Static ferromagnetic materials: from the microscopic to the mesoscopic scale

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Abstract

Thanks to averaging processes and Γ-convergence techniques, we are able to link a microscopic description of ferromagnetic materials based on spin lattices and their mesoscopic description in the static framework for the three fundamental contributions: exchange, magnetostatic and external field. The results are in accordance with the classical continuous description of ferromagnetic phenomena and justifies it. This work is a seed towards a dynamic description of ferromagnetic materials.

1 Introduction

The continuous description of ferromagnetic materials has been introduced since the 60's *via* the micromagnetism model developed by W.-F. Brown [4]. This model, based on a thermodynamical description of ferromagnetic phenomena, has proved its efficiency in numerous works *via* relevant simulations ([2, 6, 9, 5]). Nevertheless, several problems persist in the description, from the thermic effects to the magnetostrictive behaviors. These problems are very sharp and, in order to understand their modeling, one need to understand the microscopic behavior of magnetization (atomic scale) and the link between this scale and the mesoscopic scale (continuous magnetic matter scale of ferromagnetic effects). In this paper, we focus on the beginning of this program: the link between a microscopic description of ferromagnetic materials and their mesoscopic description in the static framework for the three fundamental contributions: exchange, magnetostatic and external field

[1, 7, 8]. Here, the microscopic scale designates the atomic scale where atom nuclei are assumed to be point electric charges bearing one magnetic moment induced by the atom's electronic cloud; the mesoscopic scale designates the continuous description of matter for which the ferromagnetic effects are significative.

At the microscopic scale, we describe the material as a regular periodic spin lattice intersected with the magnetic domain (a bounded open set of $\mathbb{R}^3$). Section 2 is dedicated to the mathematical description of the microscopic model (the spin lattice) and to an averaging process towards a mesoscopic models which leads to a constant norm magnetic field, in accordance with usual models of micromagnetism. The microscopic energies are introduced and several modeling hypotheses are set. The main hypothesis is induced by the adiabatic behavior of the Heisenberg energy compared to the global ferromagnetic energy. This hypothesis gives a constraint on neighboring magnetic moments. In fact, this constraint is verified by a set of minimizers for a given lattice.

The energy induced by the Heisenberg interaction is more difficult to treat. Section 3 addresses the study of this contribution and, in particular, its asymptotic behavior for sequences of lattices verifying the modeling hypothesis. This hypothesis ensures compactness which allows to use Γ-convergence tools in H^1. The limiting energy constructed from the discrete magnetization is the exchange energy (Theorem 1).

In Section 4, we introduce the demagnetization energy both for discrete lattices and the continuous model and finally obtain a convergence result for the sum of the Heisenberg and demagnetization contributions (Theorem 2).

2 Mathematical descriptions of a spin lattice

2.1 Atomic lattice description

We consider a collection of spins which are located on the nodes of a periodic lattice $\mathcal{L}$ in the $\mathbb{R}^d$ space ($d = 1, 2, 3$) with mesh size $a > 0$. In the scope of this paper we will restrict to the case of 1D, square or cubic lattices, $\mathcal{L}$ is simply $a\mathbb{Z}^d$, but we can think of more complex lattices. Here all the nodes play the same role to ensure a unique definition of neighbors. In the opposite case a multi-species model should be used.

The nodes are indexed by $i \in \mathbb{N}$ and we denote by x_i the ith spin location and μ_{x_i} the corresponding spin value (magnetic moment). The norm of these magnetic moments are scaled to the unit value and therefore for all $i \in \mathbb{N}$, $\mu_{x_i} \in \mathbb{S}^2$, where $\mathbb{S}^2$ is the unit sphere of $\mathbb{R}^3$.

Instead of describing a collection of magnetic moments, we can gather all the values in one single vector field μ defined by

$$\forall x \in \mathbb{R}^d, \quad \mu(x) = \sum_{i \in \mathbb{N}} \mu_{x_i} \delta_{x_i}(x),$$

where δ_{x_i} is the Dirac delta function centered at x_i.

2.2 Scaling

We want to obtain an homogenized model of the spin lattice, i.e. give a description when this lattice is seen from far. Instead of really doing this, we will perform some dual transformation, i.e. consider only nodes that are included in some fixed bounded domain Ω, and shrink the lattice (as shown on Figure 1 for $d = 2$). More precisely, we suppose that $0 \in \mathring{\Omega}$ and for all $n \in \mathbb{N}^*$, using the homothety $h_n(x) := x/n$, $\forall x \in \mathbb{R}^d$, we define

- $\mathcal{L}_n = h_n(\mathcal{L})$, the shrunk lattice;
- $\mathcal{L}_{n,\Omega} = \mathcal{L}_n \cap \Omega$, the nodes of the shrunk lattice that belong to Ω;
- $\mu_n \in (\mathbb{S}^2)^{\mathcal{L}_{n,\Omega}}$, the shrunk vector field.

We notice that for all $y \in \mathbb{R}^d$,

$$\mu_n(y) = \sum_{x \in \mathcal{L}_{n,\Omega}} \mu_{n,x} \delta_x(y),$$

where $\mu_{n,x} = \mu_{h_n^{-1}(x)}$. We assume that Ω has a sufficiently regular boundary in order that the number of nodes belonging to $\mathcal{L}_{n,\Omega}$ is

$$\#\mathcal{L}_{n,\Omega} = Cn^d(1 + O(\frac{1}{n})).$$

where C is a constant which only depends on $\mathcal{L}$, a and Ω (which are constants of our problem).

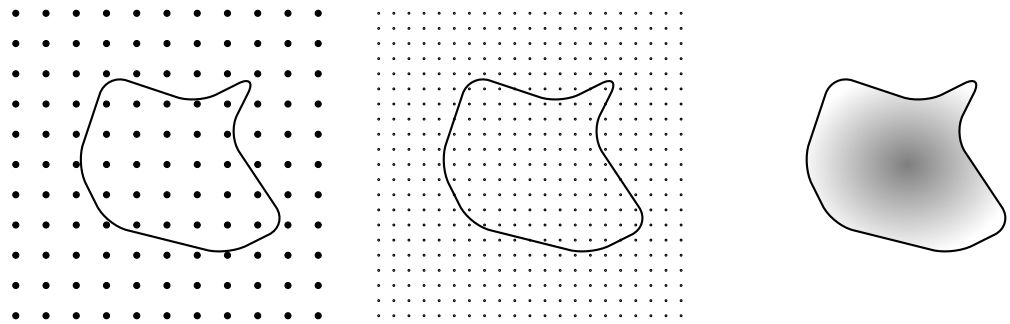

Figure 1: Scaling of a 2D spin lattice: each sub-plot represents the domain Ω and (a) the square lattice $\mathcal{L}$; (b) the shrunk square lattice $\mathcal{L}_2$; (c) the homogeneized lattice in Ω as $n \to \infty$.

2.3 Regularity assumptions

In order to pass to the limit as $n \to \infty$, we have to assume that the magnetic moments are locally almost aligned. The definition of locality is given by an integer multiple $k \in \mathbb{N}^*$ of the shrunk mesh size a/n.

We define a first regularity assumption that only depends on the distance. For all $x \in \mathbb{R}^d$ and $r > 0$, we denote by $\mathcal{B}(x, r)$ the ball of center x and radius r in $\mathbb{R}^d$.

Hypothesis 1. *For all $n \in \mathbb{N}^*$, there exists $\zeta_n > 0$ such that*

$$\forall x \in \Omega,\ \forall y, z \in \mathcal{L}_{n,\Omega} \cap \mathcal{B}\left(x, \frac{ka}{n}\right), \qquad 1 - \zeta_n \leqslant \mu_{n,y} \cdot \mu_{n,z} \leqslant 1,$$

where $\zeta_n = O(1/n^2)$.

We are indeed interested in the limit when we have a more and more dense lattice of more and more aligned spins. We therefore perform a diagonal process and correlate n and the spin alignment.

To define the averaging process we will also need to assume the Ω has the *uniform cone property.*

Hypothesis 2. *There exists an angle α and a radius r, such that for all $y \in \Omega$ there exists a cone C_y of angle α with vertex at y such that $B(y, r) \cap C_y \subset \Omega$.*

2.4 Partitions adapted to the lattices

Let us first work on the initial lattice. To this aim, we define a partition of unity $(\rho_x)_{x\in k\mathcal{L}}$ adapted to the dilated lattice $k\mathcal{L}$. Since our lattice is uniform and all the nodes are equivalent, all the ρ_x are equal up to a translation (see Figure 2), i.e. there exists $\rho^\star \in \mathcal{C}_0^\infty(\mathbb{R}^d;\mathbb{R})$ such that

$$\forall x \in k\mathcal{L},\ \forall y \in \mathbb{R}^d,\ \rho_x(y) = \rho^\star(y-x).$$

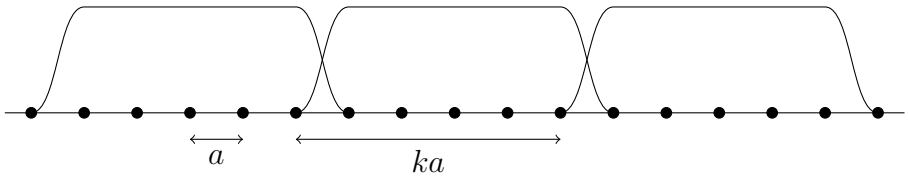

Figure 2: Partition $(\rho_x)_{x\in k\mathcal{L}}$ in dimension 1.

Without lack of generality, we assume that $\rho^\star > 0$ and $\operatorname{supp}\rho^\star \in B(ka)$. By definition of a partition

$$\forall y \in \mathbb{R}^d,\ \sum_{x\in k\mathcal{L}} \rho_x(y) = \sum_{x\in k\mathcal{L}} \rho^\star(y-x) = 1.$$

Let n_k be the number of nodes in $\mathcal{B}(0,ka)$, which is e.g. $n_k = (2k+1)^d$ for a cubic lattice. If we now sum over all the $x \in \mathcal{L}$, we have the same translation property and

$$\forall y \in \mathbb{R}^d,\ \sum_{x\in \mathcal{L}} \rho^\star(y-x) = n_k.$$

Defining $\rho = n_k^{-1}\rho^\star$, we have

$$\forall y \in \mathbb{R}^d,\ \sum_{x\in \mathcal{L}} \rho(y-x) = 1,$$

and therefore a continuous partition of unity on $\mathbb{R}^d$.

Now, we adapt this partition to the shrunk lattice $\mathcal{L}_n$. Defining

$$\forall n \in \mathbb{N}^*,\ \rho_n(x) = \rho(h_n^{-1}x),$$

we have a continuous partition adapted to the shrunk lattice (see Figure 3)

$$\forall y \in \mathbb{R}^d,\ \sum_{x\in \mathcal{L}_n} \rho_n(y-x) = 1 \text{ and } \operatorname{supp}\rho_n \subset \mathcal{B}(0,\frac{ka}{n}).$$

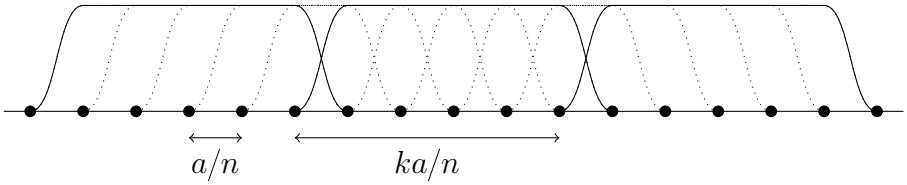

Figure 3: Partition $(\rho_x)_{x\in\mathcal{L}_n}$ in dimension $d = 1$.

Since $\nabla\rho^\star$ is uniformly bounded (i.e. $O(1)$), then $\nabla\rho_n$ is uniformly $O(n)$.

To define an averaging process we will have to use a truncated partition of unity, namely

$$\Phi_n(y) = \sum_{x\in\mathcal{L}_{n,\Omega}} \rho_n(y-x).$$

We clearly have $0 \leqslant \Phi_n(y) \leqslant 1$ and as a finite sum of $\mathcal{C}^\infty$ functions, $\Phi_n \in \mathcal{C}^\infty(\mathbb{R}^d;\mathbb{R})$. We also have a stronger result, namely $\Phi_n(y)$ is bounded from below uniformly in n and $y \in \Omega$: there exists $b > 0$ and $n_0 \in \mathbb{N}^*$ such that

$$\forall y \in \Omega,\ \forall n \geqslant n_0, \qquad b \leqslant \Phi_n(y) \leqslant 1.$$

This result stems from the "cone property" (Hypothesis 2). Besides $\nabla\Phi_n$ is uniformly $O(n)$.

2.5 Averaging process

From the sequence $(\mu_n)_{n\in\mathbb{N}*}$ of vector fields, we now define a new sequence $(m_n)_{n\geqslant n_0}$ of regular vector fields on Ω: for all $n \geqslant n_0$, we define

$$m_n = \frac{1}{\Phi_n}\mu_n \star \rho_n,$$

Remark 1. *Since ρ_n and $\Phi_n \in \mathcal{C}^\infty(\mathbb{R}^d;\mathbb{R})$, and Φ_n is bounded from below by $b > 0$, it immediately follows that $m_n \in \mathcal{C}^\infty(\Omega;\mathbb{R}^3)$. In particular, since Ω is bounded, $m_n \in H^1(\Omega;\mathbb{R}^3)$.*

Lemma 1. *The sequence $(m_n)_{n\geqslant n_0}$ is bounded in $L^\infty(\Omega;\mathbb{R}^3)$ and $L^2(\Omega;\mathbb{R}^3)$.*

Proof. Recall

$$\mu_n = \sum_{x\in\mathcal{L}_{n,\Omega}} \mu_{n,x}\delta_x,$$

hence, for all $y \in \Omega$,

$$m_n(y) = \frac{1}{\Phi_n(y)} \sum_{x \in \mathcal{L}_{n,\Omega}} \mu_{n,x} \rho_n(y-x).$$

We clearly have

$$\begin{aligned}
\left| \frac{1}{\Phi_n(y)} \sum_{x \in \mathcal{L}_{n,\Omega}} \mu_{n,x} \rho_n(y-x) \right| &\leqslant \frac{1}{\Phi_n(y)} \sum_{x \in \mathcal{L}_{n,\Omega}} |\mu_{n,x}| \rho_n(y-x) = \frac{\Phi_n(y)}{\Phi_n(y)} = 1, \\
\|m_n\|_{L^\infty(\Omega;\mathbb{R}^3)} &\leqslant 1, \\
\|m_n\|_{L^2(\Omega;\mathbb{R}^3)} &\leqslant \sqrt{|\Omega|}.
\end{aligned}$$

□

Proposition 1. *Under Hypothesis 1, $(m_n)_{n \geqslant n_0}$ is a bounded sequence in $H^1(\Omega;\mathbb{R}^3)$.*

Proof. For all $y \in \Omega$, we write

$$\begin{aligned}
\nabla m_n(y) &= \nabla \left(\frac{1}{\Phi_n(y)} \right) \sum_{x \in \mathcal{L}_{n,\Omega}} \mu_{n,x} \rho_n(y-x) + \frac{1}{\Phi_n(y)} \nabla \sum_{x \in \mathcal{L}_{n,\Omega}} \mu_{n,x} \rho_n(y-x), \\
&= -\frac{\nabla \Phi_n(y)}{\Phi_n(y)} \otimes m_n(y) + \frac{1}{\Phi_n(y)} \sum_{x \in \mathcal{L}_{n,\Omega}} \nabla \rho_n(y-x) \otimes \mu_{n,x}.
\end{aligned}$$

Let $x_y \in \mathcal{L}_{n,\Omega} \cap \operatorname{supp} \rho_n(y - \cdot)$, we can write

$$\begin{aligned}
\sum_{x \in \mathcal{L}_{n,\Omega}} \nabla \rho_n(y-x) \otimes \mu_{n,x} &= \sum_{x \in \mathcal{L}_{n,\Omega}} \nabla \rho_n(y-x) \otimes (\mu_{n,x_y} + (\mu_{n,x} - \mu_{n,x_y})) \\
&= \sum_{x \in \mathcal{L}_{n,\Omega}} \nabla \rho_n(y-x) \otimes \mu_{n,x_y} \\
&\quad + \sum_{x \in \mathcal{L}_{n,\Omega}} \nabla \rho_n(y-x) \otimes (\mu_{n,x} - \mu_{n,x_y}) \\
&= \nabla \Phi_n(y) \otimes \mu_{n,x_y} \\
&\quad + \sum_{x \in \mathcal{L}_{n,\Omega}} \nabla \rho_n(y-x) \otimes (\mu_{n,x} - \mu_{n,x_y}).
\end{aligned}$$

Hence

$$\begin{aligned}
\nabla m_n(y) &= -\frac{\nabla \Phi_n(y)}{\Phi_n(y)} \otimes m_n(y) + \frac{\nabla \Phi_n(y)}{\Phi_n(y)} \otimes \mu_{n,x_y} \\
&\quad + \left(\frac{1}{\Phi_n(y)} \right) \sum_{x \in \mathcal{L}_{n,\Omega}} \nabla \rho_n(y-x) \otimes (\mu_{n,x} - \mu_{n,x_y})
\end{aligned}$$

$$
\begin{aligned}
&= -\frac{\nabla\Phi_n(y)}{\Phi_n(y)} \otimes \left(\mu_{n,x_y} + \frac{1}{\Phi_n(y)} \sum_{x \in \mathcal{L}_{n,\Omega}} (\mu_{n,x} - \mu_{n,x_y}) \rho_n(y-x) \right) \\
&+ \frac{\nabla\Phi_n(y)}{\Phi_n(y)} \otimes \mu_{n,x_y} + \left(\frac{1}{\Phi_n(y)} \right) \sum_{x \in \mathcal{L}_{n,\Omega}} \nabla\rho_n(y-x) \otimes (\mu_{n,x} - \mu_{n,x_y}) \\
&= \frac{\nabla\Phi_n(y)}{\Phi_n(y)^2} \otimes \left(\sum_{x \in \mathcal{L}_{n,\Omega}} (\mu_{n,x_y} - \mu_{n,x}) \rho_n(y-x) \right) \\
&+ \left(\frac{1}{\Phi_n(y)} \right) \sum_{x \in \mathcal{L}_{n,\Omega}} \nabla\rho_n(y-x) \otimes (\mu_{n,x} - \mu_{n,x_y}).
\end{aligned}
$$

In both sums there is only an $O(1)$ number of terms for which ρ_n or $\nabla\rho_n$ is non zero. In the first sum, by Hypothesis 1, $|\mu_{n,x} - \mu_{n,x_y}| = O(\zeta_n^{1/2}) = O(1/n)$. Besides $|\nabla\Phi_n(y)| = O(n)$ and Φ_n is bounded from below. The first term is therefore $O(1)$. In the second sum $|\mu_{n,x} - \mu_{n,x_y}| = O(1/n)$ and $\nabla\rho_n(y-x) = O(n)$. Hence there exists $C' > 0$ such that, for all $y \in \Omega$ and $n \geqslant n_0$, $|\nabla m_n(y)| \leqslant C'$.

Finally, Ω being bounded, hence $(\|\nabla m_n\|_{L^2(\Omega;\mathbb{R}^{3d})})_{n \geqslant n_0}$ is a bounded sequence. □

2.6 Asymptotics towards a mesoscopic model

Since $H^1(\Omega;\mathbb{R}^3)$ is weakly compact, Proposition 1 implies that there exists $m \in H^1(\Omega;\mathbb{R}^3)$ such that

$$m_n \rightharpoonup m \text{ weakly in } H^1(\Omega;\mathbb{R}^3).$$

From now on, we have to assume that Ω is compact (closed) and has a piecewise $\mathcal{C}^1$ boundary, to ensure that this implies that this convergence is strong in $L^2(\Omega;\mathbb{R}^3)$.

Proposition 2. *Under Hypothesis 1, m has a constant norm equal to 1 almost everywhere on Ω.*

Remark 2. *We recover here a property of the magnetization field in Brown's model of micromagnetism [4], where the constant norm is assumed.*

Proof. We have seen that for all $n \geqslant n_0$ and $y \in \Omega$, $|m_n(y)| \leqslant 1$. We want to show that it is also bounded from below and pass to the limit. For all $y \in \Omega$,

since $|\mu_{n,x}|^2 = 1$,

$$\begin{aligned} |m_n(y)|^2 &= \Big|\frac{1}{\Phi_n(y)} \sum_{x \in \mathcal{L}_{n,\Omega}} \mu_{n,x} \rho_n(y-x)\Big|^2 \\ &= \frac{1}{\Phi_n(y)^2} \sum_{x,x' \in \mathcal{L}_{n,\Omega}} \mu_{n,x} \cdot \mu_{n,x'}\ \rho_n(y-x)\rho_n(y-x'). \end{aligned}$$

Since $\operatorname{supp} \rho_n \subset \mathcal{B}(0, ka/n)$, the sum runs indeed on $\mathcal{L}_{n,\Omega} \cap \mathcal{B}(y, ka/n)$:

$$|m_n(y)|^2 = \frac{1}{\Phi_n(y)^2} \sum_{x,x' \in \mathcal{L}_{n,\Omega} \cap \mathcal{B}(y, \frac{ka}{n})} \mu_{n,x} \cdot \mu_{n,x'}\ \rho_n(y-x)\rho_n(y-x').$$

Hypothesis 1 implies that

$$\forall x, x' \in \mathcal{L}_{n,\Omega} \cap \mathcal{B}(y, \frac{ka}{n}),\ 1 - \zeta_n \leqslant \mu_{n,x} \cdot \mu_{n,x'} \leqslant 1.$$

and we also have that

$$\forall y \in \Omega,\ \sum_{x,x' \in \mathcal{L}_{n,\Omega}} \rho_n(y-x)\rho_n(y-x') = \Phi_n(y)^2,$$

therefore

$$\begin{aligned} \frac{1}{\Phi_n(y)^2}(1-\zeta_n)\Phi_n(y)^2 \leqslant\ & |m_n(y)|^2 \ \leqslant \frac{1}{\Phi_n(y)^2}\Phi_n(y)^2, \\ 1 - \zeta_n \leqslant\ & |m_n(y)|^2 \ \leqslant 1. \end{aligned}$$

In the $L^2(\Omega; \mathbb{R}^3)$ limit, we therefore have $|m| = \chi_\Omega$ almost everywhere. □

3 Towards the exchange energy

3.1 Heisenberg interaction

The interaction of the spins is described by the Heisenberg energy, which can be written as follows:

$$e_{x,y} = -\frac{1}{2} A_{x,y}(\mu_x \cdot \mu_y - 1),$$

where $A_{x,y} \geqslant 0$ only depends on the distance between x and y. We make the assumption that each node x only interacts with its neighbors N_x.

Let $V_0 \subset \mathcal{L}$ be the set of neighboring nodes in interaction with the node $(0,0,0)$ *via* the Heisenberg energy. In the shrunk lattice, we will restrict

the computation of this energy to elements x and y in $\in \mathcal{L}_{n,\Omega}$. Since the lattice is homogeneous, the neighbors of any given node $x \in \mathcal{L}_{n,\Omega}$ can be deduced from the definition of N_0: $N_{n,\Omega,x} = (\{x\} + h_n^{-1}(N_0)) \cap \Omega$. We also assume that (a) N_0 (and hence $N_{n,\Omega,x}$) is a finite set; (b) $N_0 \subset \mathcal{B}(0, ka)$ (i.e. $N_{n,\Omega,x} \subset \mathcal{B}(x, ka/n)$).

We therefore define the node energy by

$$e_x = \sum_{y \in N_x} e_{x,y} = -\frac{1}{2} \sum_{y \in N_x} A_{x,y}(\mu_x \cdot \mu_y - 1).$$

In what follows we will restrict the study to $3D$ cubic lattices. Dimensions 1 and 2 are also possible to treat in the same way. The fact that the lattice is cubic is used in the explicit computations, but our proof may be extended to other classes of regular lattices. We also consider as neighbors only the 6 closest ones on the cubic lattice, which at at the same distance. Since $A_{x,y}$ only depends on the distance, which is now equal for all the neighbors, we can set

$$A_{x,y} = \begin{cases} A > 0, & \text{if } y \in N_x; \\ 0, & \text{else.} \end{cases}$$

For all $n \in \mathbb{N}^*$, we define the exchange energy of the domain Ω associated to the spin distribution μ_n summing up the node energies scales to

$$\mathcal{E}_{n,\mathrm{ex}}(\mu_n) = \sum_{x \in \mathcal{L}_{n,\Omega}} e_x = \frac{a}{n} \sum_{x \in \mathcal{L}_{n,\Omega}} \sum_{y \in N_{n,\Omega,x}} A|\mu_{n,y} - \mu_{n,x}|^2.$$

3.2 Spaces and convergence

We define the space sequence $(W_n)_{n \in \mathbb{N}^*}$ by $W_n = (\mathbb{R}^3)^{\mathcal{L}_{n,\Omega}}$. In the sequel, we set $W = \prod_{n \in \mathbb{N}^*} W_n$.

Hypothesis 3. *Let $\boldsymbol{\mu} = (\mu_n)_{n \in \mathbb{N}^*} \in \prod_{n \in \mathbb{N}^*} W_n$. There exists $c > 0$ such that*

$$\forall n \in \mathbb{N}^*,\ \forall x \in \mathcal{L}_{n,\Omega},\ \forall y \in N_{n,\Omega,x}, \qquad |\mu_{n,x} - \mu_{n,y}|^2 \leqslant \frac{c}{n^2},$$

except possibly for a subset $l_{n,\Omega} \subset \mathcal{L}_{n,\Omega}$ such that $\#(l_{n,\Omega}) = O(n)$, and there exists a sequence $(c_n)_{n \geqslant 1} \in \mathbb{R}^{\mathbb{N}^*}$ such that $c_n \xrightarrow[n \to \infty]{} 0$ and

$$\forall n \in \mathbb{N}^*,\ \forall x \in l_{n,\Omega},\ \forall y \in N_{n,\Omega,x},\ |\mu_{n,x} - \mu_{n,y}|^2 \leqslant c_n.$$

More precisely, given the constant c, $x \in l_{n,\Omega}$ if there exists $y \in N_{n,\Omega,x}$ such that $|\mu_{n,x} - \mu_{n,y}|^2 > c/n^2$. Hypothesis 3 is a little weaker than Hypothesis 1.

We denote by $W^{\mathfrak{h}} \subset W$ the set of $\boldsymbol{\mu} = (\mu_n)_{n\in\mathbb{N}^*}$ for which Hypothesis 3 holds and $W_1^{\mathfrak{h}} \subset W^{\mathfrak{h}}$ the set of $\boldsymbol{\mu} \in W^{\mathfrak{h}}$ for which $|\mu_{n,x}| = 1$, $\forall n \in \mathbb{N}^*$, $\forall x \in \mathcal{L}_{n,\Omega}$.

We want to define the convergence of elements of W towards elements of the limit space $H^1(\Omega;\mathbb{R}^3)$. To this aim we define a partition of the domain $\Omega \subset \mathbb{R}^3$ in tetrahedra, by groups of 5 tetrahedra (see Figure 4 and Section 3.3.1).

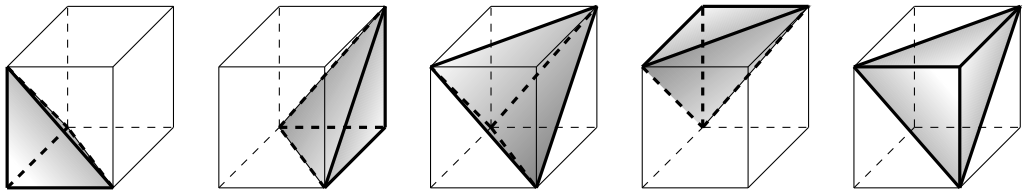

Figure 4: Partition of a single 3D lattice cell. These five tetrahedra are elements $\mathcal{T}_n$, and T_n for the corner tetrahedra, and T_n^* for the center tetrahedron (see Section 3.3.1).

Definition 1. *We define the projection $P_n : W_n \longrightarrow H^1(\Omega;\mathbb{R}^3)$ such that $P_n(\mu_n)$ is equal to μ_n on the lattice nodes and linear on each element of the partition.*

Definition 2. *We say that $\boldsymbol{\mu} \in W$ converges to $m \in H^1(\Omega;\mathbb{R}^3)$ if $P_n(\mu_n)$ converges weakly in $H^1(\Omega;\mathbb{R}^3)$ to m as $n \to \infty$. We denote this $\mu_n \xrightarrow[n\to\infty]{} m$.*

Definition 3. *We define the projection $p_n : \mathcal{C}(\Omega;\mathbb{R}^3) \longrightarrow W_n$, such that for all $m \in \mathcal{C}(\Omega;\mathbb{R}^3)$, $p_n(m) \in W_n$ and for all $x \in \mathcal{L}_{n,\Omega}$, $(p_n(m))_x = m(x)$.*

3.3 Main result

The exchange energy $\mathcal{E}_{n,\mathrm{ex}}$ is a functional defined on W_n. The main result of this paper is the following

Theorem 1. *Let $(\mu_n)_{n\in\mathbb{N}^*} \in W^{\mathfrak{h}}$. In the sense of the topology defined by Definition 2*

$$\mathcal{E}_{n,\mathrm{ex}} \xrightarrow[n\to\infty]{\Gamma} \mathcal{E}_{\infty,\mathrm{ex}},$$

where

$$\begin{aligned} \mathcal{E}_{\infty,\mathrm{ex}} : \ H^1(\Omega;\mathbb{R}^3) &\longrightarrow \mathbb{R}_+ \\ m &\longmapsto 2A\int_\Omega |\nabla m(x)|^2 \mathrm{d}x. \end{aligned}$$

Moreover, this convergence is compatible with the unit norm constraint.

Remark 3. *The Γ-convergence result is two-fold [3]:*

construction: *for all $m \in H^1(\Omega;\mathbb{R}^3)$, there exists $\boldsymbol{\mu} \in W$ such that $\mu_n \to m$ and $\limsup_{n\to\infty} \mathcal{E}_{n,\mathrm{ex}}(\mu_n) \leqslant \mathcal{E}_{\infty,\mathrm{ex}}(m)$.*

lower semi-continuity: *for all $\boldsymbol{\mu} \in W$, such that $\|\mu_n\| \leqslant B$, $\mu_n \to m_\infty \in H^1(\Omega;\mathbb{R}^3)$ and $\liminf_{n\to\infty} \mathcal{E}_{n,\mathrm{ex}}(\mu_n) \geqslant \mathcal{E}_{\infty,\mathrm{ex}}(m_\infty)$.*

Proof. The proof of Theorem 1 splits into many steps to which various lemmas are devoted, the technical proofs of which are postponed.

Lemma 2. *Let $(\mu_n)_{n\in\mathbb{N}^*} \in W^{\mathfrak{h}}$, then there exists $m_\infty \in H^1(\Omega;\mathbb{R}^3)$ such that $\mu_n \xrightarrow[n\to\infty]{} m_\infty$.*

Now this function m_∞ is only in $H^1(\Omega;\mathbb{R}^3)$, and not continuous, and we need to use pointwise values of this function. Therefore, for all ε, we approximate m_∞ by a $\mathcal{C}^1(\Omega;\mathbb{R}^3)$ which coincides with m_∞ on a smaller domain Ω_ε. We denote by λ the Lebesgue measure on $\mathbb{R}^d$.

Lemma 3. *Let $u \in H^1(\Omega;\mathbb{R}^3)$, for all $\varepsilon > 0$, there exists an open set $\omega_{u,\varepsilon}$ and a function $u_\varepsilon \in \mathcal{C}^1(\Omega;\mathbb{R}^3)$ such that for all $x \in \Omega\backslash\omega_{u,\varepsilon}$, $u_\varepsilon(x) = u(x)$, $\lambda(\omega_{u,\varepsilon}) < \varepsilon$, and*

$$\lim_{n\to\infty} \frac{\#(\mathcal{L}_{n,\Omega} \cap \omega_{u,\varepsilon})}{\#(\mathcal{L}_{n,\Omega})} < \varepsilon.$$

Corollary 1. *Let $u \in H^1(\Omega,\mathbb{R}^3)$, for all $\varepsilon > 0$, there exists an open set $\Omega_{u,\varepsilon} \subset \Omega$ with piecewise $\mathcal{C}^1$ boundary such that $\lambda(\Omega\backslash\Omega_{u,\varepsilon}) \leqslant \varepsilon$ and*

$$u_{|\Omega_{u,\varepsilon}} \in \mathcal{C}^1(\Omega_{u,\varepsilon};\mathbb{R}^3).$$

Lemma 4. *Let $u \in \mathcal{C}^1(\Omega;\mathbb{R}^3)$, then $(p_n(u))_{n\in\mathbb{N}^*} \in W^{\mathfrak{h}}$, $p_n(u) \xrightarrow[n\to\infty]{} u$ and $\lim_{n\to\infty} \mathcal{E}_{n,\mathrm{ex}}(p_n(u)) = \mathcal{E}_{\infty,\mathrm{ex}}(u)$. Moreover if u has a constant unit norm, then $(p_n(u))_{n\in\mathbb{N}^*} \in W_1^{\mathfrak{h}}$.*

For all $\varepsilon > 0$, we can therefore associate to m_∞ an open set Ω_ε on which it is $\mathcal{C}^1$ and define the approximate energies:

$$\begin{aligned}
\mathcal{E}^\varepsilon_{n,\mathrm{ex}}(\mu_n) &= \frac{a}{n} \sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y\in N_{n,\Omega_\varepsilon,x}} A|\mu_{n,y} - \mu_{n,x}|^2, \qquad \text{for all } n \in \mathbb{N}^*, \\
\mathcal{E}^\varepsilon_{\infty,\mathrm{ex}}(m_\infty) &= 2A \int_{\Omega_\varepsilon} |\nabla m_\infty(x)|^2 \mathrm{d}x.
\end{aligned}$$

Comparing $\mathcal{E}^\varepsilon_{n,\mathrm{ex}}(\mu_n)$ and $\mathcal{E}^\varepsilon_{n,\mathrm{ex}}(p_n(m_\infty))$, we first show that

Lemma 5. *For all* $\varepsilon > 0$, $\liminf_{n\to\infty} \mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n) \geqslant \mathcal{E}^{\varepsilon}_{\infty,\mathrm{ex}}(m_\infty)$.

Estimating the remainder of the sums and integrals on ω_ε, we can then prove

Lemma 6. $\liminf_{n\to\infty} \mathcal{E}_{n,\mathrm{ex}}(\mu_n) \geqslant \mathcal{E}_{\infty,\mathrm{ex}}(m_\infty)$.

□

3.3.1 Proof of Lemma 2: Limit of a lattice of spins

Lemma 2 is proved using an explicit computation of the projection $P_n(\mu_n)$. To this aim, we define, for all $n \in \mathbb{N}^*$,

- $\mathcal{T}_n$, the set of tetrahedra which form the partition of $\mathcal{L}_{n,\Omega}$;
- T_n, the set of corner tetrahedra (4 for each mesh of the lattice, see Figure 4);
- T_n^*, the set of center tetrahedra (1 for each mesh of the lattice, see Figure 4);
- E_n, the set of edges of the mesh of $\mathcal{L}_{n,\Omega}$ (given by couples of the indices of the lattice nodes);
- C_n, the set of edges of elements of T_n^*;
- S_n, the set of outer surfaces of T_n (triplets (i,j,k) where $(i,j) \in C_n$, (i,k) and $(j,k) \in E_n$).

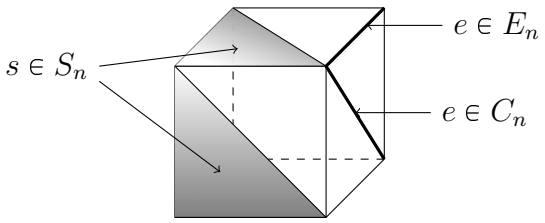

Figure 5: Different sets of tetraedra and edges.

Remark 4. *Generically* $\Omega_n \equiv \cup_{\tau\in\mathcal{T}_n} \tau \subsetneq \Omega$. *We suppose that the geometry of* Ω *is such that* $\lambda(\Omega\backslash\Omega_n) = O(1/n)$, *i.e. there are order* n^2 *tetrahedra covering the difference set. We set* $P_n(\mu_n)$ *to zero on* $\Omega\backslash\Omega_n$.

Step 1. Estimate of $\int_\Omega |P_n(\mu_n)(x)|^2 \mathrm{d}x$.

Let $x \in \Omega_n$, then there exists $\tau \in \mathcal{T}_n$ and $x \in \tau$. Since $P_n(\mu_n)$ is linear on τ, then $P_n(\mu_n)(x)$ is a pondered mean of the μ_{n,x_i^τ}, $i = 1, \dots, 4$, where $(x_1^\tau, x_2^\tau, x_3^\tau, x_4^\tau) \in (\mathcal{L}_{n,\Omega})^4$ are the vertices of τ. Therefore $|P_n(\mu_n)(x)| \leqslant 1$. Hence

$$\begin{aligned}\int_\Omega |P_n(\mu_n)(x)|^2 \mathrm{d}x &= \int_{\Omega_n} |P_n(\mu_n)(x)|^2 \mathrm{d}x = \sum_{\tau \in \mathcal{T}_n} \int_\tau |P_n(\mu_n)(x)|^2 \mathrm{d}x \\ &\leqslant \sum_{\tau \in \mathcal{T}_n} \lambda(\tau) = \lambda(\Omega_n).\end{aligned}$$

Step 2. Explicit computation of $\int_\Omega |\nabla P_n(\mu_n)(x)|^2 \mathrm{d}x$.

We compute $\int_\Omega |\nabla P_n(\mu_n)(x)|^2 \mathrm{d}x$ explicitly using the tetrahedron decomposition of the lattice. On each tetrahedron $P_n(\mu_n)$ is linear, and therefore its gradient is constant.

If $\tau \in T_n$, we can construct an orthogonal system using the lattice nodes $(x_1^\tau, x_2^\tau, x_3^\tau, x_4^\tau) \in (\mathcal{L}_{n,\Omega})^4$, for example $(\mu_{n,x_i^\tau} - \mu_{n,x_1^\tau})_{i=2,\dots,4}$. Each direction yields one component of the gradient. Since the length of the edges are a/n, the component of the gradient are the $(\mu_{n,x_i^\tau} - \mu_{n,x_1^\tau})n/a$. Besides the volume of τ is $\frac{1}{6}(a/n)^3$, therefore

$$\int_\tau |\nabla P_n(\mu_n)(x)|^2 \mathrm{d}x = \frac{a}{6n} \sum_{i=2}^4 |\mu_{n,x_i^\tau} - \mu_{n,x_1^\tau}|^2.$$

For a center tetrahedron $\tau* \in T_n^*$, it is a bit more tricky since the edges are not orthogonal. The volume is of course the complement of the volumes of the corner tetrahedra, namely $\frac{1}{3}(a/n)^3$. The computation yields

$$|\nabla P_n(\mu_n)(x)|^2 = \frac{n^2}{4a^2} \sum_{1 \leqslant i,j \leqslant 4} |\mu_{n,x_i^{\tau*}} - \mu_{n,x_j^{\tau*}}|^2$$

and hence

$$\int_{\tau*} |\nabla P_n(\mu_n)(x)|^2 \mathrm{d}x = \frac{a}{12n} \sum_{1 \leqslant i,j \leqslant 4} |\mu_{n,x_i^{\tau*}} - \mu_{n,x_j^{\tau*}}|^2.$$

Gathering all the contributions

$$\begin{aligned}
&\int_\Omega |\nabla P_n(\mu_n)(x)|^2 \mathrm{d}x \\
&\qquad = \sum_{\tau\in\mathcal{T}_n} \int_\tau |\nabla P_n(\mu_n)(x)|^2 \mathrm{d}x \\
&\qquad = \sum_{\tau\in T_n} \int_\tau |\nabla P_n(\mu_n)(x)|^2 \mathrm{d}x + \sum_{\tau*\in T_n^*} \int_{\tau*} |\nabla P_n(\mu_n)(x)|^2 \mathrm{d}x \\
&\qquad = 4 \sum_{(i,j)\in E_n} \frac{a}{6n} |\mu_{n,x_i} - \mu_{n,x_j}|^2 + 2 \sum_{(i,j)\in C_n} \frac{a}{12n} |\mu_{n,x_i} - \mu_{n,x_j}|^2 - \mathcal{S}_{n,\Omega}.
\end{aligned}$$

The coefficient 4 in front of the sum on E_n occurs because each element of E_n is an element of four $\tau \in T_n$. Similarly each element of C_n belongs to two $\tau^* \in T_n^*$. The positive error $\mathcal{S}_{n,\Omega}$ is due to an over-estimation because some of the edges $e \in E_n$ are on the outer surface of Ω_n and have been counted too many times. Following Remark 4, the contribution of $\mathcal{S}_{n,\Omega}$ will always be $O(1/n)$ less than that of the other terms, and therefore will tend to zero as $n \to \infty$.

We rewrite the first sum

$$4 \sum_{(i,j)\in E_n} \frac{a}{6n} |\mu_{n,x_i} - \mu_{n,x_j}|^2 = \sum_{x\in\mathcal{L}_{n,\Omega}} \sum_{y\in N_{n,\Omega,x}} \frac{a}{3n} |\mu_{n,x} - \mu_{n,y}|^2$$

(here each edge is counted twice through the couples (x, y) and (y, x)). For $x \in l_{n,\Omega}$, we can only estimate $(a/3n)|\mu_{n,x} - \mu_{n,y}|^2 \leqslant 4a/3n$, but there are only $O(n)$ such terms. For $x \in \mathcal{L}_{n,\Omega}\backslash l_{n,\Omega}$, $(a/3n)|\mu_{n,x} - \mu_{n,y}|^2 \leqslant ac/3n^3$ and there are $O(n^3)$ such terms. Therefore

$$4 \sum_{(i,j)\in E_n} \frac{a}{6n} |\mu_{n,x_i} - \mu_{n,x_j}|^2 = O(1).$$

For the second sum

$$\begin{aligned}
&\sum_{(i,j)\in C_n} \frac{a}{6n} |\mu_{n,x_i} - \mu_{n,x_j}|^2 = \frac{1}{2} \sum_{(i,j,k)\in S_n} \frac{a}{6n} |\mu_{n,x_i} - \mu_{n,x_k} + \mu_{n,x_k} - \mu_{n,x_j}|^2 \\
&= \sum_{(i,j,k)\in S_n} \frac{a}{12n} \Big(|\mu_{n,x_i} - \mu_{n,x_k}|^2 + |\mu_{n,x_j} - \mu_{n,x_k}|^2 \\
&\qquad\qquad + 2(\mu_{n,x_i} - \mu_{n,x_k}) \cdot (\mu_{n,x_k} - \mu_{n,x_j}) \Big) \\
&= \sum_{(i,j)\in E_n} \frac{a}{3n} |\mu_{n,x_i} - \mu_{n,x_j}|^2 + \sum_{(i,j,k)\in S_n} \frac{a}{6n} (\mu_{n,x_i} - \mu_{n,x_k}) \cdot (\mu_{n,x_k} - \mu_{n,x_j}) \\
&= \sum_{x\in\mathcal{L}_{n,\Omega}} \sum_{y\in N_{n,\Omega,x}} \frac{a}{6n} |\mu_{n,x} - \mu_{n,y}|^2 + \sum_{(i,j,k)\in S_n} \frac{a}{6n} (\mu_{n,x_i} - \mu_{n,x_k}) \cdot (\mu_{n,x_k} - \mu_{n,x_j}).
\end{aligned}$$

As for the previous sum, we can decompose these sums into two $O(1)$ contributions. There are at most $O(n)$ terms contributing to $\mathcal{S}_{n,\Omega}$ and stemming from an $x \in l_{n,\Omega}$, therefore $\mathcal{S}_{n,\Omega} = O(1)$. Therefore $\|P_n(\mu_n)\|_{H^1(\Omega;\mathbb{R}^3)}$ is uniformly bounded and $P_n(\mu_n)$ is weakly convergent in $H^1(\Omega;\mathbb{R}^3)$. This, together with our convergence definition 2, leads to Lemma 2.

A by-product of this proof is the fact that we can write

$$\|\nabla P_n(\mu_n)\|^2_{L^2(\Omega;\mathcal{L}(\mathbb{R}^3;\mathbb{R}^3))} = \int_\Omega |\nabla P_n(\mu_n)(x)|^2 \mathrm{d}x = \frac{1}{2A}\mathcal{E}_{n,\mathrm{ex}}(\mu_n) + \alpha_n(\mu_n)$$

where

$$\alpha_n(\mu_n) = \frac{a}{6n} \sum_{(i,j,k)\in S_n} (\mu_{n,x_i} - \mu_{n,x_k}) \cdot (\mu_{n,x_k} - \mu_{n,x_j}) - \mathcal{S}_{n,\Omega}.$$

3.3.2 Proof of Lemma 3: $\mathcal{C}^1$ approximation of a H^1 function

Following Ziemer theorem ([10], Theorem 3.11.6), we know that for any function $u \in H^1(\Omega;\mathbb{R}^3)$ and for all $\varepsilon > 0$, there exists a function $u_\varepsilon \in \mathcal{C}^1(\Omega;\mathbb{R}^3)$ such that $\lambda(\omega_{u,\varepsilon}) \leqslant \varepsilon$, where

$$\omega_{u,\varepsilon} := \{x \in \Omega \text{ such that } u(x) \neq u_\varepsilon(x)\}.$$

We want to extend this result and be able to localize the irregularities of u with respect to a shrinking lattice.

Let $u \in H^1(\Omega;\mathbb{R}^3)$, and X_u be the set of points where u is not $\mathcal{C}^1$. Since the gradient of $u \in H^1(\Omega;\mathbb{R}^3)$ has to be defined almost everywhere, there cannot be an open ball in X_u and therefore $\overline{\overset{\circ}{X_u}} = \varnothing$.

We now fix $\varepsilon > 0$. The Lebesgue and $\mathcal{H}^3$ Hausdorff measures coincide in $\mathbb{R}^3$ and therefore we both have $\lambda(\overline{X_u}) \leqslant \varepsilon$ and $\mathcal{H}^3(\overline{X_u}) \leqslant \varepsilon$.
Hence there exists a sequence of open balls $(B_i)_{i\in\mathbb{N}}$ such that

$$\overline{X_u} \subset \bigcup_{i\in\mathbb{N}} B_i \text{ and } \sum_{i=1}^{\infty} \mathrm{diam}(B_i)^3 < \varepsilon.$$

Since $\overline{X_u}$ is closed and bounded, it is compact and we can extract from this open cover a finite subcover.

Hence there exists $N \in \mathbb{N}$ such that

$$\overline{X_u} \subset \bigcup_{i=1}^{N} B_i \text{ and } \sum_{i=1}^{N} \mathrm{diam}(B_i)^3 < \varepsilon.$$

Obviously $\bigcup_{i=0}^{N} B_i$ is bounded with a piecewise $\mathcal{C}^1$ boundary, hence

$$\lim_{n\to\infty} \frac{\#(\mathcal{L}_{n,\Omega} \cap \bigcup_{i=1}^{N} B_i)}{\#(\mathcal{L}_{n,\Omega})} = \lambda\left(\bigcup_{i=1}^{N} B_i \cap \Omega\right) < \varepsilon$$

Besides $u_{|\cup_{i=1}^{N} B_i} \in H^1(\cup_{i=1}^{N} B_i; \mathbb{R}^3)$, and we therefore can choose u_ε such that $\omega_{u,\varepsilon} \subset \cup_{i=1}^{N} B_i$. Finally

$$\lim_{n\to\infty} \frac{\#(\mathcal{L}_{n,\Omega} \cap \omega_{u,\varepsilon})}{\#(\mathcal{L}_{n,\Omega})} \leqslant \varepsilon.$$

In our proof, we set $\Omega_\varepsilon = \Omega\overbrace{\backslash\omega_{m_\infty,\varepsilon}}^{\circ}$ and begin to work on the restricted shrunk lattice $\mathcal{L}_{n,\Omega_\varepsilon} = \mathcal{L}_{n,\Omega} \bigcap \Omega_\varepsilon$. We also denote $\mathcal{D}_{n,\Omega_\varepsilon}$ the subset of elements $x \in \mathcal{L}_{n,\Omega_\varepsilon}$ such that $\#(N_{n,\Omega,x} \cap \Omega_\varepsilon) \neq 6$, that is the set of nodes which are too close to $\partial\Omega_\varepsilon$ to have their 6 nearest neighbors in Ω_ε.

Since $\partial\Omega_\varepsilon$ is piecewise $\mathcal{C}^1$ for all $\varepsilon > 0$, we know that $\#\mathcal{D}_{n,\Omega_\varepsilon} = O(n^2)$.

3.3.3 Proof of Lemma 4: Construction

Let $x \in \mathcal{L}_{n,\Omega}$ and $y \in N_{n,\Omega,x}$. Since $u \in \mathcal{C}^1(\Omega; \mathbb{R}^3)$, ∇u is bounded by some constant C on Ω and

$$|p_n(u)_x - p_n(u)_y|^2 \leqslant C^2|x-y|^2 \leqslant C^2\left(\frac{a}{n}\right)^2 = \frac{C^2a^2}{n^2}.$$

Therefore $p_n(u) \in W^{\mathfrak{h}}$. Clearly if $|u| = 1$ on Ω, forall $x \in \mathcal{L}_{n,\Omega}$, $|p_n(u)_x| = 1$ and $p_n(u) \in W_1^{\mathfrak{h}}$.

Lemma 2 implies that there exists $u_\infty \in H^1(\Omega; \mathbb{R}^3)$ such that $p_n(u) \xrightarrow[n\to\infty]{} u_\infty$. Since $u \in \mathcal{C}^1(\Omega; \mathbb{R}^3)$, $P_n(p_n(u))$ converges towards u. This convergence is pointwise and even uniform on Ω. Hence $u_\infty = u$.

Last

$$\begin{aligned}
\mathcal{E}_{n,\mathrm{ex}}(p_n(u)) &= \frac{a}{n} \sum_{x\in\mathcal{L}_{n,\Omega}} \sum_{y\in N_{n,\Omega,x}} A|p_n(u)_y - p_n(u)_x|^2 \\
&= \frac{a}{n} \sum_{x\in\mathcal{L}_{n,\Omega}} \sum_{y\in N_{n,\Omega,x}} A|u(y) - u(x)|^2.
\end{aligned}$$

Since $u \in \mathcal{C}^1(\Omega; \mathbb{R}^3)$, for all $x \in \mathcal{L}_{n,\Omega}$ and all $y \in N_{n,\Omega,x}$,

$$\frac{|u(y)-u(x)|^2}{|y-x|^2} = \left|\nabla u(x) \cdot \frac{y-x}{|y-x|}\right|^2 + e_{n,x,y},$$

and therefore for all $x \in \mathcal{L}_{n,\Omega} \backslash \mathcal{D}_{n,\Omega}$

$$\left(\frac{n}{a}\right)^2 \sum_{y \in N_{n,\Omega,x}} |u(y) - u(x)|^2 = 2|\nabla u(x)|^2 + e_{n,x},$$

and the errors $e_{n,x}$ are uniformly $o(1)$ as $n \to \infty$. Hence

$$\mathcal{E}_{n,\mathrm{ex}}(p_n(u)) = 2A \sum_{x \in \mathcal{L}_{n,\Omega}} \left(\frac{a}{n}\right)^3 (|\nabla u(x)|^2 + e_{n,x}) + O(\frac{1}{n}),$$

where the $O(1/n)$ stems from $x \in \mathcal{D}_{n,\Omega}$. Since $\lim_{n\to\infty} \sum_{x \in \mathcal{L}_{n,\Omega}} (a/n)^3 e_{n,x} = 0$, and the border of Ω is piecewise $\mathcal{C}^1$

$$\lim_{n\to\infty} \sum_{x \in \mathcal{L}_{n,\Omega}} \left(\frac{a}{n}\right)^3 |\nabla u(x)|^2 = \int_\Omega |\nabla u(x)|^2 \mathrm{d}x$$

and

$$\lim_{n\to\infty} \mathcal{E}_{n,\mathrm{ex}}(p_n(u)) = \mathcal{E}_{\infty,\mathrm{ex}}(u).$$

3.3.4 Proof of Lemma 5: Lower semi-continuity

With Definition 2 for the convergence, $P_n(\mu_n) \rightharpoonup m_\infty$ in $H^1(\Omega;\mathbb{R}^3)$, and

$$\liminf_{n\to\infty} \|P_n(\mu_n)\|_{H^1(\Omega;\mathbb{R}^3)} \geqslant \|m_\infty\|_{H^1(\Omega;\mathbb{R}^3)}$$

(see [3], Proposition 2.3).

Since we have assumed that Ω is compact and has a piecewise $\mathcal{C}^1$ boundary, we have already seen that the convergence is strong in $L^2(\Omega;\mathbb{R}^3)$ and therefore

$$\liminf_{n\to\infty} \|\nabla P_n(\mu_n)\|^2_{L^2(\Omega;\mathcal{L}(\mathbb{R}^3;\mathbb{R}^d))} \geqslant \|\nabla m_\infty\|^2_{L^2(\Omega;\mathcal{L}(\mathbb{R}^3;\mathbb{R}^d))}.$$

Let us first fix ε and work in Ω_ε. Thanks to Proposition 4, we know that m_∞ is continuous and

$$\|\nabla P_n(p_n(m_\infty))\|_{L^2(\Omega_\varepsilon;\mathcal{L}(\mathbb{R}^3;\mathbb{R}^d))} \xrightarrow[n\to\infty]{} \|\nabla m_\infty\|_{L^2(\Omega_\varepsilon;\mathcal{L}(\mathbb{R}^3;\mathbb{R}^d))}.$$

This implies that

$$\liminf_{n\to\infty} \left(\|\nabla P_n(\mu_n)\|^2_{L^2(\Omega_\varepsilon;\mathcal{L}(\mathbb{R}^3;\mathbb{R}^d))} - \|\nabla P_n(p_n(m_\infty))\|^2_{L^2(\Omega_\varepsilon;\mathcal{L}(\mathbb{R}^3;\mathbb{R}^d))} \right) \geqslant 0.$$

According to Lemma 2, we can write

$$\|\nabla P_n(\mu_n)\|^2_{L^2(\Omega_\varepsilon;\mathcal{L}(\mathbb{R}^3;\mathbb{R}^d))} = \frac{1}{2A}(\mathcal{E}^\varepsilon_{n,\mathrm{ex}}(\mu_n) + \alpha^\varepsilon_n(\mu_n)).$$

We therefore know that

$$\liminf_{n\to\infty}\left(\frac{1}{2A}\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n)-\frac{1}{2A}\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(p_n(m_\infty))+\alpha^{\varepsilon}_n(\mu_n)-\alpha^{\varepsilon}_n(p_n(m_\infty))\right)\geqslant 0.$$

We split this into 5 parts, namely

$$\begin{aligned}\frac{1}{2A}\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n)-\frac{1}{2A}\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(p_n(m_\infty)) &= a_n+b_n,\\ \alpha^{\varepsilon}_n(\mu_n)-\alpha^{\varepsilon}_n(p_n(m_\infty)) &= c_n+d_n+e_n+f_n,\end{aligned}$$

which can be expressed using $\psi_{n,x}:=\mu_{n,x}-m_\infty(x)$, defined for all $n\in\mathbb{N}^*$ and $x\in\mathcal{L}_{n,\Omega_\varepsilon}$:

$$\begin{aligned}a_n &= \frac{a}{2n}\sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}}\sum_{y\in N_{n,\Omega_\varepsilon,x}}|\psi_{n,x}-\psi_{n,y}|^2,\\ b_n &= \frac{a}{2n}\sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}}\sum_{y\in N_{n,\Omega_\varepsilon,x}}2(m_\infty(x)-m_\infty(y))\cdot(\psi_{n,x}-\psi_{n,y}),\\ c_n &= \frac{a}{6n}\sum_{(i,j,k)\in S_n}(m_\infty(x_i)-m_\infty(x_k))\cdot(\psi_{n,x_k}-\psi_{n,x_j}),\\ d_n &= \frac{a}{6n}\sum_{(i,j,k)\in S_n}(\psi_{n,x_i}-\psi_{n,x_k})\cdot(m_\infty(x_k)-m_\infty(x_j)),\\ e_n &= \frac{a}{6n}\sum_{(i,j,k)\in S_n}(\psi_{n,x_i}-\psi_{n,x_k})\cdot(\psi_{n,x_k}-\psi_{n,x_j}),\\ f_n &= \mathcal{S}_{n,\Omega_\varepsilon}(p_n(m_\infty))-\mathcal{S}_{n,\Omega_\varepsilon}(\mu_n).\end{aligned}$$

We show below that $e_n\leqslant a_n$, and b_n, c_n, d_n and f_n tend to zero. This implies that

$$\liminf_{n\to\infty}(\alpha_n(\mu_n)-\alpha_n(p_n(m_\infty)))\leqslant\frac{1}{2A}\liminf_{n\to\infty}(\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n)-\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(p_n(m_\infty)))$$

and therefore

$$\liminf_{n\to\infty}(\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n)-\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(p_n(m_\infty)))\geqslant 0.$$

Lemma 4 implies that $\lim_{n\to\infty}\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(p_n(m_\infty))=\mathcal{E}^{\varepsilon}_{\infty,\mathrm{ex}}(m_\infty)$, hence

$$\liminf_{n\to\infty}\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n)\geqslant\mathcal{E}^{\varepsilon}_{\infty,\mathrm{ex}}(m_\infty).$$

which ends the proof.

Proof of $e_n \leqslant a_n$. For all x_i, x_j, $x_k \in \mathcal{L}_{n,\Omega_\varepsilon}$,

$$(\psi_{n,x_i} - \psi_{n,x_k}) \cdot (\psi_{n,x_k} - \psi_{n,x_j}) \leqslant \frac{1}{2}(|\psi_{n,x_i} - \psi_{n,x_k}|^2 + |\psi_{n,x_k} - \psi_{n,x_j}|^2).$$

Since each couple $(i,j) \in E_n$ is an element of 4 triples in S_n, we have

$$\begin{aligned}\sum_{(i,j,k)\in S_n} (\psi_{n,x_i} - \psi_{n,x_k}) \cdot (\psi_{n,x_k} - \psi_{n,x_j}) &\leqslant 2 \sum_{(i,j)\in E_n} |\psi_{n,x_i} - \psi_{n,x_j}|^2 \\ &\leqslant \sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y\in N_{n,\Omega_\varepsilon,x}} |\psi_{n,x} - \psi_{n,y}|^2,\end{aligned}$$

which is a much stronger result than $e_n \leqslant a_n$.

Proof of c_n and $d_n \to 0$. Let $(\psi_{n,x} - \psi_{n,y}) \cdot (m_\infty(y) - m_\infty(z))$ be one term of the sum in c_n and set $v = z - y$. Then

$$(\psi_{n,x} - \psi_{n,y}) \cdot (m_\infty(y) - m_\infty(z)) = (\psi_{n,x} - \psi_{n,y}) \cdot (m_\infty(y) - m_\infty(y+v))$$

and in the same sum there is also a term $(\psi_{n,x} - \psi_{n,y}) \cdot (m_\infty(y) - m_\infty(y-v))$, except for $y \in \mathcal{D}_{n,\Omega_\varepsilon}$.

Now since $\mu_n \in W^\mathfrak{h}$, there exists a constant $C_\psi \geqslant 0$ such that

$$|\psi_{n,x} - \psi_{n,y}| \leqslant C_\psi \frac{a}{n},$$

except for $y \in l_{n,\Omega_\varepsilon}$, but since there are $O(n)$ such nodes, their contribution in c_n tends to 0. We also have

$$\begin{aligned}&\frac{n}{a}((m_\infty(y) - m_\infty(y-v)) + (m_\infty(y) - m_\infty(y+v))) \\ &\qquad\qquad \xrightarrow[n\to\infty]{} (\nabla m_\infty(y) - \nabla m_\infty(y)) \cdot \frac{v}{|v|} = 0,\end{aligned}$$

and therefore

$$\frac{a}{6n} \sum_{(i,j,k)\in S_n} (\psi_{n,x_i} - \psi_{n,x_k}) \cdot (m_\infty(x_k) - m_\infty(x_j)) = O(\frac{1}{n})O(n^3)O(\frac{1}{n})o(\frac{1}{n}) = o(1).$$

Remark 5. *When $y \in \mathcal{D}_{n,\Omega_\varepsilon}$, we can only say that $|\psi_{n,x} - \psi_{n,y}| \leqslant C_\psi a/n$ (except on l_{n,Ω_ε}) and $|m_\infty(y) - m_\infty(z)| \leqslant C_m a/n$, and since $\#\mathcal{D}_{n,\Omega_\varepsilon} = O(n^2)$, the contribution of these nodes in c_n is a*

$$O(n^2)O(\frac{1}{n})O(\frac{1}{n})O(\frac{1}{n}) + O(n)O(\frac{1}{n})O(\frac{1}{n}) = O(\frac{1}{n}).$$

The sum d_n is treated in the same way.

Proof of $f_n \to 0$. The quantity $\mathcal{S}_{n,\Omega_\varepsilon}(\mu_n)$ is a sum of $O(n^2)$ terms reading like $(a/6n)|\mu_{n,x_i} - \mu_{n,x_j}|^2$ for $(i,j) \in E_n$, or $(a/12n)|\mu_{n,x_i} - \mu_{n,x_j}|^2$ for $(i,j) \in C_n$. By Hypothesis 3, only $O(n)$ among these terms can be only $o(1/n)$ and the others are $O(1/n^3)$. Hence $\mathcal{S}_{n,\Omega_\varepsilon}(\mu_n) = o(1)$.
On the other hand, the fact that $u_\infty \in \mathcal{C}^1(\Omega_\varepsilon, \mathbb{R}^3)$ ensures that all the terms in $\mathcal{S}_{n,\Omega_\varepsilon}(p_n(m_\infty))$ are $O(1/n^3)$, and therefore is $\mathcal{S}_{n,\Omega_\varepsilon}(p_n(m_\infty)) = O(1/n)$.

Proof of $b_n \to 0$. We use the fact that $\mathcal{C}^\infty(\Omega_\varepsilon; \mathbb{R}^3)$ is dense in $H^1(\Omega_\varepsilon; \mathbb{R}^3)$ for the $\| \cdot \|_{H^1(\Omega_\varepsilon;\mathbb{R}^3)}$ norm. Let $\eta > 0$, there exists $m_\eta \in \mathcal{C}^\infty(\Omega_\varepsilon; \mathbb{R}^3)$ such that $\|m_\infty - m_\eta\|_{H^1(\Omega_\varepsilon;\mathbb{R}^3)} \leqslant \eta$. Then b_n can be split into two contributions $b_n = b_n^\eta + b_n^{'\eta}$ where

$$\begin{aligned} b_n^\eta &= \frac{a}{n} \sum_{x \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y \in N_{n,\Omega_\varepsilon,x}} (m_\eta(x) - m_\eta(y)) \cdot (\psi_{n,x} - \psi_{n,y}), \\ b_n^{'\eta} &= \frac{a}{n} \sum_{x \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y \in N_{n,\Omega_\varepsilon,x}} ((m_\infty - m_\eta)(x) - (m_\infty - m_\eta)(y)) \cdot (\psi_{n,x} - \psi_{n,y}). \end{aligned}$$

For the first term, we notice that

$$\begin{aligned} b_n^\eta &= \frac{a}{n} \sum_{x \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y \in N_{n,\Omega,x}} (m_\eta(x) - m_\eta(y)) \cdot \psi_{n,x} \\ &- \frac{a}{n} \sum_{y \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{x \in N_{n,\Omega,y}} (m_\eta(x) - m_\eta(y)) \cdot \psi_{n,y}. \end{aligned}$$

As in the previous proof, we write y as $x + v$ and

$$b_n^\eta = \frac{a}{n} \sum_{x \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{v \in V_{n,0}} ((m_\eta(x) - m_\eta(x+v)) - (m_\eta(x-v) - m_\eta(x))) \cdot \psi_{n,x}.$$

We estimate

$$\begin{aligned} (m_\eta(x) - m_\eta(x+v)) &- (m_\eta(x-v) - m_\eta(x)) \\ &= \int_{t=1}^{0} \nabla m_\eta(x+tv) \cdot v \, \mathrm{d}t - \int_{t=0}^{-1} \nabla m_\eta(x+tv) \cdot v \, \mathrm{d}t \\ &= -\nabla m_\eta(x) \cdot \frac{v}{|v|} + \nabla m_\eta(x) \cdot \frac{v}{|v|} + O(|v|^2) \leqslant \frac{ca^2}{n^2}, \end{aligned}$$

where the constant c only depends on the second derivative of m_η, which is bounded on Ω_ε. Thus

$$|b_n^\eta| \leqslant \frac{ca^3}{n^3} \sum_{x \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y \in N_{n,\Omega,x}} |\psi_{n,x}|.$$

Thanks to the compact injection of $H^1(\Omega;\mathbb{R}^3)$ in $L^1(\Omega;\mathbb{R}^3)$, we deduce that this term vanishes. We obviously have

$$|b_n'^{\eta}| \leqslant \frac{a^2 C_\psi}{n^2} \sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y\in N_{n,\Omega_\varepsilon,x}} |(m_\infty - m_\eta)(x) - (m_\infty - m_\eta)(y)|.$$

For any function $u \in \mathcal{C}^1(\Omega;\mathbb{R}^3)$, and $y = x + v$, if $[x, y] \subset \Omega$, then

$$\begin{aligned} u(y) - u(x) &= \int_{t=1}^{0} \nabla u(x+tv)\cdot v \ \mathrm{d}t \\ &= \nabla u(x)\cdot v + \int_{t=1}^{0} (\nabla u(x+tv) - \nabla u(x))\cdot v \ \mathrm{d}t \end{aligned}$$

Applying this to m_∞ and m_η,

$$\begin{aligned} (m_\infty - m_\eta)(y) - (m_\infty - m_\eta)(x) &= (\nabla m_\infty(x) - \nabla m_\eta(x))\cdot v \\ &+ \int_{t=1}^{0} (\nabla m_\infty(x+tv) - \nabla m_\infty(x))\cdot v \ \mathrm{d}t \\ &- \int_{t=1}^{0} (\nabla m_\eta(x+tv) - \nabla m_\eta(x))\cdot v \ \mathrm{d}t. \end{aligned}$$

$\star$ By definition of m_η, $\|m_\infty - m_\eta\|_{H^1(\Omega;\mathbb{R}^3)} \leqslant \eta$, which implies that $\|\nabla m_\infty(x) - \nabla m_\eta(x)\|_{L^2(\Omega_\varepsilon;\mathbb{R}^3)} \leqslant \eta$. Hence

$$\begin{aligned} &\frac{a^2 C_\psi}{n^2} \left| \sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y\in N_{n,\Omega_\varepsilon,x}} (\nabla m_\infty(x) - \nabla m_\eta(x)).(y-x) \right| \\ &\quad \leqslant 2C_\psi \sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}} \left(\frac{a}{n}\right)^3 |\nabla m_\infty(x) - \nabla m_\eta(x)| \\ &\quad \leqslant 2C_\psi \left(\sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}} \left(\frac{a}{n}\right)^3 \right)^{1/2} \left(\sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}} \left(\frac{a}{n}\right)^3 |\nabla m_\infty(x) - \nabla m_\eta(x)|^2 \right)^{1/2}. \end{aligned}$$

Since

$$\lim_{n\to\infty} \sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}} \left(\frac{a}{n}\right)^3 |\nabla m_\infty(x) - \nabla m_\eta(x)|^2 = \int_{\Omega_\varepsilon} |\nabla m_\infty(x) - \nabla m_\eta(x)|^2 \mathrm{d}x,$$

$$\begin{aligned} \lim_{n\to\infty} \frac{a^2 C_\psi}{n^2} \sum_{x\in\mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y\in N_{n,\Omega_\varepsilon,x}} &(\nabla m_\infty(x) - \nabla m_\eta(x)).(y-x)| \\ &\leqslant C\|\nabla m_\infty(x) - \nabla m_\eta(x)\|_{L^2(\Omega_\varepsilon;\mathbb{R}^3)} \leqslant C\eta. \end{aligned}$$

$\star$ Let us treat the second contribution involving the $\mathcal{C}^\infty$ function m_η. Since

$$\int_{t=1}^{0} (\nabla m_\eta(x+tv) - \nabla m_\eta(x)) \cdot v \ \mathrm{d}t = \int_{t=1}^{0} \int_{t'=0}^{t} \nabla^2 m_\eta(x+t'v) \cdot v \otimes v \ \mathrm{d}t' \mathrm{d}t,$$

and $\nabla^2 m_\eta$ is uniformly bounded on Ω_ε, we can estimate

$$\frac{a^2 C_\psi}{n^2} \sum_{x \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y \in N_{n,\Omega_\varepsilon,x}} \int_{t=1}^{0} (\nabla m_\eta(x+t(y-x)) - \nabla m_\eta(x)) \cdot (y-x) \ \mathrm{d}t = O(\frac{1}{n}).$$

$\star$ In the last contribution, function m_∞ is only $\mathcal{C}^1$.

$$\begin{aligned}
&\frac{a^2 C_\psi}{n^2} \sum_{x \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{y \in N_{n,\Omega_\varepsilon,x}} \left| \int_{t=1}^{0} (\nabla m_\infty(x+t(y-x)) - \nabla m_\infty(x)) \cdot (y-x) \ \mathrm{d}t \right| \\
&\qquad \leqslant \frac{a^2 C_\psi}{n^2} \sum_{x \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{v \in N_{n,0}} \int_{t=0}^{1} |(\nabla m_\infty(x+tv) - \nabla m_\infty(x)) \cdot v| \ \mathrm{d}t \\
&\qquad \leqslant \frac{a^3 C_\psi}{n^3} \int_{t=0}^{1} \sum_{x \in \mathcal{L}_{n,\Omega_\varepsilon}} \sum_{v \in N_{n,0}} |(\nabla m_\infty(x+tv) - \nabla m_\infty(x)) \cdot \frac{v}{|v|}| \ \mathrm{d}t.
\end{aligned}$$

Since $m_\infty \in \mathcal{C}^1(\Omega_\varepsilon; \mathbb{R}^3)$, the elements of the sum converge uniformly towards 0 as $n \to \infty$, and therefore the integral is $o(n^3)$.

Hence $\lim_{n\to\infty} |b_n'^{\eta}| \leqslant \eta$ and therefore $\lim_{n\to\infty} |b_n| \leqslant \eta$, for all $\eta > 0$. This leads to $\lim_{n\to\infty} |b_n| = 0$, and the lemma is proved.

3.3.5 Proof of Lemma 6

The terms that occur in $\mathcal{E}_{n,\mathrm{ex}}(\mu_n)$ but not in $\mathcal{E}^\varepsilon_{n,\mathrm{ex}}(\mu_n)$ are those involing couples (x,y) where one at least of the nodes belong to $\Omega \backslash \Omega_\varepsilon$. There are $\varepsilon O(n^3)$ such nodes. Hence, by Hypothesis 3, the contribution of $l_{n,\Omega}$ in $\mathcal{E}_{n,\mathrm{ex}}(\mu_n)$ tends to zero, and there exists $c > 0$ such that for all $\{\mu_n\}_{n\in\mathbb{N}^*} \in W^{\mathfrak{h}}$,

$$\lim_{n\to\infty} |\mathcal{E}^\varepsilon_{n,\mathrm{ex}}(\mu_n) - \mathcal{E}_{n,\mathrm{ex}}(\mu_n)| \leqslant c\varepsilon.$$

We have already estimated $P_n(\mu)$ on $\Omega \backslash \Omega_{n,\varepsilon}$, where $\Omega_{n,\varepsilon}$ is a polyhedral subset of Ω which, like ω_ε has an $O(\varepsilon)$ Lebesgue measure. We already know that $P_n(\mu_n)_{|\Omega\backslash\Omega_{n,\varepsilon}} \in H^1(\Omega\backslash\Omega_{n,\varepsilon}; \mathbb{R}^3)$ and $P_n(u_n)_{|\omega_\varepsilon} \rightharpoonup m_{\infty|\Omega\backslash\Omega_{n,\varepsilon}}$ in the sense of $H^1(\Omega\backslash\Omega_{n,\varepsilon}; \mathbb{R}^3)$, therefore

$$\int_{\Omega\backslash\Omega_{n,\varepsilon}} |\nabla m_\infty(x)|^2 \ \mathrm{d}x \leqslant \liminf_{n\to\infty} \int_{\Omega\backslash\Omega_{n,\varepsilon}} |\nabla P_n(\mu_n)(x)|^2 \ \mathrm{d}x \leqslant C\varepsilon.$$

$$\begin{aligned}
\liminf_{n\to\infty} \mathcal{E}_{n,\mathrm{ex}}(\mu_n) &= \liminf_{n\to\infty} (\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n) + (\mathcal{E}_{n,\mathrm{ex}}(\mu_n) - \mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n))) \\
&\geqslant \liminf_{n\to\infty} (\mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n)) + \liminf_{n\to\infty} (\mathcal{E}_{n,\mathrm{ex}}(\mu_n) - \mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n)) \\
&\geqslant \mathcal{E}^{\varepsilon}_{\infty,\mathrm{ex}}(m_\infty) + \liminf_{n\to\infty} (\mathcal{E}_{n,\mathrm{ex}}(\mu_n) - \mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n)) \\
&\geqslant \mathcal{E}_{\infty,\mathrm{ex}}(m_\infty) + (\mathcal{E}^{\varepsilon}_{\infty,\mathrm{ex}}(m_\infty) - \mathcal{E}_{\infty,\mathrm{ex}}(m_\infty)) \\
&\quad + \liminf_{n\to\infty} (\mathcal{E}_{n,\mathrm{ex}}(\mu_n) - \mathcal{E}^{\varepsilon}_{n,\mathrm{ex}}(\mu_n)) \\
&\geqslant \mathcal{E}_{\infty,\mathrm{ex}}(m_\infty) - (c + c_1)\varepsilon.
\end{aligned}$$

Since this holds for all $\varepsilon > 0$, we finally deduce that

$$\liminf_{n\to\infty} \mathcal{E}_{n,\mathrm{ex}}(\mu_n) \geqslant \mathcal{E}_{\infty,\mathrm{ex}}(m_\infty).$$

4 Other energy contributions

4.1 Magnetostatics: demagnetizing energy

We can define a mapping $h_{\mathrm{d}} : L^2(\mathbb{R}^3;\mathbb{R}^3) \mapsto L^2(\mathbb{R}^3;\mathbb{R}^3)$ by: for all $u \in L^2(\mathbb{R}^3;\mathbb{R}^3)$, $h_{\mathrm{d}}(u)$ is solution in the sense of distributions to

$$\left\{ \begin{array}{rcl} \mathrm{rot}\, h_{\mathrm{d}}(u) &=& 0, \\ \mathrm{div}\, h_{\mathrm{d}}(u) &=& -\mathrm{div}\, u. \end{array} \right.$$

When u is the magnetization, $h_{\mathrm{d}}(u)$ is the demagnetizing field. Its energy is

$$\mathcal{E}_{\mathrm{d}}(u) = \frac{\mu_0}{2} \|h_{\mathrm{d}}(u)\|_{L^2(\mathbb{R}^3;\mathbb{R}^3)}.$$

For $u \in L^2(\Omega;\mathbb{R}^3)$, we denote by $\tilde{u}$ the $L^2(\mathbb{R}^3;\mathbb{R}^3)$ function which equals u inside Ω, and 0 outside Ω. Hence for a spin distribution $\mu_n \in (\mathbb{S}^2)^{\mathcal{L}_{n,\Omega}}$, the demagnetizing energy is defined by

$$\mathcal{E}_{n,\mathrm{d}}(\mu_n) = \frac{\mu_0}{2} \left\| h_{\mathrm{d}} \left(\widetilde{P_n(\mu_n)} \right) \right\|_{L^2(\mathbb{R}^3;\mathbb{R}^3)}.$$

4.2 Total energy

We define the total energy summing up the exchange and demagnetizing energies both in the lattice context:

$$\forall \mu_n \in (\mathbb{S}^2)^{\mathcal{L}_{n,\Omega}},\ \mathcal{E}_n(\mu_n) = \mathcal{E}_{n,\mathrm{ex}}(\mu_n) + \mathcal{E}_{n,\mathrm{d}}(\mu_n),$$

and the limit continuous one:

$$\forall u \in H^1(\Omega;\mathbb{R}^3),\ \mathcal{E}_\infty(u) = \mathcal{E}_{\infty,\mathrm{ex}}(u) + \mathcal{E}_{\infty,\mathrm{d}}(u).$$

Theorem 2. *Let $(\mu_n)_{n\in\mathbb{N}^*} \in W^\mathfrak{h}$. In the sense of the topology defined by Definition 2*

$$\mathcal{E}_n \xrightarrow[n\to\infty]{\Gamma} \mathcal{E}_\infty.$$

Moreover, this convergence is compatible with the unit norm constraint.

Proof. We have already shown that

$$\mathcal{E}_{n,\mathrm{ex}} \xrightarrow[n\to\infty]{\Gamma} \mathcal{E}_{\infty,\mathrm{ex}}.$$

Moreover $h_\mathrm{d} : L^2(\mathbb{R}^3;\mathbb{R}^3) \mapsto L^2(\mathbb{R}^3;\mathbb{R}^3)$ is linear and continuous. We therefore choose $(\mu_n)_{n\in\mathbb{N}^*} \in W^\mathfrak{h}$ such that $\mu_n \xrightarrow[n\to\infty]{} \mu \in H^1(\Omega;\mathbb{R}^3)$. This means that the sequence$(P_n(\mu_n))$ is weakly convergent in $H^1(\Omega;\mathbb{R}^3)$ to μ. Hence

$$P_n(\mu_n) \xrightarrow[n\to\infty]{L^2(\Omega;\mathbb{R}^3)} \mu \text{ and } \widetilde{P_n(\mu_n)} \xrightarrow[n\to\infty]{L^2(\mathbb{R}^3;\mathbb{R}^3)} \tilde{\mu}.$$

In particular $\mathcal{E}_{n,\mathrm{d}}(\mu_n) \xrightarrow[n\to\infty]{} \mathcal{E}_{\infty,\mathrm{d}}(\mu)$.

Besides if $\mu \in H^1(\Omega;\mathbb{R}^3)$, we know that $p_n(\mu) \xrightarrow[n\to\infty]{} \mu$ in $H^1(\Omega;\mathbb{R}^3)$, which ends the proof of

$$\mathcal{E}_{n,\mathrm{d}} \xrightarrow[n\to\infty]{\Gamma} \mathcal{E}_{\infty,\mathrm{d}}$$

and Theorem 2. □

5 Conclusion

In this paper, we prove a Γ-convergence result from a discrete description of ferromagnetic materials at the microscopic scale to the continuous one. This result has been shown thanks to a rigidity hypothesis on the lattice of magnetic moments. This modeling hypothesis is based on the Heisenberg interaction phenomenon and could be justified by a time multi-scale study. The new hypothesis would take into account the speed of the Heisenberg relaxation compared to the Larmor precession process.

The results in this paper are the seed in order to address the micro–mesoscopic limit for dynamic processes to be able to better understand the dissipation phenomena involved in the mesoscopic Landau–Lifchitz system.

References

[1] Amikam Aharoni. *Introduction to the theory of ferromagnetism*. Oxford Science Publications, 1996.

[2] Fabrice Boust, Nicolas Vukadinovic, and Stéphane Labbé. 3D dynamic micromagnetic simulations of susceptibility spectra in soft ferromagnetic particles. *ESAIM Proceedings*, 22:127–131, February 2008.

[3] Andrea Braides. *Gamma-Convergence for Beginners*, Oxford University Press, 2002.

[4] William Fuller Brown, Jr. *Micromagnetics*, volume 18 of *Interscience Tracts on Physics and Astronomy*. John Wiley and Sons, 1963.

[5] William Fuller Brown, Jr and Anton E. LaBonte. Structure and energy of one-dimensional domain walls in ferromagnetic thin films. *Journal of Applied Physics*, 36(4):1380–1386, 1965.

[6] R. Fisher, Thomas Shrefl, Helmut Kronmüller, and Josef Fidler. Grain-size dependence of remanence and coercive field of isotropic nanocrystalline composite permanent magnets. *Journal of Magnetism and Magnetic Materials*, 153:35–49, 1996.

[7] Laurence Halpern and Stéphane Labbé. La théorie du micromagnétisme. Modélisation et simulation du comportement des matériaux magnétiques. *Matapli*, 66:77–92, 2001.

[8] Stéphane Labbé and Pierre-Yves Bertin. Microwave polarizability of ferrite particles with non-uniform magnetization. *Journal of Magnetism and Magnetic Materials*, 206:93–105, 1999.

[9] Nicolas Vukadinovic, Jamal Ben Youssef, and Henri Le Gall. Influence of magnetic parameters on microwave absorption of domain mode ferromagnetic resonance. *Journal of Magnetism and Magnetic Materials*, 150:213–222, 1995.

[10] William P. Ziemer. *Weakly differentiable functions: Sobolev Spaces and Functions of Bounded Variation*, volume 120 of *Graduate Texts in Mathematics*. Springer, 1989.