. Discrete-to-continuum convergence

In what follows we identify each discrete function $u$ with its piecewise-constant extension \( \tilde{u} \) defined by \( \tilde{u}(t) = u(\alpha) \) if $t \in \alpha + [0, \varepsilon)^m$. We introduce the sets:

$$
\mathcal{A}_\varepsilon(\Omega; \mathcal{S}^{N-1}) := \left\{ \tilde{u} : \mathbb{R}^m \to \mathcal{S}^{N-1} : \tilde{u}(t) \equiv u(\alpha) \text{ if } t \in \alpha + [0, \varepsilon)^m, \text{ for } \alpha \in \mathcal{Z}_\varepsilon(\Omega) \right\}.
$$

If no confusion is possible, we will simply write $u$ instead of $\tilde{u}$. If $\varepsilon = 1$ we will simply write $\mathcal{A}(\Omega; \mathcal{S}^{N-1})$ in the place of $\mathcal{A}_1(\Omega; \mathcal{S}^{N-1})$.

Up to the identification of each function $u$ with its piecewise-constant extension, we can consider energies $E_\varepsilon : L^\infty(\Omega, \mathcal{S}^{N-1}) \to \mathbb{R} \cup \{+\infty\}$ of the following form:

$$
E_\varepsilon(u; \Omega) = \begin{cases} 
\sum_{\xi \in \mathbb{Z}^m} \sum_{|\xi| \leq R} \varepsilon^m G^\xi \left( \frac{\Omega}{\varepsilon}, u(\alpha), u(\alpha + \xi \varepsilon) \right) & \text{if } u \in \mathcal{A}_\varepsilon(\Omega; \mathcal{S}^{N-1}), \\
+\infty & \text{otherwise}.
\end{cases}
$$

(2.6)

Let $\varepsilon_j \to 0$ and let $\{u_j\}$ be a sequence of functions $u_j : \mathcal{Z}_{\varepsilon_j}(\Omega) \to \mathcal{S}^{N-1}$. We will say that $\{u_j\}$ converges to a function $u$ if $\tilde{u}_j$ is converging to $u$ weakly* in $L^\infty$. Then we will say that the functionals defined in (2.5) $\Gamma$-converge to $E_0$ if $E_\varepsilon$ defined in (2.6) $\Gamma$-converge to $E_0$ with respect to that convergence.

2.4. The homogenization theorem

We will prove the following discrete-to-continuum homogenization theorem.

**Theorem 2.1.** Let $E_\varepsilon$ be the energy defined in (2.5) and suppose that (2.1)–(2.3) hold. Then $E_\varepsilon$ $\Gamma$-converge to the functional

$$
E_0(u) = \int_\Omega G_{\text{hom}}(u) \, dx
$$

(2.7)

defined for functions $u \in L^\infty(\Omega, B_1^N)$. The function $G_{\text{hom}}$ is given by the following asymptotic formula

$$
G_{\text{hom}}(z) = \lim_{T \to \infty} \frac{1}{T^m} \inf \left\{ E_1(u; Q_T) : \langle u \rangle_{Q_T}^1 = z \right\}.
$$

(2.8)

The treatment of the average condition in (2.8) will be performed using a geometric lemma which exploits the geometry of $\mathcal{S}^{N-1}$, as shown in the next section.

3. Two geometric lemmas

In this section we provide two general lemmas. The first one is a simple observation on the characterisation of sums of vectors in $\mathcal{S}^{N-1}$, while the second one allows to satisfy conditions on the average of discrete functions with values in $\mathcal{S}^{N-1}$.
**Lemma 3.1.** Let \( u \) be a vector in the ball \( B_1^N \) in \( \mathbb{R}^N \) centered in the origin and with radius \( k \geq 2 \); then \( u \) can be written as the sum of \( k \) vectors on \( S^{N-1} \):

\[
    u = \sum_{i=1}^{k} u_i \quad u_i \in S^{N-1}.
\]

Equivalently, given \( u \in B_1^N \) and \( k \geq 2 \), \( u \) can be written as the average of \( k \) vectors on \( S^{N-1} \):

\[
    u = \frac{1}{k} \sum_{i=1}^{k} u_i \quad u_i \in S^{N-1}.
\]

**Proof.** We proceed by induction on \( k \).

Let \( k = 2 \) and let \( u \in B_2^N \). The set \((u + S^{N-1}) \cap S^{N-1}\) is not empty set. If we choose \( v \in (u + S^{N-1}) \cap S^{N-1} \) then the first induction step is proven with \( u_1 = v \) and \( u_2 = (u - v) \).

Suppose that the claim holds for \( k - 1 \). Let \( u \in B_k^N \) and note that the set \((u + S^{N-1}) \cap B_{k-1}^N\) is not empty.

If \( v \in (u + S^{N-1}) \cap B_{k-1}^N \) by the inductive hypothesis we may write \( v = u_1 + \cdots + u_{k-1} \) with \( u_j \in S^{N-1} \). The claim is then proved by setting \( u_k = u - v \). \( \square \)

**Lemma 3.2.** Let \( A \subset \mathbb{R}^m \) be an open bounded set with Lipschitz boundary. Let \( \delta_i > 0 \) be a spacing parameter and \( u_j : Z_{\delta_j}(A) \to S^{N-1} \) be a sequence of discrete function. Suppose that \( u_j \rightharpoonup^* u \) in \( L^\infty(A,B_1^n) \) and that the average of \( u \) on \( A \) satisfies \( |\langle u \rangle_A| < 1 \). Then, for all \( j \) there exist \( \tilde{u}_j \) such that

1. the discrete average \( \langle \tilde{u}_j \rangle_A^d := \frac{1}{\#Z_{\delta_j}(A)} \sum_{i \in Z_{\delta_j}(A)} \tilde{u}_j(i) \) is equal to \( \langle u \rangle_A \);

2. the function \( \tilde{u}_j \) is obtained by modifying the function \( u_j \) in at most \( 2P_j \) points, with \( \frac{P_j}{\#Z_{\delta_j}(A)} \to 0 \).

**Proof.** To simplify the notation we set \( Z_j(A) = Z_{\delta_j}(A) \) and \( u_j^i = u_j(i) \).

Note that, by the weak convergence of \( u_j \),

\[
    \eta_j := |\langle u_j \rangle^d - \langle u \rangle_A| = o(1) \quad (3.1)
\]

as \( j \to +\infty \). We will treat the case that \( \eta_j \neq 0 \) since otherwise we simply take \( \tilde{u}_j = u_j \).

Since \( \langle u_j \rangle_A^d \to \langle u \rangle_A \), by the hypothesis that \( |\langle u \rangle_A| < 1 \) we may suppose that

\[
    |\langle u_j \rangle_A^d| \leq 1 - 2b \quad (3.2)
\]

for all \( j \), for some \( b \in (0,1/2) \).

**Claim:** setting \( B = b/(4 - 2b) \), for every \( i \in Z_j(A) \) there exist at least \( B \# Z_j(A) \) indices \( l \in Z_j(A) \) such that \( (u_j^i, u_j^l) \leq 1 - b \).

Indeed, otherwise there exists at least one index \( i \) for which the set

\[
    \mathcal{A}_b := \{ l \in Z_j(A) : (u_j^i, u_j^l) > 1 - b, \ l \neq i \}
\]

(3.3)
is such that \( \# \mathcal{A}_b \geq (1 - B) \# \mathcal{Z}_j(A) \) and we have

\[
|\langle u_j \rangle^d_A| \geq \langle \langle u_j \rangle^d, u_j^i \rangle = \frac{1}{\# \mathcal{Z}_j(A)} \sum_{l \in \mathcal{Z}_j(A)} (u_j^l, u_j^i) \\
= \frac{1}{\# \mathcal{Z}_j(A)} \sum_{l \in \mathcal{A}_b} (u_j^l, u_j^i) + \frac{1}{\# \mathcal{Z}_j(A)} \sum_{l \in \mathcal{Z}_j(A) \setminus \mathcal{A}_b} (u_j^l, u_j^i) \\
\geq \frac{1}{\# \mathcal{Z}_j(A)} (\# \mathcal{A}_b (1 - b) - (\# \mathcal{Z}_j(A) - \# \mathcal{A}_b)) \\
= \frac{1}{\# \mathcal{Z}_j(A)} ((2 - b) \# \mathcal{A}_b - \# \mathcal{Z}_j(A)) \\
\geq (2 - b)(1 - B) - 1 = 1 - \frac{3}{2}b \\
> |\langle u_j \rangle^d_A|,
\]

where we have used (3.2) in the last estimate. We then obtain a contradiction, thus proving the claim.

By the Claim above, there exist \((B/2) \# \mathcal{Z}_j(A)\) pairs of indices \((i_s, l_s)\) with \(\{i_s, l_s\} \cap \{i_r, l_r\} = \emptyset\) if \(r \neq s\) and

\[
(u_j^{i_s}, u_j^{l_s}) \leq 1 - b. \tag{3.4}
\]

Since \(\eta_j \to 0\), with fixed \(c > 0\) we may suppose that

\[
B \# \mathcal{Z}_j(A) > 2 \left\lfloor \frac{\eta_j}{c} \# \mathcal{Z}_j(A) \right\rfloor + 1 \tag{3.5}
\]

for all \(j\).

We now set

\[
P_j = \left\lfloor \frac{\eta_j}{c} \# \mathcal{Z}_j(A) \right\rfloor + 1, \tag{3.6}
\]

so that by (3.5) there exist pairs \((i_s, l_s)\) as above, with \(s \in I_j := \{1, \ldots, P_j\}\). Note that \(P_j\) satisfies the second claim of the theorem.

If for fixed \(j\) we define the vector

\[
w = \sum_{i \in \mathcal{Z}_j(A)} u_j^i - \langle \mathcal{Z}_j(A) \rangle \langle u \rangle_A - \sum_{s \in I_j} (u_j^{i_s} + u_j^{l_s}),
\]

then we have

\[
|w| \leq \langle \mathcal{Z}_j(A) \rangle |\langle u_j \rangle^d - \langle u \rangle_A| + \sum_{s \in I_j} |u_j^{i_s} + u_j^{l_s}| \\
\leq \langle \mathcal{Z}_j(A) \rangle \eta_j + \sum_{s \in I_j} \sqrt{2 + 2(u_j^{i_s}, u_j^{l_s})} \\
\leq \langle \mathcal{Z}_j(A) \rangle \eta_j + P_j \sqrt{4 - 2b}.
\]
Since \( \#Z_j(A) \eta_j < c P_j \) by (3.6), we then have \( |w| \leq c P_j + P_j \sqrt{4 - 2b} \). We finally choose \( c > 0 \) such that \( \sqrt{4 - 2b} < 2 - c \), so that

\[
|w| < 2P_j.
\]

By Lemma 3.1, applied with \( u = -w \) and \( k = 2P_j \), there exists a set of \( 2P_j \) vectors in \( \mathcal{S}^{N-1} \), that we may label as

\[
\{ \tilde{\pi}_j^i, \tilde{\pi}_j^s : s \in I_j \},
\]

such that

\[
\sum_{s \in I_j} (\tilde{\pi}_j^i + \tilde{\pi}_j^s) = -w. \quad (3.7)
\]

If we now define \( \tilde{u}_j \) by setting

\[
\tilde{u}_j = \begin{cases} 
\tilde{\pi}_j^i & \text{if } i \in \{i_s, l_s : s \in I_j\} \\
\tilde{\pi}_j^s & \text{otherwise},
\end{cases} \quad (3.8)
\]

we have

\[
\langle \tilde{u}_j \rangle_A^d = \frac{1}{\#Z_j(A)} \left( \sum_{i \in Z_j(A)} u_j^i - \sum_{s \in I_j} (u_j^{i_s} + u_j^{l_s}) + \sum_{s \in I_j} (\tilde{\pi}_j^i + \tilde{\pi}_j^s) \right)
= \frac{1}{\#Z_j(A)} \left( \sum_{i \in Z_j(A)} u_j^i - \sum_{s \in I_j} (u_j^{i_s} + u_j^{l_s}) - w \right)
= \langle u \rangle_A,
\]

and the proof is concluded.

**Remark 3.3.** The assumption \( |\langle u \rangle_A| < 1 \) in Lemma 3.2 is sharp: if \( |\langle u \rangle_A| = 1 \), we may have \( u_j \rightharpoonup^* u \), such that \( u_j \neq u \) and \( |\langle u_j \rangle_A^{d,\delta_j}| = 1 \) at every point (for example take \( u \) and \( u_j \) constant vectors in \( \mathcal{S}^{N-1} \)). In this case, in order to have \( \langle u_j \rangle_A^{d,\delta_j} = \langle u \rangle_A \), we should change the function \( u_j \) in every point.

4. The homogenization formula

In this section we prove that the homogenization formula characterizing \( G_{\text{hom}} \) in Theorem 2.1 is well defined, and derive some properties of that function.

**Proposition 4.1.** Let \( G \) be a function satisfying (2.1)–(2.3) and let \( G^\xi \) be defined as in (2.4). For all \( T > 0 \) consider an arbitrary \( x_T \in \mathbb{R}^m \), then the limit

\[
\lim_{T \to \infty} \frac{1}{T} \inf \left\{ E_1(u; x_T + Q_T) : \langle u \rangle_{x_T+Q_T}^{d,1} = z \right\} \quad (4.1)
\]

exists for all \( z \in B_1^N \).

**Proof.** Let \( z \in B_1^N \) be fixed. In the following we will assume \( G \) to be 1-periodic (which means that in (2.2) we consider \( l = 1 \)) and \( x_T = 0 \), since the general case can be derived similarly following arguments already present
for example in [1, 3] and only needing a heavier notation. Let $t > 0$ and consider the function

$$g_t(z) = \frac{1}{tm} \inf \left\{ E_1(u, \zeta; Q_t) : \langle u \rangle_{Q_t}^{d,1} = z \right\}. \quad (4.2)$$

In the rest of the proof we will drop the dependence on $z$. Let $u_t$ be a test function for $g_t$ such that

$$\frac{1}{tm} E_1(u_t; Q_t) \leq g_t + \frac{1}{t}, \quad (4.3)$$

For every $s > t$ we want to prove that $g_s < g_t$ up to a controlled error.

For fixed $s, t$, we introduce the following notation:

$$I := \left\{ 0, \ldots, \left\lfloor \frac{s}{t} \right\rfloor - 1 \right\}^m.$$ 

We can construct a test functions for $g_s$ as

$$u_s(\beta) = \begin{cases} u_t(\beta - ti) & \text{if } \beta \in ti + Q_t, i \in I \\ \bar{u}(\beta) & \text{otherwise}, \end{cases}$$

where $\bar{u}$ is a $S^{N-1}$-valued function such that $\langle u_s \rangle_{Q_s}^{d,1} = z$. We can choose such $\bar{u}$ thanks to Lemma 3.1: define

$$Z(Q_s) = Z^m \cap Q_s, \quad Q_{s,t} = \left( \bigcup_{i \in I} (ti + Q_t) \cap Z(Q_s) \right).$$

We want $\bar{u}$ to be such that

$$\sum_{\beta \in Z(Q_s)} u_s(\beta) = z \#(Z(Q_s)).$$

Equivalently

$$\sum_{\beta \in Q_{s,t}} u_t(\beta - ti) + \sum_{\beta \in Z(Q_s) \setminus Q_{s,t}} \bar{u}(\beta) = z \#(Z(Q_s)),$$

which means that

$$\sum_{\beta \in Z(Q_s) \setminus Q_{s,t}} \bar{u}(\beta) = z \left( \#(Z(Q_s)) - \#(Q_{s,t}) \right). \quad (4.4)$$

On the left-hand side of (4.4) we are summing $\#(Z(Q_s)) - \#(Q_{s,t})$ vectors in $S^{N-1}$ while on the right-hand side we have a vector which belongs to a ball whose radius is at most $\#(Z(Q_s)) - \#(Q_{s,t})$.

If $|z| < 1$, thanks to Lemma 3.1 we know that it is possible to choose the values of $\bar{u}$ in such a way that the relation (4.4) is satisfied.

If $|z| = 1$, we simply set $\bar{u}(\beta) \equiv z$, and again (4.4) is satisfied. Moreover, we observe that

$$R^z_1(Q_s) \subseteq \left( \bigcup_{i \in I} R^z_1(ti + Q_t) \right) \cup \left( R^z_1\left( Q_s \setminus \bigcup_{i \in I} (ti + Q_t) \right) \right) \cup \left( \bigcup_{i \in I} (ti + ([0, \ldots, t + R]^N \setminus [0, \ldots, t - R]^N)) \right)$$
and if $\beta$ belongs to one of the last two set of indices, then $D^2_{\xi}\zeta_{\beta}(\beta) = M(\xi/|\xi|)$.

Recalling now (2.1), for some $C > 0$ big enough, we have that

$$g_s \leq \frac{1}{s^m} E_1(u_s; Q_s) \leq \left[\frac{s}{t}\right]^m \frac{1}{s^m} E_1(u_t; Q_t) + \frac{1}{s^m} C \left(s^m - \left[\frac{s}{t}\right]^m t^m + \left[\frac{s}{t}\right]^m \left((t + R)^m - (t - R)^m\right)\right).$$

Using now (4.3) we get

$$g_s \leq \left[\frac{s}{t}\right]^m t^m \left(g_t + \frac{1}{t}\right) + \frac{1}{s^m} C \left(s^m - \left[\frac{s}{t}\right]^m t^m + \left[\frac{s}{t}\right]^m \left((t + R)^m - (t - R)^m\right)\right).$$

Letting now $s \to +\infty$ and then $t \to +\infty$, we have that

$$\limsup_{s \to +\infty} g_s(z) \leq \liminf_{t \to +\infty} g_t(z),$$

which concludes the proof.

**Remark 4.2.** Note that for $z \in S^{N-1}$ the only test function for the minimum problem in (4.1) is the constant $z$, so that the limit is actually an average over the period with $u = z$.

**Proposition 4.3.** The function $G_{\text{hom}}$ as defined in (2.8) is convex and lower semicontinuous in $B_1^N$.

**Proof.** We want to show that for every $0 \leq t \leq 1$ and for every $z_1, z_2 \in B_1^N$ it holds:

$$G_{\text{hom}}(tz_1 + (1 - t)z_2, M) \leq t G_{\text{hom}}(z_1, M) + (1 - t) G_{\text{hom}}(z_2, M).$$

(4.5)

Let $k \in \mathbb{N}$ be fixed; having (2.2) in mind, and thanks to Proposition 4.1, it is not restrictive to take $k \in \mathbb{N}$. We define

$$g_k(z) = \frac{1}{k^m} \inf \left\{ E_1(u; Q_k) : \langle u, Q_k \rangle = z \right\}.$$  

(4.6)

In the following we will denote $g_k^1 = g_k(z_1)$, $g_k^2 = g_k(z_2)$.

Let $u_k^1$ and $u_k^2$ be functions such that

$$\frac{1}{k^m} E_1(u_k^1; Q_k) \leq g_k^1 + \frac{1}{k},$$

(4.7)

$$\frac{1}{k^m} E_1(u_k^2; Q_k) \leq g_k^2 + \frac{1}{k}.$$  

(4.8)

Let $h > k$ be such that $h/k \in \mathbb{N}$. Denote $g_h = g_h(tz_1 + (1 - t)z_2)$, we define the following test function for $g_h$:

$$u_h(\beta) =$$

$$\begin{cases} u_k^1(\beta - ki) & \text{if } \beta \in ki + Q_k \quad i \in \left\{0, \ldots, \frac{h}{k} - 1\right\}^{m-1} \times \left\{0, \ldots, \left\lfloor\frac{h}{k}\right\rfloor - 1\right\}, \\ u_k^2(\beta - ki) & \text{if } \beta \in ki + Q_k \quad i \in \left\{0, \ldots, \frac{h}{k} - 1\right\}^{m-1} \times \left\{\frac{h}{k} - \left\lfloor\frac{h(1-t)}{k}\right\rfloor, \ldots, \frac{h}{k} - 1\right\}, \\ \bar{u}(\beta) & \text{otherwise}, \end{cases}$$
Reasoning as in Proposition 4.1, thanks to Lemma 3.1 we can choose the values of \( \bar{u} \) such that

\[
\langle u_h \rangle_{Q_s}^{d,1} = tz_1 + (1 - t)z_2.
\]

By (2.1) and (2.2), for some \( \bar{C} > 0 \) we get

\[
g_h \leq \frac{1}{h^m} E_1(u_h, \xi_h; Q_h) \\
\leq \frac{1}{h^m} \left( \frac{h}{k} \right)^{m-1} \left( \frac{h}{k} \right) E_1(u_{1,1}^k, Q_k) + \frac{1}{h^m} \left( \frac{h}{k} \right)^{m-1} \left( \frac{h(1 - t)}{k} \right) E_1(u_{2,1}^k, Q_k) \\
+ \frac{1}{h^m} \bar{C} \left( h^m - \left( \frac{h}{k} \right)^{m-1} \left( \frac{h}{k} \right) \right) k^m \\
+ \frac{1}{h^m} \bar{C} \left( \frac{h}{k} \right)^m ((k + R)^m - (k - R)^m).
\]

Then, thanks to (4.7) and (4.8), we can rewrite the above relation as

\[
g_h \leq \frac{k^m}{h^m} \left( \frac{h}{k} \right)^{m-1} \left( \frac{h}{k} \right) \left( \frac{h + 1}{k} \right) + \frac{k^m}{h^m} \left( \frac{h}{k} \right)^{m-1} \left( \frac{h(1 - t)}{k} \right) \left( \frac{g_k + 1}{k} \right) \\
+ \frac{1}{h^m} \bar{C} \left( h^m - \left( \frac{h}{k} \right)^{m-1} \left( \frac{h}{k} \right) \right) k^m \\
+ \frac{1}{h^m} \bar{C} \left( \frac{h}{k} \right)^m ((k + R)^m - (k - R)^m).
\]

Letting \( h \to +\infty \) and then \( k \to +\infty \), we can conclude the proof of the convexity.

From the convexity and the boundedness of \( G_{\text{hom}} \) we deduce that it is continuous in the interior of \( B_1^N \). Moreover, by (2.3) it is lower semicontinuous at points on the boundary of \( B_1^N \). \( \square \)

**Remark 4.4.** Note that the function \( G_{\text{hom}} \) may not be continuous on \( B_1^N \), even if it is convex. It suffices to take a nearest-neighbor energy \( G = G^\xi \) independent on \( \alpha \), with \( G(e_1, e_1) = 0 \) and \( G(u, v) = 1 \) otherwise. In this case, in particular \( G_{\text{hom}}(e_1) = 0 \) and \( G_{\text{hom}}(z) = 1 \) if \( z \in S^{N-1} \), \( z \neq e_1 \).

**5. Proof of the Homogenization Theorem**

Thanks to the geometric lemmas in Section 3, we can now easily give a proof of the homogenization theorem. We remark that it will be sufficient to prove a lower bound, since we may resort to the homogenization result of Alicandro, Cicalese and Gloria [3] in order to give an upper bound for the homogenized functional. Indeed, by (1.1) we have \( \overline{G}_{\text{hom}} \leq G_{\text{hom}} \), so that functional (2.7) is an upper bound for the homogenized energy. Note that we could directly proof the upper bound using approximation results and constructions starting from the formula for \( G_{\text{hom}} \), but this would be essentially a repetition of the arguments in [3].

In order to prove a lower bound we will make use of Lemma 3.2 and of the Fonseca-Müller blow-up technique [11, 18]. Let \( \varepsilon_j \to 0 \) be a vanishing sequence of parameters, let \( u \in L^\infty(\Omega, B_1^N) \) and let \( u_j \to u \) with \( u \in L^\infty(\Omega, B_1^N) \). We define the measures \( \mu_j \) by setting

\[
\mu_j(A) = \sum_{\xi \in \mathbb{Z}^m} \sum_{|\xi| \leq R} \varepsilon_j^m G^\xi \left( \frac{\alpha}{\varepsilon_j}, u_j(\alpha), u_j(\alpha + \varepsilon_j \xi) \right) \delta_{\alpha + \varepsilon_j \xi}(A)
\]
for all $A \in \mathcal{B}(\mathbb{R}^n)$, where $\delta_x$ denotes the usual Dirac delta measure at $x$. Since the measures are equibounded, by the weak* compactness of measures there exists a limit measure $\mu$ on $\Omega$ such that, up to subsequences, $\mu_j \rightharpoonup^* \mu$. We consider the Radon-Nikodym decomposition of the limit measure $\mu$ with respect to the $m$-dimensional Lebesgue measure $\mathcal{L}^m$:

$$\mu = \frac{d\mu}{dx} \mathcal{L}^m + \mu^s, \quad \mu^s \perp \mathcal{L}^m.$$  

Besicovitch Derivation Theorem [4] states that almost every point in $\Omega$ with respect to $\mathcal{L}^m$ is a Lebesgue point for $\mu$. So, we may suppose that $x_0 \in Z_{\varepsilon_j}(\Omega)$ be a Lebesgue point both for $u$ and for $\mu$ and let $Q_\rho(x_0) = x_0 + (-\rho/2, \rho/2)^m$. We then have

$$\frac{d\mu}{dx}(x_0) = \lim_{\rho \to 0^+} \frac{\mu(Q_\rho(x_0))}{\mathcal{L}^m(Q_\rho(x_0))} = \lim_{\rho \to 0^+} \frac{1}{\rho^m} \mu(Q_\rho(x_0)). \quad (5.1)$$

Recalling that

$$\mu(Q_\rho(x_0)) = \lim_{j \to +\infty} \mu_j(Q_\rho(x_0)) \quad (5.2)$$

except for a countable set of $\rho$, by a diagonalization argument on (5.1) and (5.2) we can extract a subsequence $\{\rho_j\}$ such that

$$\frac{d\mu}{dx}(x_0) = \lim_{j \to +\infty} \frac{1}{\rho_j^m} \mu_j(Q_{\rho_j}(x_0))$$

holds. This means that

$$\frac{d\mu}{dx}(x_0) = \lim_{j \to +\infty} \left(\frac{\varepsilon_j}{\rho_j}\right)^m \sum_{\varepsilon_j \in \mathbb{Z}^m} \sum_{\alpha \in R^m_{\varepsilon_j}(\Omega)} G^\varepsilon\left(\frac{\alpha}{\varepsilon_j}, u_j(\alpha), u_j(\alpha + \varepsilon_j \xi)\right) \delta_{\alpha^*} \frac{\varepsilon_j}{\rho_j^m}(Q_{\rho_j}(x_0)). \quad (5.3)$$

Also note that, by the weak* convergence of $u_j$ to $u$, we have

$$\langle u \rangle_{Q_\rho(x_0)} = \lim_j \langle u_j \rangle_{Q_\rho(x_0)} = \lim_j \langle u_j \rangle_{Q_\rho(x_0)}^{d,\varepsilon_j},$$

and that for almost every $x_0$ we have

$$\lim_{\rho \to 0^+} \langle u \rangle_{Q_\rho(x_0)} = u(x_0),$$

so that we may assume that

$$\lim_j \langle u_j \rangle_{Q_\rho(x_0)}^{d,\varepsilon_j} = u(x_0).$$

We can parameterizing functions on a common unit cube, by setting

$$v_j(\gamma) = u_j(x_0 + \rho_j \gamma) \quad \text{and} \quad \delta_j = \frac{\varepsilon_j}{\rho_j}. $$
With this parameterization, (5.3) reads
\[
\frac{d\mu}{dx}(x_0) = \lim_{j \to +\infty} \delta_j^m \sum_{\xi \in \mathbb{Z}^m} \sum_{|\xi| \leq R} G^\xi \left( \frac{x_0}{\varepsilon_j} + \gamma \delta_j, \nu_j(\gamma), \nu_j(\gamma + \delta_j \xi) \right) \delta_{\gamma - \frac{x_0}{\varepsilon_j} + \frac{\delta_j}{2} \xi} (Q_j(0)).
\]

Note that we have \( \lim_j \langle \nu_j \rangle_{Q_j(0)}^{d, \delta_j} = u(x_0) \). We can then apply Lemma 3.2 with \( \nu_j \) in the place of \( u_j \) and \( A = Q_j(0) \). We obtain a family \( \tilde{\nu}_j \) with
\[
\langle \tilde{\nu}_j \rangle_{Q_j(0)}^{d, \delta_j} = u(x_0), \tag{5.4}
\]
and such that \( \tilde{\nu}_j(\gamma) = v_j(\gamma) \) except for a set \( P_j \) of \( \gamma \) with \#\( P_j = o(\delta_j^{-m}) \). From this, the finiteness of the range of interactions and the boundedness of \( G^\xi \), we further rewrite as
\[
\frac{d\mu}{dx}(x_0) = \lim_{j \to +\infty} \delta_j^m \sum_{\xi \in \mathbb{Z}^m} \sum_{|\xi| \leq R} G^\xi \left( \frac{x_0}{\varepsilon_j} + \gamma \delta_j, \tilde{\nu}_j(\gamma), \tilde{\nu}_j(\gamma + \delta_j \xi) \right) \delta_{\gamma - \frac{x_0}{\varepsilon_j} + \frac{\delta_j}{2} \xi} (Q_j(0)).
\]

We now set
\[
T_j = \frac{\rho_j}{\varepsilon_j} = \delta_j^{-1}, \quad x_{T_j} = \frac{x_0}{\varepsilon_j},
\]
so that
\[
\frac{d\mu}{dx}(x_0) \leq \lim_{j \to +\infty} \frac{1}{T_j} \sum_{\xi \in \mathbb{Z}^m} \sum_{|\xi| \leq R} G^\xi \left( x_{T_j} + \gamma \delta_j, \tilde{\nu}_j(\gamma), \tilde{\nu}_j(\gamma + \delta_j \xi) \right) \delta_{\gamma - \frac{x_{T_j}}{\varepsilon_j} + \frac{\delta_j}{2} \xi} (Q_j(0))
\]

We now set \( w_j(\eta) = v_j(\frac{\eta}{T_j}) \) and use the boundedness of \( G^\xi \) and \( R \) to deduce that
\[
\frac{d\mu}{dx}(x_0) \geq \lim_{j \to +\infty} \frac{1}{T_j} \sum_{\xi \in \mathbb{Z}^m} \sum_{|\xi| \leq R} G^\xi \left( x_{T_j} + \eta, \tilde{\nu}_j(\eta), \tilde{\nu}_j(\eta + \xi) \right) \delta_{\eta - x_{T_j} + \frac{\delta_j}{2} \xi} (Q_j(0)).
\]

Note indeed that by considering interactions in \( R^1_j(Q_j(0)) \) we neglect a contribution of a number of interactions of order \( O(T_j^{-1}) \); i.e., an energy contribution of order \( O(T_j^{-1}) \). Noting that \( w_j \) satisfies the constraint
\[
\langle \tilde{\nu}_j \rangle_{x_{T_j} + Q_j(0)}^{d,1} = u(x_0),
\]
thanks to (5.4), by Proposition 4.1 we finally deduce that

\[ \frac{d\mu}{dx}(x_0) \geq \lim_{j \to \infty} \frac{1}{T_{m_j}^\infty} \inf \left\{ E_1(w; x_{T_j} + Q_{T_j}) : \langle w \rangle_{x_{T_j} + Q_{T_j}} = u(x_0) \right\} = G_{\text{hom}}(u(x_0)). \]

Since this holds for almost all \( x_0 \in \Omega \), we have proved the desired lower bound, and hence the convergence result.

**REFERENCES**

[1] R. Alicandro and M. Cicalese, A general integral representation result for continuum limits of discrete energies with superlinear growth. *SIAM J. Math. Anal.* 36 (2004) 1–37.

[2] R. Alicandro and M. Cicalese, Variational analysis of the asymptotics of the XY Model. *Arch Rational Mech Anal* 192 (2006) 501–536.

[3] R. Alicandro, M. Cicalese and A. Gloria, Variational description of bulk energies for bounded and unbounded spin systems. *Nonlinearity* 21 (2008) 1881–1910.

[4] L. Ambrosio, N. Fusco and D. Pallara, Function of Bounded Variations and Free Discontinuity Problems. Oxford University Press Oxford (2000).

[5] R. Berardi, A.P.J. Emerson and C. Zannoni, Monte Carlo investigations of a Gay-Berne liquid crystal. *J. Chem. Soc. Faraday Trans.* 89 (1993) 4069–4078.

[6] B.J. Berne and J.G. Gay, Modification of the overlap potential to mimic linear site-site potential. *J. Chem. Phys.* 74 (1981) 3316.

[7] A. Braides, Γ-convergence for Beginners. Oxford University Press (2002).

[8] A. Braides, A handbook of Γ-convergence In Handbook of Differential Equations. Stationary Partial Differential Equations Edited by M. Chipot and P. Quittner. Elsevier, Amsterdam (2006).

[9] A. Braides, M. Cicalese and F. Solombrino, Q-tensor continuum energies as limits of head-to-tail symmetric spin systems. *SIAM J. Math. Anal.* 47 (2015) 2832–2867.

[10] A. Braides, A.J. Lew and M. Ortiz, Effective cohesive behavior of layers of interatomic planes. *Arch. Ration. Mech. Anal.* 180 (2006) 151–182.

[11] A. Braides, M. Maslennikov and L. Sigalotti, Homogenization by blow-up. *Appl. Anal.* 87 (2008) 1341–1356.

[12] A. Braides and M. Solci, Asymptotic analysis of Lennard-Jones systems beyond the nearest-neighbour setting: a one-dimensional prototypical case. *Math. Mech. Solids* 21 (2016) 915–930.

[13] A. Braides and L. Truskinovsky, Asymptotic expansions by Γ-convergence. *Cont. Mech. Therm.* 20 (2008) 21–62.

[14] M. Cicalese, G. Orlando and M. Ruf, From the N-clock model to the XY model: emergence of concentration effects in the variational analysis. Preprint (2019) http://cvgmt.sns.it/paper/4432/.

[15] M. Cicalese, M. Ruf and F. Solombrino, Chirality transitions in frustrated \( S^2 \)-valued spin systems. *M3AS* 26 (2016) 1481–1529.

[16] M. Cicalese and F. Solombrino, Frustrated ferromagnetic spin chains: a variational approach to chirality transitions. *J. Nonlinear Sci.* 25 (2015) 291–313.

[17] P.G. de Gennes, *The Physics of Liquid Crystals*. Clarendon Press, Oxford (1974).

[18] I. Fonseca and S. Müller, Quasiconvex integrands and lower semicontinuity in \( L^1 \). *SIAM J. Math. Anal.* 23 (1992) 1081–1098.

[19] E.G. Virga, *Variational Theories for Liquid Crystals*. Chapman and Hall, London (1994).

[20] J. Wu, *Variational Methods in Molecular Modeling*. Springer, Berlin (2017).