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VARIATIONAL APPROXIMATION OF INTERFACE ENERGIES AND APPLICATIONS

SAMUEL AMSTUTZ, DANIEL GOURION, AND MOHAMMED ZABIBA

ABSTRACT. Minimal partition problems consist in finding a partition of a domain into a given number of components in order to minimize a geometric criterion. In applicative fields such as image processing or continuum mechanics, it is standard to incorporate in this objective an interface energy that accounts for the lengths of the interfaces between components. The present work is focused on the theoretical and numerical treatment of minimal partition problems with such interface energies. The considered approach is based on a Γ -convergence approximation combined with convex analysis techniques.

1. INTRODUCTION

Consider a partition of a bounded domain Ω of \mathbb{R}^d into relatively closed subsets $\Omega_1, \dots, \Omega_N$, called phases, that may intersect only through their boundaries:

$$\Omega = \bigcup_{j=1}^N \Omega_j, \quad \text{with } \Omega_i \cap \Omega_j = \partial\Omega_i \cap \partial\Omega_j \cap \Omega \text{ for } i \neq j.$$

Denote the interface separating Ω_i and Ω_j by Γ_{ij} :

$$\Gamma_{ij} = \partial\Omega_i \cap \partial\Omega_j \cap \Omega \text{ for } i \neq j,$$

with the additional convention $\Gamma_{ii} = \emptyset$, see Figure 1. The prototype problem of minimal partition can be written as

$$\text{minimize } \sum_{i=1}^N \int_{\Omega_i} g_i(x) dx + \mathcal{I}(\Omega_1, \dots, \Omega_N) \quad (1.1)$$

over all partitions $(\Omega_1, \dots, \Omega_N)$ of Ω , where g_1, \dots, g_N are given functions in $L^1(\Omega)$, and $\mathcal{I}(\Omega_1, \dots, \Omega_N)$ is the total interface energy. This energy is here chosen as

$$\mathcal{I}(\Omega_1, \dots, \Omega_N) = \frac{1}{2} \sum_{1 \leq i < j \leq N} \alpha_{ij} \mathcal{H}^{d-1}(\Gamma_{ij}), \quad (1.2)$$

where $\alpha_{ij} \geq 0$ is a coefficient called surface tension associated with Γ_{ij} and $\mathcal{H}^{d-1}(\Gamma_{ij})$ is the $d-1$ dimensional Hausdorff measure of Γ_{ij} . It is convenient to assume that the surface tensions satisfy $\alpha_{ij} = \alpha_{ji}$ whenever $i \neq j$ and $\alpha_{ii} = 0$. We denote

$$S_N = \{(\alpha_{ij}) \in \mathbb{R}^{N \times N} : \alpha_{ij} = \alpha_{ji} \text{ and } \alpha_{ii} = 0\}.$$

In order to guarantee the lower semicontinuity of the interface energy, it is required that the surface tensions be nonnegative and satisfy the triangle inequality [4]

$$\alpha_{ij} \leq \alpha_{ik} + \alpha_{kj} \quad \forall i, j, k. \quad (1.3)$$

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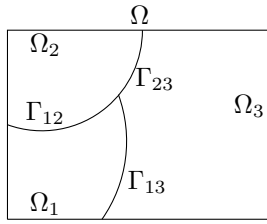


FIGURE 1. A partition of a domain into sets (Ω_j) that intersect only at their boundaries. Interface Γ_{ij} separates Ω_i from Ω_j .

This condition is also discussed in [15, 16, 19]. We will therefore mainly place ourselves in the classes of surface tensions

$$S_N^+ = \{(\alpha_{ij}) \in S_N : \alpha_{ij} \geq 0\},$$

$$T_N = \{(\alpha_{ij}) \in S_N^+ : \alpha_{ij} \leq \alpha_{ik} + \alpha_{kj} \forall i, j, k\}.$$

For the rigorous mathematical analysis, the lower semicontinuity of (1.2) needs to be formulated in an appropriate framework, namely the space of sets of finite perimeter, or Caccioppoli sets [6, 9, 23]. In this setting, the total interface energy writes

$$\frac{1}{2} \sum_{1 \leq i < j \leq N} \alpha_{ij} \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega), \quad (1.4)$$

where $\Omega_1, \dots, \Omega_N$ are now assumed to be sets of finite perimeter in Ω such that $\Omega = \cup_{i=1}^N \Omega_i$ up to a Lebesgue negligible set and $|\Omega_i \cap \Omega_j| = 0$ for all $i \neq j$, denoting by $|\cdot|$ the d -dimensional Lebesgue measure. Moreover, $\partial_M \Omega_i$ is the measure theoretical (or essential) boundary of Ω_i in Ω . We refer to [6, 9, 23] for details on sets of finite perimeter and geometric measure theory.

Domain functionals of perimetric type are known to be difficult to handle within numerical optimization procedures. The most direct approach in shape optimization relies on the concept of shape derivative, often implemented by means of level-sets, see e.g. the seminal paper [3] and [2] for a multiphase application. Drawbacks of this setting are that it does not allow all types of topology changes, and that it raises the difficulty, when perimetric terms are involved, of the numerical evaluation of curvatures. In this paper we follow another path, and propose an approximation of the energy (1.4) by a Γ -converging parameterized functional. This latter is constructed upon the solutions of auxiliary elliptic boundary value problems, in the spirit of [7, 8]. This is in contrast with the celebrated Modica-Mortola Γ -convergence approximation of the perimeter [26] which, borrowing the terminology of numerical schemes, could be qualified as explicit. The Modica-Mortola functional, special case of the Ginzburg Landau free energy, has been used in particular by several authors to address minimal partition problems, see e.g. [10–12, 27], and specifically [15] where the energy (1.4) is considered. Closely related to our approach is the parabolic approximation, applied to (1.4) in [19], see also [1, 25] for the two phase case. Nonlocal functionals, either elliptic or parabolic, lend themselves to optimization procedures which are less sensitive to the spatial discretization than local, explicit ones. In particular, descent steps are unrelated to mesh size. As we will see, the elliptic framework has a further advantage: it provides a variational formulation which enables the implementation of alternating minimization schemes. The separated subproblems may be linear or quadratic and be solved in one shot without line search. Finally, different from Γ -convergence based methods, we mention the convex approximation of minimal partition problems from [17].

On the mathematical side, two main questions are addressed in the present work. The first one is the Γ -convergence of the approximating functionals, which we establish under two alternative sets of assumptions. In the first setting we assume that the surface tensions satisfy an algebraic property, denoted by $(\alpha_{ij}) \in B_N^+$, implying that the total interface energy can be written as a conical combination of perimeters of clusters of phases. This allows to use results on the two-phase

case from [7,8], under generalized forms. In the second setting we only assume that $(\alpha_{ij}) \in T_N$, but we suppose that Ω is a Cartesian product of intervals. To prove the Γ -lim inf inequality we follow a very different approach, to a large extent inspired from [19]. Our most novel contribution deals with the second issue, namely the construction of the aforementioned variational formulation. It is based on Legendre-Fenchel duality arguments, therefore it involves convexity assumptions. We actually propose two complementary formulations in order to cope with all surface tensions $(\alpha_{ij}) \in T_N$.

The paper is organized as follows. In section 2 we recall and extend some useful results from [7,8]. In section 3 we introduce our interface energy approximation and analyze its pointwise convergence. Section 4 deals with the lower semicontinuity and equicoercivity properties. In section 5 we recall and complement known combinatorial issues concerning the decomposition of the interface energy as a weighted sum of perimeters, and prove our two Γ -convergence results. Sections 6 and 7 are dedicated to the variational formulation. The resulting algorithm is presented in section 8, together with some numerical examples. In section 9 we describe an enrichment of the algorithm in order to take into account volume constraints. A technical lemma is deferred in appendix.

2. PRELIMINARY: A GRADIENT-FREE PERIMETER APPROXIMATION

To set up the mathematical framework, we assume that the hold-all Ω is an open and bounded subset of \mathbb{R}^d , $d \in \{2, 3\}$, with Lipschitz boundary, and we first define the functional $F : L^\infty(\Omega, \{0, 1\}) \rightarrow \mathbb{R} \cup \{+\infty\}$ by

$$F(u) = \begin{cases} \frac{1}{2}|Du|(\Omega) & \text{if } u \in BV(\Omega, \{0, 1\}), \\ +\infty & \text{otherwise.} \end{cases}$$

We recall that the total variation of u satisfies $|Du|(\Omega) = \mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \Omega)$ whenever $u \in BV(\Omega, \{0, 1\})$ and u is the characteristic function of a Lebesgue-measurable subset Ω_1 of Ω , denoted by $u = \chi_{\Omega_1}$, see again [6, 9, 23]. Then we say that Ω_1 is a set of finite perimeter and that $\mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \Omega)$ is the relative perimeter of Ω_1 in Ω . We also define the extended functional \tilde{F} over the convex set $L^\infty(\Omega, [0, 1])$ by

$$\tilde{F}(u) = \begin{cases} F(u) & \text{if } u \in L^\infty(\Omega, \{0, 1\}), \\ +\infty & \text{otherwise.} \end{cases}$$

In all what follows we denote

$$\langle u, v \rangle = \int_{\Omega} u(x) \cdot v(x) dx$$

for every pair of scalar or vector valued functions u, v having suitable regularity. It is shown in [7,8] that a variational approximation of \tilde{F} , in the sense of Γ -convergence, is provided by the family of functionals $(\tilde{F}_\varepsilon)_{\varepsilon>0}$ defined by

$$\tilde{F}_\varepsilon(u) = \inf_{v \in H^1(\Omega)} \left\{ \varepsilon \|\nabla v\|_{L^2(\Omega)}^2 + \frac{1}{\varepsilon} \left(\|v\|_{L^2(\Omega)}^2 + \langle u, 1 - 2v \rangle \right) \right\}. \quad (2.1)$$

We recall below some results proven in [7, 8]. The first one is a straightforward reformulation of (2.1) with the help of Euler-Lagrange equations.

Proposition 2.1. *Let $u \in L^2(\Omega)$ be given and $L_\varepsilon u := v_\varepsilon \in H^1(\Omega)$ be the (weak) solution of*

$$\begin{cases} -\varepsilon^2 \Delta v_\varepsilon + v_\varepsilon = u & \text{in } \Omega, \\ \partial_n v_\varepsilon = 0 & \text{on } \partial\Omega. \end{cases} \quad (2.2)$$

Then we have

$$\tilde{F}_\varepsilon(u) = \frac{1}{\varepsilon} \langle 1 - L_\varepsilon u, u \rangle.$$

It follows straightforwardly from (2.2) that $L_\varepsilon 1 = 1$. Also, the weak formulation yields for all $u, v \in L^2(\Omega)$

$$\langle L_\varepsilon u, v \rangle = \int_{\Omega} (\varepsilon^2 \nabla(L_\varepsilon u) \cdot \nabla(L_\varepsilon v) + (L_\varepsilon u) \cdot (L_\varepsilon v)) dx,$$

whereby the operator $L_\varepsilon : L^2(\Omega) \rightarrow L^2(\Omega)$ is self-adjoint and positive definite. It follows that

$$\tilde{F}_\varepsilon(u) = \frac{1}{\varepsilon} \langle L_\varepsilon u, 1 - u \rangle.$$

Moreover, the weak maximum principle yields $0 \leq u \leq 1 \Rightarrow 0 \leq L_\varepsilon u \leq 1$.

The second result will be useful for existence issues at ε fixed.

Lemma 2.2. *The functional \tilde{F}_ε is continuous on $L^\infty(\Omega, [0, 1])$ for the weak-* topology of $L^\infty(\Omega)$.*

The third result establishes the lim inf inequality of the Γ -convergence of the approximating functionals. From now on, convergence statements for $\varepsilon \rightarrow 0$ will refer to the convergence of the corresponding quantity considering any sequence (ε_k) of positive numbers such that $\lim_{k \rightarrow +\infty} \varepsilon_k = 0$.

Proposition 2.3. *Let $u \in L^\infty(\Omega, [0, 1])$ and (u^ε) be a sequence of functions of $L^\infty(\Omega, [0, 1])$ such that $u^\varepsilon \rightarrow u$ strongly in $L^1(\Omega)$. Then we have*

$$\liminf_{\varepsilon \rightarrow 0} \tilde{F}_\varepsilon(u^\varepsilon) \geq \tilde{F}(u).$$

Proofs of the lim sup inequality of the Γ -convergence may involve more geometrical aspects, with a possible influence of the space dimension and the shape of Ω . In [8] it was proved for a Lipschitz domain Ω in any dimension, with the help of a recovery sequence (u^ε) . However, recovery sequences become problematic in the multiphase case, since independent recovery sequences $(u_i^\varepsilon)_{1 \leq i \leq N}$ have no reason to satisfy $\sum_{i=1}^N u_i^\varepsilon = 1$, even if this property is verified at the limit. In [7] the lim sup inequality was proved for the constant recovery sequence $u^\varepsilon = u$, which is obviously a remedy to the above limitation, in two dimensions for Ω rectangular. Here we extend this result to Lipschitz domains in dimension $d \in \{2, 3\}$.

Proposition 2.4. *For all $u \in BV(\Omega, \{0, 1\})$ and all $\varepsilon > 0$ we have*

$$\limsup_{\varepsilon \rightarrow 0} \tilde{F}_\varepsilon(u) \leq \frac{1}{2} |Du|(\Omega).$$

Proof. We first note that for all $u \in BV(\Omega, \{0, 1\})$ we can write

$$\tilde{F}_\varepsilon(u) = F_\varepsilon(u) := \frac{1}{\varepsilon} \langle u - L_\varepsilon u, u \rangle.$$

Moreover, standard arguments provide the variational formulation

$$F_\varepsilon(u) = \inf_{w \in H^1(\Omega)} \left\{ \varepsilon \|\nabla w\|_{L^2(\Omega)}^2 + \frac{1}{\varepsilon} \|w - u\|_{L^2(\Omega)}^2 \right\}.$$

We will estimate $F_\varepsilon(u)$ through three steps.

Step 1. In the first step we assume that $u \in H^1(\Omega, [0, 1])$. We have in particular for all $w \in \mathcal{C}^2(\bar{\Omega})$

$$F_\varepsilon(u) \leq \varepsilon \|\nabla w\|_{L^2(\Omega)}^2 + \frac{1}{\varepsilon} \|w - u\|_{L^2(\Omega)}^2,$$

which rewrites

$$F_\varepsilon(u) \leq \varepsilon \int_{\partial\Omega} \partial_n w (w - u) ds + \varepsilon \int_{\Omega} \nabla w \cdot \nabla u dx + \frac{1}{\varepsilon} \int_{\Omega} (-\varepsilon^2 \Delta w + w - u)(w - u) dx. \quad (2.3)$$

Here we have used the Green formula for BV functions [6, 9], which applies in Lipschitz domains. We recall that u admits a trace in $L^1_{\mathcal{H}^{d-1}}(\partial\Omega)$, and that this trace can be lifted by a function in $W^1_1(\tilde{\Omega} \setminus \bar{\Omega})$, where $\tilde{\Omega}$ is a bounded open smooth set containing $\bar{\Omega}$, see [6, 20]. Call \tilde{u} the obtained extension of u , further extended by 0 outside $\tilde{\Omega}$. Inequality (2.3) extends by density to any function $w \in \mathcal{C}^1(\tilde{\Omega})$ with $\Delta w \in L^2(\tilde{\Omega})$. We choose $w = w_\varepsilon := \Phi_\varepsilon \star \tilde{u}$ where Φ_ε is the fundamental solution

of the operator $-\varepsilon^2\Delta + I$. By construction, it holds $-\varepsilon^2\Delta w_\varepsilon + w_\varepsilon = \tilde{u}$ a.e. in $\tilde{\Omega}$. Hence, since $\tilde{u} \in W^{1,1}(\tilde{\Omega})$, $w_\varepsilon \in C^1(\tilde{\Omega})$ [21] and

$$F_\varepsilon(u) \leq \varepsilon \int_{\partial\Omega} \partial_n w_\varepsilon (w_\varepsilon - u) ds + \varepsilon \int_{\Omega} \nabla w_\varepsilon \cdot \nabla u dx. \quad (2.4)$$

The construction from [20] permits to assume the $0 \leq \tilde{u} \leq 1$ a.e. in $\tilde{\Omega}$. Using $\Phi_\varepsilon(x) = \varepsilon^{-d}\Phi_1(\varepsilon^{-1}x)$ we obtain

$$\varepsilon \nabla w_\varepsilon(x) = \int_{\mathbb{R}^d} \nabla \Phi_1(z) \tilde{u}(x - \varepsilon z) dz.$$

Let ν be a unit vector of \mathbb{R}^d . We infer

$$\varepsilon \nabla w_\varepsilon(x) \cdot \nu = \int_{\mathbb{R}^d} \nabla \Phi_1(z) \cdot \nu \tilde{u}(x - \varepsilon z) dz \leq \int_{\mathbb{R}^d} \max(\nabla \Phi_1(z) \cdot \nu, 0) dz.$$

Due to the radial symmetry of Φ_1 we can without loss of generality assume that ν is oriented along the first basis vector of \mathbb{R}^d . It follows that

$$\varepsilon \nabla w_\varepsilon(x) \cdot \nu \leq \int_{\mathbb{R}^d} \max(\partial_{x_1} \Phi_1(z), 0) dz.$$

We subsequently infer

$$\varepsilon \nabla w_\varepsilon(x) \cdot \nu \leq \int_{\mathbb{R}} \max\left(\int_{\mathbb{R}^{d-1}} \partial_{x_1} \Phi_1(z_1, \bar{z}) d\bar{z}, 0\right) dz_1$$

because, due to radial symmetry, the sign of $\partial_{x_1} \Phi_1(z_1, \bar{z})$ only depends on the coordinate z_1 . By uniqueness, the function

$$z_1 \mapsto \int_{\mathbb{R}^{d-1}} \Phi_1(z_1, \bar{z}) d\bar{z}$$

is the one dimensional fundamental solution, i.e.,

$$\int_{\mathbb{R}^{d-1}} \Phi_1(z_1, \bar{z}) d\bar{z} = \frac{1}{2} e^{-|z_1|}.$$

We arrive at

$$\varepsilon \nabla w_\varepsilon(x) \cdot \nu \leq \int_0^{+\infty} \frac{1}{2} e^{-z_1} dz_1 = \frac{1}{2},$$

whereby, since ν is arbitrary,

$$\varepsilon |\nabla w_\varepsilon(x)| \leq \frac{1}{2}.$$

Coming back to (2.4) we obtain

$$F_\varepsilon(u) \leq \frac{1}{2} \int_{\partial\Omega} |w_\varepsilon - u| ds + \frac{1}{2} \int_{\Omega} |\nabla u| dx = \frac{1}{2} \int_{\partial\Omega} |\Phi_\varepsilon \star \tilde{u} - u| ds + \frac{1}{2} \int_{\Omega} |\nabla u| dx. \quad (2.5)$$

Step 2. We now assume that $u \in BV(\Omega, [0, 1])$. By density of $C^\infty(\bar{\Omega})$ in $BV(\Omega)$ for the intermediate convergence [6, 9], there exists a sequence of functions $u_k \in H^1(\Omega)$ such that $u_k \rightarrow u$ in $L^1(\Omega)$ and $|Du_k|(\Omega) \rightarrow |Du|(\Omega)$. The construction by mollifiers allows to assume that $0 \leq u_k \leq 1$. By Parseval's equality, as the Fourier transform of Φ_1 is $\mathcal{F}\Phi_1(\xi) = 1/(1 + |\xi|^2)$, we infer that $\Phi_1 \in L^2(\mathbb{R}^d)$. Since obviously $u_k \rightarrow u$ also in $L^2(\Omega)$, $\tilde{u}_k \rightarrow \tilde{u}$ in $L^2(\mathbb{R}^d)$ by continuity of the trace operator for the intermediate convergence, and F_ε is continuous on $L^2(\Omega)$, taking limits in (2.5) yields

$$F_\varepsilon(u) \leq \frac{1}{2} \int_{\partial\Omega} |\Phi_\varepsilon \star \tilde{u} - u| ds + \frac{1}{2} \int_{\Omega} |Du|. \quad (2.6)$$

Step 3. It remains to estimate the first integral in (2.6), which denoting $w_\varepsilon = \Phi_\varepsilon \star \tilde{u}$ can be rewritten

$$\int_{\partial\Omega} |w_\varepsilon - u| ds = \int_{\partial\Omega} \left| \int_{\mathbb{R}^d} \Phi_1(y) (\tilde{u}(x - \varepsilon y) - \tilde{u}(x)) dy \right| ds(x).$$

Let $\alpha > 0$. Due to the decay of Φ_1 at infinity there exists $\rho > 0$ such that

$$\int_{\partial\Omega} \left| \int_{\mathbb{R}^d \setminus B_\rho(0)} \Phi_1(y) (\tilde{u}(x - \varepsilon y) - \tilde{u}(x)) dy \right| ds(x) \leq \alpha.$$

The Cauchy-Schwarz inequality yields

$$\int_{\partial\Omega} |w_\varepsilon - u| ds \leq \mathcal{H}^{d-1}(\partial\Omega)^{1/2} \|\Phi_1\|_{L^2(\mathbb{R}^d)} \left(\int_{\partial\Omega} \int_{B_\rho(0)} |\tilde{u}(x - \varepsilon y) - \tilde{u}(x)| dy ds(x) \right)^{1/2} + \alpha.$$

By a change of variable this rewrites as

$$\int_{\partial\Omega} |w_\varepsilon - u| ds \leq \mathcal{H}^{d-1}(\partial\Omega)^{1/2} \|\Phi_1\|_{L^2(\mathbb{R}^d)} \left(\int_{\partial\Omega} \varepsilon^{-d} \int_{B_{\varepsilon\rho}(0)} |\tilde{u}(x - z) - \tilde{u}(x)| dz ds(x) \right)^{1/2} + \alpha.$$

Theorem 3.87 of [6] states the following: for \mathcal{H}^{d-1} - a.e. $x \in \partial\Omega$ it holds

$$\lim_{t \rightarrow 0} t^{-d} \int_{\Omega \cap B_t(x)} |u(y) - u(x)| dy = 0.$$

Obviously the same limit holds for the exterior part, which entails

$$\lim_{\varepsilon \rightarrow 0} \varepsilon^{-d} \rho^{-d} \int_{B_{\varepsilon\rho}(0)} |\tilde{u}(x - z) - \tilde{u}(x)| dz = 0$$

for \mathcal{H}^{d-1} - a.e. $x \in \partial\Omega$. Then it follows from Lebesgue's dominated convergence theorem that

$$\lim_{\varepsilon \rightarrow 0} \int_{\partial\Omega} \varepsilon^{-d} \int_{B_{\varepsilon\rho}(0)} |\tilde{u}(x - z) - \tilde{u}(x)| dz ds(x) = 0.$$

We infer that, for ε small enough,

$$\int_{\partial\Omega} |w_\varepsilon - u| ds \leq 2\alpha.$$

This completes the proof. \square

As straightforward consequences of Propositions 2.3 and 2.4, one obtains the desired Γ -convergence and pointwise convergence results.

Theorem 2.5. *When $\varepsilon \rightarrow 0$, the functionals \tilde{F}_ε Γ -converge in $L^\infty(\Omega, [0, 1])$ endowed with the strong topology of $L^1(\Omega)$ to the functional \tilde{F} defined by*

$$\tilde{F}(u) = \begin{cases} \frac{1}{2} |Du|(\Omega) & \text{if } u \in BV(\Omega, \{0, 1\}), \\ +\infty & \text{otherwise.} \end{cases}$$

Theorem 2.6. *For all $u \in L^\infty(\Omega, [0, 1])$ it holds*

$$\lim_{\varepsilon \rightarrow 0} \tilde{F}_\varepsilon(u) = \tilde{F}(u). \quad (2.7)$$

3. APPROXIMATION OF INTERFACE ENERGIES: POINTWISE CONVERGENCE

Given two subsets Ω_i and Ω_j of Ω , we look for an approximation of the interface energy $\mathcal{H}^1(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega)$. The starting point is the following result established within the proof of Proposition 1 of [5].

Lemma 3.1. *Let Ω_i, Ω_j be sets of finite perimeter such that $|\Omega_i \cap \Omega_j| = 0$. There exists an \mathcal{H}^{d-1} -negligible set L such that*

$$\partial_M(\Omega_i \cup \Omega_j) \setminus L \subset \partial_M \Omega_i \Delta \partial_M \Omega_j \subset \partial_M(\Omega_i \cup \Omega_j).$$

We obtain the following extension of Proposition 1 of [5].

Proposition 3.2. *Let $(\Omega_i)_{i=1,\dots,m}$ be sets of finite perimeter such that $|\Omega_i \cap \Omega_j| = 0$ for any $i \neq j$. Then*

$$\mathcal{H}^{d-1}(\partial_M(\cup_{i=1}^m \Omega_i) \cap \Omega) = \sum_{i=1}^m \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \Omega) - 2 \sum_{1 \leq i < j \leq m} \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega).$$

Proof. First we derive from Lemma 3.1 that if $|\Omega_i \cap \Omega_j| = 0$ then

$$\mathcal{H}^{d-1}(\partial_M(\Omega_i \cup \Omega_j) \cap \Omega) = \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \Omega) + \mathcal{H}^{d-1}(\partial_M \Omega_j \cap \Omega) - 2\mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega). \quad (3.1)$$

This proves the proposition for $m = 2$. The general case is obtained by induction. For readability we present the proof for $m = 3$. Using (3.1) we obtain

$$\begin{aligned} \mathcal{H}^{d-1}(\partial_M(\Omega_1 \cup \Omega_2 \cup \Omega_3) \cap \Omega) &= \mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \Omega) + \mathcal{H}^{d-1}(\partial_M \Omega_2 \cap \Omega) + \mathcal{H}^{d-1}(\partial_M \Omega_3 \cap \Omega) \\ &\quad - 2\mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \partial_M \Omega_2 \cap \Omega) - 2\mathcal{H}^{d-1}(\partial_M(\Omega_1 \cup \Omega_2) \cap \partial_M \Omega_3 \cap \Omega). \end{aligned}$$

Using Lemma 3.1 we get

$$\mathcal{H}^{d-1}(\partial_M(\Omega_1 \cup \Omega_2) \cap \partial_M \Omega_3 \cap \Omega) = \mathcal{H}^{d-1}((\partial_M \Omega_1 \cap \partial_M \Omega_3 \cap \Omega) \Delta (\partial_M \Omega_2 \cap \partial_M \Omega_3 \cap \Omega)).$$

Now, we will prove that

$$\mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \partial_M \Omega_2 \cap \partial_M \Omega_3) = 0. \quad (3.2)$$

Call $\Omega_i^{\frac{1}{2}}$ the set of points of density $\frac{1}{2}$ relatively to Ω_i , see e.g. [6]. By definition we have

$$\Omega_1^{\frac{1}{2}} \cap \Omega_2^{\frac{1}{2}} \cap \Omega_3^{\frac{1}{2}} = \emptyset.$$

As a consequence, it follows that

$$0 = \mathcal{H}^{d-1}(\Omega_1^{\frac{1}{2}} \cap \Omega_2^{\frac{1}{2}} \cap \Omega_3^{\frac{1}{2}}) = \mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \partial_M \Omega_2 \cap \partial_M \Omega_3), \quad (3.3)$$

since the two sets above coincide up to an \mathcal{H}^{d-1} -negligible set, see [6]. We infer that

$$\begin{aligned} \mathcal{H}^{d-1}((\partial_M \Omega_1 \cap \partial_M \Omega_3 \cap \Omega) \Delta (\partial_M \Omega_2 \cap \partial_M \Omega_3 \cap \Omega)) \\ = \mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \partial_M \Omega_3 \cap \Omega) + \mathcal{H}^{d-1}(\partial_M \Omega_2 \cap \partial_M \Omega_3 \cap \Omega) \end{aligned}$$

and subsequently

$$\begin{aligned} \mathcal{H}^{d-1}(\partial_M(\Omega_1 \cup \Omega_2 \cup \Omega_3) \cap \Omega) &= \mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \Omega) + \mathcal{H}^{d-1}(\partial_M \Omega_2 \cap \Omega) + \mathcal{H}^{d-1}(\partial_M \Omega_3 \cap \Omega) \\ &\quad - 2\mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \partial_M \Omega_2 \cap \Omega) - 2\mathcal{H}^{d-1}(\partial_M \Omega_1 \cap \partial_M \Omega_3 \cap \Omega) - 2\mathcal{H}^{d-1}(\partial_M \Omega_2 \cap \partial_M \Omega_3 \cap \Omega). \end{aligned}$$

This proves the result for $m = 3$. \square

We have now all the ingredients to prove the pointwise convergence result.

Theorem 3.3. *Let Ω_i, Ω_j be two subsets of finite perimeter of Ω such that $|\Omega_i \cap \Omega_j| = 0$. If $u_i = \chi_{\Omega_i}$ and $u_j = \chi_{\Omega_j}$, then*

$$\mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega) = \lim_{\varepsilon \rightarrow 0} \frac{2}{\varepsilon} \langle L_\varepsilon u_i, u_j \rangle.$$

Proof. By Proposition 3.2, we have

$$\mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega) = \frac{1}{2} [\mathcal{H}^{d-1}(\partial_M \Omega_i \cap \Omega) + \mathcal{H}^{d-1}(\partial_M \Omega_j \cap \Omega) - \mathcal{H}^{d-1}(\partial_M(\Omega_i \cup \Omega_j) \cap \Omega)].$$

Using Theorem 2.6 we obtain

$$\begin{aligned} \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega) &= \lim_{\varepsilon \rightarrow 0} [\tilde{F}_\varepsilon(u_i) + \tilde{F}_\varepsilon(u_j) - \tilde{F}_\varepsilon(u_i + u_j)] \\ &= \lim_{\varepsilon \rightarrow 0} \left[\frac{1}{\varepsilon} \langle 1 - L_\varepsilon u_i, u_i \rangle + \frac{1}{\varepsilon} \langle 1 - L_\varepsilon u_j, u_j \rangle - \frac{1}{\varepsilon} \langle 1 - L_\varepsilon(u_i + u_j), u_i + u_j \rangle \right] \\ &= \lim_{\varepsilon \rightarrow 0} \frac{2}{\varepsilon} \langle L_\varepsilon u_i, u_j \rangle. \end{aligned}$$

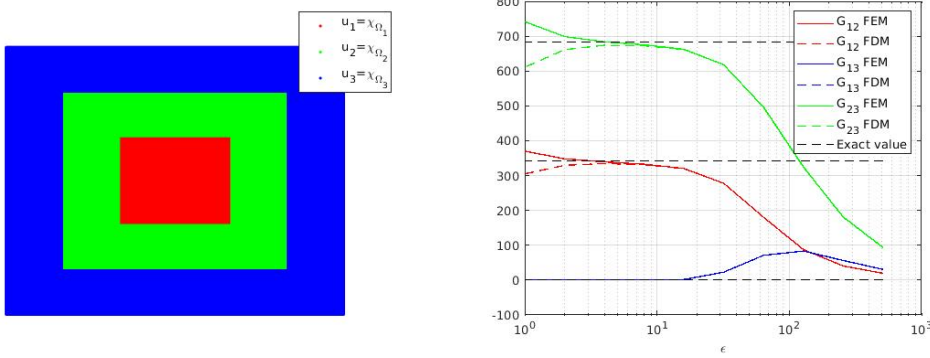


FIGURE 2. (left) given partition, (right) convergence history of $G_\varepsilon(u_i, u_j)$ computed with the FEM (solid lines), the FDM (dashed lines) and the exact values (horizontal lines).

□

We denote

$$G_\varepsilon(u_i, u_j) = \frac{1}{\varepsilon} \langle L_\varepsilon u_i, u_j \rangle. \quad (3.4)$$

We present an example to illustrate the pointwise convergence of the functional G_ε in Figure 2. The values of the function G_ε are computed using two discretization methods, namely the finite element method (FEM) with Q1 elements and the finite difference method (FDM) with 5 points stencil. The parameter ε has the dimension of a length. In fact, in view of (2.2), it is a characteristic width of the diffuse interface represented by the slow variable v_ε . Thus we start with a characteristic size of Ω , namely $\varepsilon_0 = \varepsilon_{\max} = \max(m, n)$ where (m, n) is the size of the grid (its stepsize is fixed as unitary). Then we divide ε by two between each computation, that is, we choose $\varepsilon_i = \varepsilon_{\max}/2^i$. In order to approximate (2.2) properly, ε must not be taken significantly smaller than the grid resolution. Thus we stop the algorithm as soon as $\varepsilon_i \leq \varepsilon_{\min} = 1$. We observe that the computed values of $G_\varepsilon(u_i, u_j)$ are always smaller using the FDM than using the FEM. This is due to higher diffusion of the FEM.

4. LOWER SEMICONTINUITY AND EQUICOERCIVITY

4.1. Lower semicontinuity. The following important result is found in [4]. An alternative proof is given in [19] when Ω is a Cartesian product of intervals, in which case it is also a consequence of Theorem 5.11.

Theorem 4.1. *Let $(\alpha_{ij}) \in S_N^+$. The condition (1.3) is necessary and sufficient for the function*

$$\mathcal{I} : (\Omega_1, \dots, \Omega_N) \mapsto \frac{1}{2} \sum_{1 \leq i < j \leq N} \alpha_{ij} \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega)$$

to be lower semicontinuous for the convergence in measure in the set of N -tuples $(\Omega_1, \dots, \Omega_N)$ of Lebesgue-measurable subsets of Ω such that $\chi_{\Omega_i} \in BV(\Omega)$ for all i and $\sum_{i=1}^N \chi_{\Omega_i} = 1$.

This property will lead to the existence of minimizers for the exact minimal partition problem in Theorem 5.2. In addition, lower-semicontinuity is a necessary condition for Γ -convergence [9, 14], which will be addressed later. Equicoercivity is another important property. Basically, together with Γ -convergence, it implies that sequences of minimizers of approximating functionals converge up to a subsequence to a minimizer of the limiting functional, see again, e.g., [9, 14].

4.2. Equicoercivity. We will rely on the following theorem from [7].

Theorem 4.2. *Let u^ε be a sequence of functions of $L^\infty(\Omega, [0, 1])$ such that $\sup_{\varepsilon>0} \tilde{F}_\varepsilon(u^\varepsilon) < +\infty$. There exists $u \in L^\infty(\Omega, \{0, 1\})$ such that $u^\varepsilon \rightarrow u$ strongly in $L^1(\Omega)$ for a subsequence.*

We set

$$\mathcal{I}_\varepsilon(u_1, \dots, u_N) = \sum_{1 \leq i < j \leq N} \alpha_{ij} G_\varepsilon(u_i, u_j) = \frac{1}{\varepsilon} \sum_{1 \leq i < j \leq N} \alpha_{ij} \langle L_\varepsilon u_i, u_j \rangle.$$

We now prove the equicoercivity of the functionals \mathcal{I}_ε .

Theorem 4.3. *Assume that $(\alpha_{ij}) \in S_N^+$ with $\alpha_{ij} \geq \underline{\alpha} > 0$. Let $(u_1^\varepsilon, \dots, u_N^\varepsilon)$ be a sequence of N -tuples of functions in $L^\infty(\Omega, [0, 1])$ such that $\sum_{i=1}^N u_i^\varepsilon = 1$ for all ε and $\sup_{\varepsilon>0} \mathcal{I}_\varepsilon(u_1^\varepsilon, \dots, u_N^\varepsilon) < +\infty$. For all i , there exists $u_i \in L^\infty(\Omega, \{0, 1\})$ such that $u_i^\varepsilon \rightarrow u_i$ strongly in $L^1(\Omega)$ for a subsequence. Moreover we have $\sum_{i=1}^N u_i = 1$.*

Proof. Using (3.4), we obtain

$$\begin{aligned} \sum_{1 \leq i < j \leq N} \alpha_{ij} G_\varepsilon(u_i^\varepsilon, u_j^\varepsilon) &= \frac{1}{\varepsilon} \sum_{1 \leq i < j \leq N} \alpha_{ij} \langle L_\varepsilon u_i^\varepsilon, u_j^\varepsilon \rangle \\ &\geq \frac{\underline{\alpha}}{\varepsilon} \sum_{1 \leq i < j \leq N} \langle L_\varepsilon u_i^\varepsilon, u_j^\varepsilon \rangle = \frac{\underline{\alpha}}{2\varepsilon} \sum_{1 \leq i \neq j \leq N} \langle L_\varepsilon u_i^\varepsilon, u_j^\varepsilon \rangle = \frac{\underline{\alpha}}{2\varepsilon} \sum_{i=1}^N \langle L_\varepsilon u_i^\varepsilon, \sum_{\substack{j=1 \\ j \neq i}}^N u_j^\varepsilon \rangle. \end{aligned}$$

Due to $\sum_{j \neq i} u_j^\varepsilon = 1 - u_i^\varepsilon$ we infer

$$\sum_{1 \leq i < j \leq N} \alpha_{ij} G_\varepsilon(u_i^\varepsilon, u_j^\varepsilon) \geq \frac{\underline{\alpha}}{2} \sum_{i=1}^N \frac{1}{\varepsilon} \langle L_\varepsilon u_i^\varepsilon, 1 - u_i^\varepsilon \rangle = \frac{\underline{\alpha}}{2} \sum_{i=1}^N \tilde{F}_\varepsilon(u_i^\varepsilon).$$

The result follows from Theorem 4.2. \square

5. CONICAL COMBINATIONS OF PERIMETERS AND Γ -CONVERGENCE

In this section we rewrite the interface energy as a linear combination of perimeters of aggregated phases. If all coefficients can be taken nonnegative (conical combination) then the Γ -convergence of the approximating functional is straightforward. Therefore special attention is paid to the signs of the coefficients.

Let $S \subset \{1, \dots, N\}$. From now on, we will denote $\Omega_S = \cup_{i \in S} \Omega_i$ and $\bar{S} = \{1, \dots, N\} \setminus S$.

5.1. Algebraic properties of interface energies.

Lemma 5.1. *Let $\Omega_1, \dots, \Omega_N$ be subsets of finite perimeter of Ω such that $|\Omega \setminus \cup_{i=1}^N \Omega_i| = 0$ and $|\Omega_i \cap \Omega_j| = 0$ for $i \neq j$. Let $\mathbb{L}_{ij} = \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega)$, $\mathbb{P}_S = \mathcal{H}^{d-1}(\partial_M \Omega_S \cap \Omega)$. Then*

$$\mathbb{P}_S = \sum_{\substack{i \in S \\ j \notin S}} \mathbb{L}_{ij} = \mathbb{P}_{\bar{S}}.$$

Proof. By the definition of the essential boundary, we have

$$\partial_M \Omega_i = \partial_M (\mathbb{R}^d \setminus \Omega_i) = \partial_M \left(\bigcup_{j \neq i} \Omega_j \cup (\mathbb{R}^d \setminus \Omega) \right).$$

As an elementary property of the essential boundary, we have that $\partial_M(A \cup B) \subset \partial_M A \cup \partial_M B$. Moreover, as Ω is open, we have $\partial_M \Omega \cap \Omega = \emptyset$. This yields

$$\partial_M \left(\bigcup_{j \neq i} \Omega_j \cup (\mathbb{R}^d \setminus \Omega) \right) \cap \Omega \subset \left(\bigcup_{j \neq i} \partial_M \Omega_j \right) \cap \Omega,$$

which implies that

$$\partial_M \Omega_i \cap \Omega = \bigcup_{j \neq i} (\partial_M \Omega_j \cap \partial_M \Omega_i \cap \Omega). \quad (5.1)$$

For $i \neq j, i \neq k, j \neq k$, following (3.2), we have

$$\mathcal{H}^{d-1}((\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega) \cap (\partial_M \Omega_i \cap \partial_M \Omega_k \cap \Omega)) = \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \partial_M \Omega_k \cap \Omega) = 0. \quad (5.2)$$

We deduce from (5.1),(5.2) that

$$\mathbb{P}_{\{i\}} = \sum_{j \neq i} \mathbb{L}_{ij}.$$

From this fact and Proposition 3.2, we obtain that

$$\mathbb{P}_S = \sum_{i \in S} \mathbb{P}_{\{i\}} - 2 \sum_{\substack{(i,j) \in S^2 \\ i < j}} \mathbb{L}_{ij} = \sum_{\substack{i \in S \\ j \notin S}} \mathbb{L}_{ij}.$$

□

We arrive at the announced existence result.

Theorem 5.2. *Assume that $(\alpha_{ij}) \in T_N$ with $\alpha_{ij} \geq \underline{\alpha} > 0$. Let $g_1, \dots, g_N \in L^1(\Omega)$. The problem*

$$\text{minimize } \mathcal{J}(\Omega_1, \dots, \Omega_N) := \sum_{i=1}^N \int_{\Omega_i} g_i(x) dx + \mathcal{I}(\Omega_1, \dots, \Omega_N), \quad (5.3)$$

in the set of N -tuples $(\Omega_1, \dots, \Omega_N)$ of Lebesgue-measurable subsets of Ω such that $\chi_{\Omega_i} \in BV(\Omega)$ for all i and $\sum_{i=1}^N \chi_{\Omega_i} = 1$, admits at least a solution.

Proof. We have the inequality

$$\mathcal{J}(\Omega_1, \dots, \Omega_N) \geq - \sum_{i=1}^N \|g_i\|_{L^1(\Omega)} + \frac{\alpha}{2} \sum_{1 \leq i < j \leq N} \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega).$$

Lemma 5.1 entails

$$\mathcal{J}(\Omega_1, \dots, \Omega_N) \geq - \sum_{i=1}^N \|g_i\|_{L^1(\Omega)} + \frac{\alpha}{4} \sum_{i=1}^N \mathcal{H}^{d-1}(\partial_M \Omega_i \cap \Omega).$$

Therefore, for a minimizing sequence $(\Omega_1^k, \dots, \Omega_N^k)$, the quantity $\sum_{i=1}^N \mathcal{H}^{d-1}(\partial_M \Omega_i^k \cap \Omega)$ is bounded. By a standard property of bounded sequences of sets of finite perimeters, see e.g. [6, 9, 23], there exists a family $(\Omega_1, \dots, \Omega_N)$ of subsets of finite perimeters of Ω such that $\Omega_i^k \rightarrow \Omega_i$ in measure for each i , for a non-relabelled subsequence. Equivalently, $\chi_{\Omega_i^k} \rightarrow \chi_{\Omega_i}$ in $L^1(\Omega)$, which implies that $\sum_{i=1}^N \chi_{\Omega_i} = 1$. The lower-semicontinuity of Theorem 4.1 shows that $(\Omega_1, \dots, \Omega_N)$ is a global minimizer. □

5.2. Algebraic properties of approximate interface energies. We now prove the approximate counterpart of Lemma 5.1.

Lemma 5.3. *Let $\Omega_i, \dots, \Omega_N$ be subsets of finite perimeter of Ω such that $|\Omega \setminus \cup_{i=1}^N \Omega_i| = 0$ and $|\Omega_i \cap \Omega_j| = 0$ for $i \neq j$. Let $u_i = \chi_{\Omega_i}$, $\mathbb{L}_{ij}^\varepsilon = \frac{1}{\varepsilon} \langle L_\varepsilon u_i, u_j \rangle$, $\mathbb{P}_S^\varepsilon = \frac{1}{\varepsilon} \langle 1 - L_\varepsilon \sum_{i \in S} u_i, \sum_{i \in S} u_i \rangle$. Then*

$$\mathbb{P}_S^\varepsilon = \sum_{\substack{i \in S \\ j \notin S}} \mathbb{L}_{ij}^\varepsilon = \mathbb{P}_S^\varepsilon.$$

Proof. We have

$$\mathbb{P}_S^\varepsilon = \frac{1}{\varepsilon} \left\langle 1 - L_\varepsilon \sum_{i \in S} u_i, \sum_{i \in S} u_i \right\rangle = \frac{1}{\varepsilon} \left\langle L_\varepsilon \sum_{i \in S} u_i, 1 - \sum_{i \in S} u_i \right\rangle.$$

Using $1 - \sum_{i \in S} u_i = \sum_{j \notin S} u_j$ we obtain

$$\mathbb{P}_S^\varepsilon = \frac{1}{\varepsilon} \left\langle L_\varepsilon \sum_{i \in S} u_i, \sum_{j \notin S} u_j \right\rangle = \frac{1}{\varepsilon} \sum_{\substack{i \in S \\ j \notin S}} \langle L_\varepsilon u_i, u_j \rangle = \sum_{\substack{i \in S \\ j \notin S}} \mathbb{L}_{ij}^\varepsilon.$$

□

We emphasize that the properties stated in Lemmas 5.1 and 5.3 are formally the same. This will allow to obtain similar reformulations for the interface energy and its approximation. The approximate counterpart of Theorem 5.2 is stated below.

Theorem 5.4. *Assume that $(\alpha_{ij}) \in S_N^+$ with $\alpha_{ij} \geq \underline{\alpha} > 0$. Let $g_1, \dots, g_N \in L^1(\Omega)$. The problem*

$$\text{minimize } \mathcal{J}_\varepsilon(u_1, \dots, u_N) := \sum_{i=1}^N \int_{\Omega} u_i g_i(x) dx + \mathcal{I}_\varepsilon(u_1, \dots, u_N), \quad (5.4)$$

in the set of N -tuples $(u_1, \dots, u_N) \in L^\infty(\Omega, [0, 1])^N$ such that $\sum_{i=1}^N u_i = 1$ a.e., admits at least a solution.

Proof. Consider a minimizing sequence $(u_1^k, \dots, u_N^k) \in L^\infty(\Omega, [0, 1])^N$ such that $\sum_{i=1}^N u_i^k = 1$. Up to a subsequence, this sequence converges weakly-* to some $(u_1, \dots, u_N) \in L^\infty(\Omega, [0, 1])^N$. Obviously it holds $\sum_{i=1}^N u_i = 1$. By Lemma 2.2, (u_1, \dots, u_N) is a minimizer of (5.4). □

5.3. Matrix representation of algebraic properties. We define the column vector \mathbb{L} made of the values (\mathbb{L}_{ij}) in a chosen order. Similarly we define the column vector α of the surface tensions (α_{ij}) and \mathbb{P} the vector gathering the values \mathbb{P}_S , for $S \in \mathcal{S} \subset \mathcal{P}(\{1, \dots, N\})$. The set \mathcal{S} is made as small as possible by exploiting the property of complementation. We adopt the following construction: when N is odd the elements of \mathcal{S} are the subsets of $\{1, \dots, N\}$ containing between 1 and $(N-1)/2$ elements; when N is even the elements of \mathcal{S} are the subsets of $\{1, \dots, N\}$ containing between 1 and $N/2 - 1$ elements and the subsets containing $N/2$ elements including 1 (see Table 1 for $N \leq 5$). An alternative - bijective - set could be taken as the set of nonempty subsets of $\{1, \dots, N-1\}$, so that $\#\mathcal{S} = 2^{N-1} - 1$. In view of Lemma 5.1, we can define a matrix $\mathbb{M} = (m_{ij}) \in \mathbb{R}^{\#\mathcal{S} \times \binom{N}{2}}$ such that

$$\mathbb{P} = \mathbb{M}\mathbb{L}. \quad (5.5)$$

Note that $m_{ij} \in \{0, 1\}$.

Let $\beta = (\beta_S)_{S \in \mathcal{S}}$. Starting from the dot products

$$\beta \cdot \mathbb{P} = \beta \cdot \mathbb{M}\mathbb{L} = \mathbb{M}^\top \beta \cdot \mathbb{L},$$

one infers that

$$\sum_{1 \leq i < j \leq N} \alpha_{ij} \mathbb{L}_{ij} = \sum_{S \in \mathcal{S}} \beta_S \mathbb{P}_S \quad (5.6)$$

holds for any \mathbb{L} and corresponding \mathbb{P} as soon as the columns of coefficients satisfy the linear system

$$\mathbb{M}^\top \beta = \alpha. \quad (5.7)$$

Due to

$$\mathbb{L}_{ij} = \frac{1}{2}(\mathbb{P}_i + \mathbb{P}_j - \mathbb{P}_{ij}), \quad (5.8)$$

N=2	$\{\{1\}\}$
N=3	$\{\{1\}, \{2\}, \{3\}\}$
N=4	$\{\{1\}, \{2\}, \{3\}, \{4\}, \{12\}, \{13\}, \{14\}\}$
N=5	$\{\{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \{12\}, \{13\}, \{14\}, \{15\}, \{23\}, \{24\}, \{25\}, \{34\}, \{35\}, \{45\}\}$

TABLE 1. The set \mathcal{S} of values of S .

it turns out that \mathbb{M} has full rank. However there are in general multiple ways to find a β corresponding to a given α . For the purpose of proving a Γ -convergence property, possible nonnegative solutions of this system will be privileged.

5.4. Existence of conical combination. We define the set

$$B_N^+ = \{(\alpha_{ij}) \in S_N : \exists(\beta_S) \geq 0 \text{ s.t. } \alpha = \mathbb{M}^\top \beta\} \subset S_N^+.$$

We now address the identification of the set B_N^+ . We consider S_N , T_N and B_N^+ as subsets of the Euclidean space $\mathbb{R}^{N(N-1)/2}$. Note that S_N is the full linear space, while T_N and B_N^+ are polyhedral convex cones. Indeed, T_N is defined as intersection of half-spaces of $\mathbb{R}^{N(N-1)/2}$, and B_N^+ is the convex cone generated by the row vectors of \mathbb{M} . The sets T_N and B_N^+ are sometimes called the semimetric cone (or metric cone) and the cut cone (or Hamming cone), respectively, see for example [18]. For the sake of completeness, we recall that a matrix $(\alpha_{ij}) \in S_N$ is called ℓ^1 -embeddable if there exists some integer K and N points $x_1, \dots, x_N \in \mathbb{R}^K$ such that $\alpha_{ij} = \|x_i - x_j\|_1$ for all $1 \leq i < j \leq N$. It is known that the set of ℓ^1 -embeddable matrices is equal to B_N^+ (see for example [18], proposition 4.2.2). It is also known that $B_N^+ \subset T_N$ for any $N \geq 2$ and that $B_N^+ = T_N$ for $N \leq 4$. Nevertheless we present our own proofs of these results, without using the concept of ℓ^1 -embeddability.

Theorem 5.5. *For any $N \geq 2$ it holds $B_N^+ \subset T_N$.*

Proof. Using the conic descriptions of B_N^+ and T_N , we only have to check that any row vector of \mathbb{M} is an element of T_N . Consider an arbitrary row of \mathbb{M} . It corresponds to a set $S \in \mathcal{S}$. Call (m_{ij}) the entries of this row vector in the system of indices associated with phases. Recall that $m_{ij} \in \{0, 1\}$. Consider a nontrivial triangle inequality $m_{ij} \leq m_{ik} + m_{kj}$ (with i, j and k distinct integers) defining T_N . In view of Lemma 5.1, if both i and j are in S , then $m_{ij} = 0$ and the inequality is satisfied. The same holds if both i and j are not in S . If $i \in S$ and $j \notin S$, then $m_{ij} = 1$. In this case, either $k \in S$ and $m_{kj} = 1$, or $k \notin S$ and $m_{ik} = 1$. In both cases the triangle inequality is satisfied. Obviously the same occurs if $i \notin S$ and $j \in S$. Thus any row vector of \mathbb{M} belongs to T_N , which implies that $B_N^+ \subset T_N$. \square

Theorem 5.6. *If $N = 3, 4$ then $T_N \subset B_N^+$.*

Proof. We will use the notations β_i for $\beta_{\{i\}}$ and β_{ij} for $\beta_{\{ij\}}$. We treat separately the two cases.

- Case 1: $N = 3$. The unique solution of (5.7) is

$$\beta_1 = \frac{-\alpha_{23} + \alpha_{12} + \alpha_{13}}{2}, \quad \beta_2 = \frac{-\alpha_{13} + \alpha_{12} + \alpha_{23}}{2}, \quad \beta_{12} = \frac{-\alpha_{12} + \alpha_{13} + \alpha_{23}}{2}.$$

If $(\alpha_{ij}) \in T_3$, then β_1, β_2 , and β_{12} are nonnegative, which implies that $T_3 \subset B_3^+$.

- Case 2: $N = 4$. Solving (5.7) for $N = 4$, we choose the particular solution

$$\begin{aligned} \beta_{12} &= \frac{-\alpha_{12} + \alpha_{14} + \alpha_{24}}{2}, \quad \beta_{13} = \frac{-\alpha_{13} + \alpha_{14} + \alpha_{34}}{2}, \quad \beta_{23} = \frac{-\alpha_{23} + \alpha_{24} + \alpha_{34}}{2}, \\ \beta_1 &= \frac{\alpha_{12} + \alpha_{13} - \alpha_{24} - \alpha_{34}}{2}, \quad \beta_2 = \frac{\alpha_{12} + \alpha_{23} - \alpha_{14} - \alpha_{34}}{2}, \\ \beta_3 &= \frac{\alpha_{13} + \alpha_{23} - \alpha_{14} - \alpha_{24}}{2}, \quad \beta_4 = 0. \end{aligned}$$

It is immediate to see that if $(\alpha_{ij}) \in T_4$, then β_{12}, β_{13} , and β_{23} are nonnegative. Now, we want to prove that if $(\alpha_{ij}) \in T_4$, then β_1, β_2 , and β_3 are nonnegative too. Let us define for $i = 1, \dots, 4$, $\Sigma_i = \sum_{j \neq i} \alpha_{ij}$. Up to reordering the phases, we assume that $\Sigma_4 \leq \Sigma_3 \leq \Sigma_2 \leq \Sigma_1$. Then we have

$$\begin{aligned} \begin{cases} \Sigma_4 \leq \Sigma_1 \\ \Sigma_4 \leq \Sigma_2 \\ \Sigma_4 \leq \Sigma_3 \end{cases} &\Rightarrow \begin{cases} \alpha_{14} + \alpha_{24} + \alpha_{34} \leq \alpha_{12} + \alpha_{13} + \alpha_{14} \\ \alpha_{14} + \alpha_{24} + \alpha_{34} \leq \alpha_{12} + \alpha_{23} + \alpha_{24} \\ \alpha_{14} + \alpha_{24} + \alpha_{34} \leq \alpha_{13} + \alpha_{23} + \alpha_{34} \end{cases} \\ &\Rightarrow \begin{cases} \alpha_{24} + \alpha_{34} \leq \alpha_{12} + \alpha_{13} \\ \alpha_{14} + \alpha_{34} \leq \alpha_{12} + \alpha_{23} \\ \alpha_{14} + \alpha_{24} \leq \alpha_{13} + \alpha_{23} \end{cases} \Rightarrow \begin{cases} \beta_1 \geq 0 \\ \beta_2 \geq 0 \\ \beta_3 \geq 0 \end{cases} . \end{aligned}$$

□

We now discuss the numerical search for some $(\beta_S) \geq 0$, given coefficients (α_{ij}) . Let us first recall the definition of a conical combination and Carathéodory's theorem. Given a finite number of vectors v_1, v_2, \dots, v_p in a real vector space, a conical combination of these vectors is a vector of the form

$$\lambda_1 v_1 + \lambda_2 v_2 + \dots + \lambda_p v_p,$$

where the real numbers $\lambda_1, \dots, \lambda_p$ are non-negative.

Theorem 5.7 (Carathéodory). *In a vector space of dimension n , all conical combination of m vectors ($m > n$), can be written as a conical combination of n of these vectors.*

By the above theorem and the linear system (5.7), when $\alpha = (\alpha_{ij}) \in B_N^+$, α can be written as a conical combination of $\binom{N}{2}$ rows of the matrix \mathbb{M} . Calling \mathbb{B} the corresponding submatrix, we have $\mathbb{B}\beta = \alpha$, with $\beta \geq 0$. Denoting $k = \text{rank } \mathbb{B}$, then α belongs to the space spanned by k linearly independent columns of \mathbb{B} . By Carathéodory's theorem again, α is a conical combination of k columns of \mathbb{B} . By completion of these vectors (since \mathbb{M}^\top has full rank), α writes as a conical combination of $\binom{N}{2}$ linearly independent columns of \mathbb{M}^\top . This leads to Algorithm 1.

Data: Given $\alpha = (\alpha_{ij}) \in \mathbb{R}^{\binom{N}{2} \times 1}$, $\mathbb{M} \in \mathbb{R}^{\#S \times \binom{N}{2}}$.

- 1 **repeat**
- 2 Loop on the set of square invertible submatrices $\Lambda \in \mathbb{R}^{\binom{N}{2} \times \binom{N}{2}}$ of \mathbb{M}^\top ;
- 3 Compute $\beta = \Lambda^{-1}\alpha$;
- 4 **until** $\beta \geq 0$;
- 5 Complete β by zeros at the entries corresponding to the columns of \mathbb{M}^\top that have been removed.

Algorithm 1: Search for $(\beta_S) \geq 0$.

Using Algorithm 1 we are in particular able to find counterexamples to Theorem 5.6 when $N = 5$. For instance, it is immediately seen that the matrix

$$(\alpha_{ij}) = \begin{pmatrix} 0 & 2 & 3 & 2 & 1 \\ 2 & 0 & 1 & 2 & 3 \\ 3 & 1 & 0 & 3 & 3 \\ 2 & 2 & 3 & 0 & 1 \\ 1 & 3 & 3 & 1 & 0 \end{pmatrix}$$

satisfies the triangle inequality, but Algorithm 1 terminates without finding any $\beta \geq 0$.

The complexity of Algorithm 1 rapidly grows with N : for example for $N = 6$, there are 300540195 $\binom{N}{2} \times \binom{N}{2}$ submatrices of \mathbb{M}^\top . Hence, it is impossible in practice to use this algorithm for $N > 5$. For this reason we propose a second algorithm. Let $(B_N^+)^{\circ}$ denote the polar cone

of B_N^+ . Moreau's decomposition theorem directly implies that $\alpha \in B_N^+$ if and only if the projection of α on $(B_N^+)^{\circ}$ is 0. This leads us to the following positive definite quadratic program:

$$\min_{\alpha: y \leq 0 \forall i} \|\alpha - y\|^2, \quad (5.9)$$

where (a_i) are the rows of \mathbb{M} . Then $\alpha \in B_N^+$ if and only if the optimal value of this program is 0. This program is easily tractable up to $N = 13$. This technique, however, does not provide any possible β . Note that the algorithms developed in sections 8 and 9 do not require the knowledge of such β .

5.5. Γ -convergence with nonnegative coefficients. Define the set

$$\tilde{\mathcal{E}}_N = \left\{ (u_1, \dots, u_N) \in L^\infty(\Omega, [0, 1])^N : \sum_{i=1}^N u_i = 1 \text{ a.e.} \right\}$$

and the functional $\tilde{\mathcal{I}} : \tilde{\mathcal{E}}_N \rightarrow \mathbb{R}$ such that

$$\tilde{\mathcal{I}}(u_1, \dots, u_N) = \begin{cases} \frac{1}{2} \sum_{1 \leq i < j \leq N} \alpha_{ij} \mathcal{H}^1(\partial_M \Omega_i \cap \partial_M \Omega_j \cap \Omega) & \text{if } u_i \in BV(\Omega, \{0, 1\}) \forall i, u_i = \chi_{\Omega_i}, \\ +\infty & \text{otherwise.} \end{cases}$$

Theorem 5.8. *If $(\alpha_{ij}) \in B_N^+$, then the functionals \mathcal{I}_ε Γ -converge to $\tilde{\mathcal{I}}$ in $\tilde{\mathcal{E}}_N$ endowed with the strong topology of $L^1(\Omega)^N$.*

Proof. We first prove the liminf inequality. Let $(u_i^\varepsilon) \in \tilde{\mathcal{E}}_N$ be a sequence such that (u_i^ε) converges to u_i . From (3.4), (5.6) and Lemma 5.3 we have

$$\sum_{1 \leq i < j \leq N} \alpha_{ij} G_\varepsilon(u_i^\varepsilon, u_j^\varepsilon) = \frac{1}{\varepsilon} \sum_{S \in \mathcal{S}} \beta_S \left\langle 1 - L_\varepsilon \sum_{i \in S} u_i^\varepsilon, \sum_{i \in S} u_i^\varepsilon \right\rangle. \quad (5.10)$$

This entails

$$\liminf_{\varepsilon \rightarrow 0} \sum_{1 \leq i < j \leq N} \alpha_{ij} G_\varepsilon(u_i^\varepsilon, u_j^\varepsilon) \geq \sum_{S \in \mathcal{S}} \liminf_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} \beta_S \left\langle 1 - L_\varepsilon \sum_{i \in S} u_i^\varepsilon, \sum_{i \in S} u_i^\varepsilon \right\rangle.$$

We infer from Theorem 2.5 and (5.6) that

$$\liminf_{\varepsilon \rightarrow 0} \sum_{1 \leq i < j \leq N} \alpha_{ij} G_\varepsilon(u_i^\varepsilon, u_j^\varepsilon) \geq \tilde{\mathcal{I}}(u_1, \dots, u_N).$$

Second, due to the pointwise convergence (Theorem 3.3), the limsup inequality holds for the constant recovery sequence. \square

5.6. Γ -convergence in the general case. Here we generalize Theorem 5.8 to arbitrary surface tensions when Ω is a Cartesian product of intervals. Our proof is widely inspired from [19], nevertheless it incorporates some adaptations to our context. In [19] the functional

$$E_\varepsilon(u_1, \dots, u_N) = \frac{1}{\varepsilon} \sum_{1 \leq i < j \leq N} \alpha_{ij} \int_D \mathcal{G}_\varepsilon \star u_i u_j dx \quad (5.11)$$

is considered. The convolution kernel \mathcal{G}_ε is mainly chosen as the Gaussian, and more generally it is assumed to fulfill some properties which are not all satisfied in our case. The main ingredient in the proof of [19] is an approximate monotonicity argument. Here we follow the same path. We start with a rough estimate of derivative, however different from [19] since we exploit here the underlying boundary value problems instead of the convolution structure. Therefore, we do not need at this stage any geometric assumption on Ω .

Lemma 5.9. For all $(u_1, \dots, u_N) \in \tilde{\mathcal{E}}_N$ we have

$$\frac{d}{d\varepsilon} \mathcal{I}_\varepsilon(u_1, \dots, u_N) = \frac{1}{2\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (-3v_i^\varepsilon u_j + 2v_i^\varepsilon v_j^\varepsilon) dx, \quad (5.12)$$

with $v_i^\varepsilon := L_\varepsilon u_i$, and

$$\frac{d}{d\varepsilon} (\varepsilon^3 \mathcal{I}_\varepsilon(u_1, \dots, u_N)) \geq 0.$$

Proof. For arbitrary N -tuples $v = (v_1, \dots, v_N) \in H^1(\Omega)^N$, $w = (w_1, \dots, w_N) \in H^1(\Omega)^N$, we define the Lagrangian

$$\mathcal{L}(\varepsilon, v, w) = \frac{1}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} v_i u_j dx + \sum_{i=1}^N \int_{\Omega} (\varepsilon^2 \nabla v_i \cdot \nabla w_i + v_i w_i - u_i w_i) dx.$$

Whenever $v_i = v_i^\varepsilon$ the last integral vanishes, which results in

$$\mathcal{L}(\varepsilon, v^\varepsilon, w) = \mathcal{I}_\varepsilon(u_1, \dots, u_N) \quad \forall w \in H^1(\Omega)^N. \quad (5.13)$$

Differentiating the Lagrangian with respect to v in the direction \hat{v} yields

$$\frac{\partial \mathcal{L}}{\partial v}(\varepsilon, v, w) \hat{v} = \frac{1}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \hat{v}_i u_j dx + \sum_{i=1}^N \int_{\Omega} (\varepsilon^2 \nabla \hat{v}_i \cdot \nabla w_i + \hat{v}_i w_i) dx,$$

which can be rearranged as

$$\frac{\partial \mathcal{L}}{\partial v}(\varepsilon, v, w) \hat{v} = \sum_{i=1}^N \left(\int_{\Omega} (\varepsilon^2 \nabla w_i \cdot \nabla \hat{v}_i + w_i \hat{v}_i) dx + \frac{1}{2\varepsilon} \sum_{j=1}^N \alpha_{ij} \int_{\Omega} u_j \hat{v}_i dx \right).$$

This vanishes as soon as, for all $i = 1, \dots, N$,

$$w_i = -\frac{1}{2\varepsilon} \sum_{j=1}^N \alpha_{ij} v_j^\varepsilon =: w_i^\varepsilon. \quad (5.14)$$

Going back to (5.13) we infer

$$\frac{d}{d\varepsilon} \mathcal{I}_\varepsilon(u_1, \dots, u_N) = \frac{\partial \mathcal{L}}{\partial \varepsilon}(\varepsilon, v^\varepsilon, w^\varepsilon).$$

By definition of the Lagrangian this entails

$$\frac{d}{d\varepsilon} \mathcal{I}_\varepsilon(u_1, \dots, u_N) = -\frac{1}{2\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} v_i^\varepsilon u_j dx + \sum_{i=1}^N \int_{\Omega} 2\varepsilon \nabla v_i^\varepsilon \cdot \nabla w_i^\varepsilon dx.$$

Using now the expression (5.14) of the adjoint state we arrive at

$$\frac{d}{d\varepsilon} \mathcal{I}_\varepsilon(u_1, \dots, u_N) = -\frac{1}{2\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} v_i^\varepsilon u_j dx - \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \nabla v_i^\varepsilon \cdot \nabla v_j^\varepsilon dx.$$

Using that

$$\int_{\Omega} (\varepsilon^2 \nabla v_i^\varepsilon \cdot \nabla v_j^\varepsilon + v_i^\varepsilon v_j^\varepsilon) dx = \int_{\Omega} u_i v_j^\varepsilon dx$$

we infer

$$\frac{d}{d\varepsilon} \mathcal{I}_\varepsilon(u_1, \dots, u_N) = -\frac{3}{2\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} v_i^\varepsilon u_j dx + \frac{1}{\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} v_i^\varepsilon v_j^\varepsilon dx,$$

that is (5.12). We recognize that

$$\frac{d}{d\varepsilon} \mathcal{I}_\varepsilon(u_1, \dots, u_N) = -\frac{3}{\varepsilon} \mathcal{I}_\varepsilon(u_1, \dots, u_N) + \frac{1}{\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} v_i^\varepsilon v_j^\varepsilon dx.$$

This implies that

$$\frac{d}{d\varepsilon} (\varepsilon^3 \mathcal{I}_\varepsilon(u_1, \dots, u_N)) = \varepsilon \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} v_i^\varepsilon v_j^\varepsilon dx \geq 0.$$

□

The key estimate is the following.

Lemma 5.10. *If $(\alpha_{ij}) \in T_N$ and Ω is a Cartesian product of open intervals, then for all $\varepsilon \leq \varepsilon_0$ and $(u_1, \dots, u_N) \in \tilde{\mathcal{E}}_N$ we have*

$$\mathcal{I}_\varepsilon(u_1, \dots, u_N) \geq \left(\frac{\varepsilon_0}{\varepsilon_0 + \varepsilon} \right)^3 \mathcal{I}_{\varepsilon_0}(u_1, \dots, u_N). \quad (5.15)$$

Proof. We assume that $\Omega = (0, L_1) \times \dots \times (0, L_d)$ and we define the extended domain $D = (0, 2L_1) \times \dots \times (0, 2L_d)$. We extend the functions u_1, \dots, u_N to D by successive symmetries, then to \mathbb{R}^d by periodicity, keeping the same notation. This leads to the representation $L_\varepsilon u_i = \Phi_\varepsilon \star u_i$, with the convolution kernel

$$\Phi_\varepsilon(x) = \frac{1}{\varepsilon^d} \Phi\left(\frac{x}{\varepsilon}\right), \quad (5.16)$$

$$\Phi(x) = \frac{1}{2\pi} K_0(|x|) \text{ for } d = 2, \quad \Phi(x) = \frac{1}{4\pi|x|} e^{-|x|} \text{ for } d = 3,$$

involving the modified Bessel function K_0 in the two-dimensional case. Indeed, Φ_ε is the fundamental solution of the operator $-\varepsilon^2 \Delta + I$, and the construction yields the Neumann boundary condition on $\partial\Omega$. We obtain

$$f(\varepsilon) := \mathcal{I}_\varepsilon(u_1, \dots, u_N) = \frac{1}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \Phi_\varepsilon \star u_i u_j dx = \frac{1}{2^{d+1}} \frac{1}{\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \int_D \Phi_\varepsilon \star u_i u_j dx.$$

This formulation is identical to (5.11), except that the kernel is different, in particular it admits here a singularity at 0. A change of variable using (5.16) and the symmetry of the kernel yields

$$f(\varepsilon) = \frac{1}{2^{d+1}} \frac{1}{\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \int_D \int_{\mathbb{R}^d} \Phi(h) u_i(x + \varepsilon h) u_j(x) dh dx.$$

This rewrites as

$$f(\varepsilon) = \frac{1}{2^{d+1}} \frac{1}{\varepsilon} \int_{\mathbb{R}^d} \Phi(h) \Psi(\varepsilon h) dh, \quad (5.17)$$

with

$$\Psi(h) = \sum_{i,j=1}^N \alpha_{ij} \int_D u_i(x + h) u_j(x) dx.$$

For the above function Ψ (note that it does not involve the kernel), it is shown in [19] (proof of Lemma A.2) that

$$\Psi(h + h') \leq \Psi(h) + \Psi(h') \quad \forall h, h' \in \mathbb{R}^d. \quad (5.18)$$

This obviously entails $\Psi(nh) \leq n\Psi(h)$ for all $n \in \mathbb{N} \setminus \{0\}$, and, in view of (5.17)

$$f(n\varepsilon) \leq f(\varepsilon) \quad \forall n \in \mathbb{N} \setminus \{0\}. \quad (5.19)$$

We conclude similarly to [19], choosing n such that

$$n - 1 < \frac{\varepsilon_0}{\varepsilon} \leq n$$

and combining (5.19) and Lemma 5.9 to derive

$$f(\varepsilon) \geq f(n\varepsilon) = (n\varepsilon)^{-3} (n\varepsilon)^3 f(n\varepsilon) \geq (n\varepsilon)^{-3} \varepsilon_0^3 f(\varepsilon_0) = \left(\frac{\varepsilon_0}{n\varepsilon} \right)^3 f(\varepsilon_0) > \left(\frac{\varepsilon_0}{\varepsilon_0 + \varepsilon} \right)^3 f(\varepsilon_0).$$

□

The exponent 3 appearing in (5.15) is not necessarily the same as the exponent $d + 1$ obtained in [19], but it enables the same proof of Γ -convergence, as shown below.

Theorem 5.11. *If $(\alpha_{ij}) \in T_N$ and Ω is a Cartesian product of open intervals, then the functionals \mathcal{I}_ε Γ -converge to $\tilde{\mathcal{I}}$ in $\tilde{\mathcal{E}}_N$ endowed with the strong topology of $L^1(\Omega)^N$.*

Proof. As in Theorem 5.8 only the liminf inequality needs to be checked. We exploit the approximate monotonicity in the same way as in [19]. Let $(u_i^\varepsilon) \in \tilde{\mathcal{E}}_N$ be a sequence such that (u_i^ε) converges to u_i . For any $\varepsilon_0 > 0$, owing to Lemma 5.10 and the continuity of $\mathcal{I}_{\varepsilon_0}$, we have

$$\liminf_{\varepsilon \rightarrow 0} \mathcal{I}_\varepsilon(u^\varepsilon) \geq \mathcal{I}_{\varepsilon_0}(u).$$

It suffices then to pass to the limit when $\varepsilon_0 \rightarrow 0$ using the pointwise convergence to achieve the proof. \square

6. CONVEXITY ISSUES

6.1. Conditional negative semidefiniteness.

Definition 6.1. *A real symmetric $N \times N$ matrix $Q = (\alpha_{ij})$ is said to be conditionally negative semidefinite if $\sum_{i,j=1}^N \alpha_{ij} \xi_i \xi_j \leq 0$ for all $\xi = (\xi_1, \dots, \xi_N)^\top \in \mathbb{R}^N$ such that $\sum_{i=1}^N \xi_i = 0$. We denote $Q \preceq 0$.*

In contrast we use the standard notation $Q \leq 0$ if Q is negative semidefinite.

We define the $(N - 1) \times (N - 1)$ submatrix of $Q = (\alpha_{ij})$ by

$$\tilde{Q} = (\alpha_{ij})_{1 \leq i, j \leq N-1}$$

and the column vector $C = (C_i)$ by

$$C = (\alpha_{iN})_{1 \leq i \leq N-1}. \quad (6.1)$$

We also define the $(N - 1) \times (N - 1)$ matrix

$$\bar{Q} = \tilde{Q} - \mathbb{1}C^\top - C\mathbb{1}^\top =: (\bar{\alpha}_{ij}), \quad (6.2)$$

where $\mathbb{1} = (1, \dots, 1)^\top$. Let $\xi = (\xi_1, \dots, \xi_N)^\top \in \mathbb{R}^N$, $\tilde{\xi} = (\xi_i)_{1 \leq i \leq N-1}$. If $Q \in S_N$ and $\sum_{i=1}^N \xi_i = 0$ it is immediately obtained that $Q\xi \cdot \xi = \tilde{Q}\tilde{\xi} \cdot \tilde{\xi}$. This leads to the following characterization.

Lemma 6.1. *Let $Q \in S_N$. Then $Q \preceq 0$ if and only if $\bar{Q} \leq 0$.*

6.2. Sufficient condition for conditional negative semidefiniteness. According to [19], a sufficient condition for a matrix to be conditionally negative semidefinite is its ℓ^1 -embeddability. Since Q is ℓ^1 -embeddable if and only if $Q \in B_N^+$, we infer the following statement, for which we provide a direct proof.

Theorem 6.2. *If $Q \in B_N^+$, then $Q \preceq 0$.*

Proof. The set of conditionally negative semidefinite matrices is a convex cone, and B_N^+ is the polyhedral cone generated by the row vectors of the matrix \mathbb{M} . Therefore, as in the proof of Theorem 5.5, it is enough to prove that any row vector of \mathbb{M} defines a conditionally negative semidefinite matrix Q . Consider an arbitrary row vector of \mathbb{M} with entries (m_{ij}) in the system of indices associated with phases, and denote by $S \in \mathcal{S}$ its row index in the same system. Let $\xi \in \mathbb{R}^N$

such that $\sum_{i=1}^N \xi_i = 0$. We have

$$\begin{aligned} \sum_{1 \leq i < j \leq N} m_{ij} \xi_i \xi_j &= \sum_{i=1}^{N-1} \xi_i \left(m_{iN} \xi_N + \sum_{j=i+1}^{N-1} m_{ij} \xi_j \right) \\ &= \sum_{i=1}^{N-1} \xi_i \left(m_{iN} (-\xi_1 - \dots - \xi_{N-1}) + \sum_{j=i+1}^{N-1} m_{ij} \xi_j \right) \\ &= - \sum_{i=1}^{N-1} m_{iN} \xi_i^2 + \sum_{1 \leq i < j \leq N-1} (m_{ij} - m_{iN} - m_{jN}) \xi_i \xi_j. \end{aligned}$$

Since $m_{iN} \in \{0, 1\}$ then $m_{iN} = m_{iN}^2$. Moreover, we claim that

$$m_{ij} - m_{iN} - m_{jN} = -2m_{iN}m_{jN}.$$

Indeed, if either $i \in S$, $j \in S$ and $N \notin S$ or $i \notin S$, $j \notin S$ and $N \in S$, then $m_{ij} - m_{iN} - m_{jN} = -2m_{iN}m_{jN} = -2$. In the other cases we check that $m_{ij} - m_{iN} - m_{jN} = -2m_{iN}m_{jN} = 0$. We derive

$$\begin{aligned} \sum_{1 \leq i < j \leq N} m_{ij} \xi_i \xi_j &= - \sum_{i=1}^{N-1} m_{iN}^2 \xi_i^2 - 2 \sum_{1 \leq i < j \leq N-1} m_{iN} m_{jN} \xi_i \xi_j \\ &= - \left(\sum_{i=1}^{N-1} m_{iN} \xi_i \right)^2 \leq 0. \end{aligned}$$

□

By Theorem 5.6 we obtain the following useful implication.

Corollary 6.3. *If $N = 3, 4$ and $Q \in T_N$, then $Q \preceq 0$.*

The converse of Corollary 6.3 is false. For $N = 3$ a counterexample is given by the matrix

$$Q = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 3 \\ 1 & 3 & 0 \end{pmatrix}. \quad (6.3)$$

We have $\det(\bar{Q}) = 3$ and $\text{trace}(\bar{Q}) = -8$, which implies that $Q \preceq 0$, but $\alpha_{23} > \alpha_{12} + \alpha_{13}$.

Corollary 6.3 is not true for $N \geq 5$. A counterexample is given by

$$Q = \begin{pmatrix} 0 & 1 & 2 & 1 & 1 \\ 1 & 0 & 2 & 2 & 2 \\ 2 & 2 & 0 & 1 & 1 \\ 1 & 2 & 1 & 0 & 2 \\ 1 & 2 & 1 & 2 & 0 \end{pmatrix}.$$

This matrix satisfies the triangle inequality, but the corresponding \bar{Q} admits a positive eigenvalue.

7. VARIATIONAL FORMULATIONS OF THE APPROXIMATE INTERFACE ENERGY

For algorithmic purposes we give in this section variational formulations of the approximate interface energy \mathcal{I}_ε . Our approach relies on Legendre-Fenchel duality. Since this is strongly related to convexity we distinguish between two cases. In the first case we assume that $Q \preceq 0$, which covers a rather wide range of situations as seen in Corollary 6.3. Then the energy is concave with respect to its natural variables and the Legendre-Fenchel transform directly provides a formulation as a minimization problem. In the second case we assume that $Q \succeq 0$, which corresponds to a convex energy. We follow a parametric duality approach to obtain concavity with respect to well-chosen perturbation variables. The general case is obtained by additive decomposition of the quadratic form.

Other variational formulations, based on the representation of the total interface energy as a linear combination of perimeters, are given in [28].

7.1. Case $Q \preceq 0$. We assume that Q is a conditionally negative semidefinite symmetric $N \times N$ matrix. Note that, with the aforementioned additive decomposition in mind, we do not assume that $Q \in T_N$, not even that $Q \in S_N$. Therefore we will use the expression of the approximate energy

$$\mathcal{I}_\varepsilon(u_1, \dots, u_N) = \frac{1}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \langle u_i, L_\varepsilon u_j \rangle. \quad (7.1)$$

We set for all $u, v \in H^1(\Omega)$

$$\langle u, v \rangle_{H_\varepsilon^1} = \int_{\Omega} (\varepsilon^2 \nabla u \cdot \nabla v + uv) \, dx, \quad (7.2)$$

and for all $u, v \in H^1(\Omega, \mathbb{R}^N)$

$$[u, v] = \sum_{i=1}^N \langle u_i, v_i \rangle_{H_\varepsilon^1}. \quad (7.3)$$

We first state a small technical lemma.

Lemma 7.1. *Let $\xi \in H^1(\Omega, \mathbb{R}^N)$ such that $\sum_{i=1}^N \xi_i = 0$. Then $[Q\xi, \xi] \leq 0$.*

Proof. We have by definition

$$[Q\xi, \xi] = \sum_{i=1}^N \int_{\Omega} (\varepsilon^2 \nabla(Q\xi)_i \cdot \nabla \xi_i + (Q\xi)_i \xi_i) \, dx,$$

which yields

$$\begin{aligned} [Q\xi, \xi] &= \int_{\Omega} \sum_{i,j=1}^N \alpha_{ij} (\varepsilon^2 \nabla \xi_i \cdot \nabla \xi_j + \xi_i \xi_j) \, dx \\ &= \int_{\Omega} \left[\sum_{k=1}^d \varepsilon^2 (Q \partial_k \xi) \cdot \partial_k \xi + Q\xi \cdot \xi \right] \, dx. \end{aligned}$$

The fact that $Q \preceq 0$ implies $[Q\xi, \xi] \leq 0$. □

With the help of the canonical embeddings $H^1(\Omega) \hookrightarrow L^2(\Omega) \hookrightarrow H^1(\Omega)'$, where $H^1(\Omega)'$ is the continuous dual space of $H^1(\Omega)$, we consider the extended operator $L_\varepsilon : H^1(\Omega)' \rightarrow H^1(\Omega)$, defined by $L_\varepsilon u = u_\varepsilon$ such that

$$\int_{\Omega} (\varepsilon^2 \nabla u_\varepsilon \cdot \nabla \varphi + u_\varepsilon \varphi) \, dx = \langle u, \varphi \rangle \quad \forall \varphi \in H^1(\Omega). \quad (7.4)$$

Here the notation $\langle \cdot, \cdot \rangle$ is used for the duality pairing between $H^1(\Omega)'$ and $H^1(\Omega)$. Clearly this defines a linear and continuous operator. If $u, v \in H^1(\Omega)'$, then choosing $\varphi = v_\varepsilon := L_\varepsilon v$ in (7.4) yields

$$\langle u, L_\varepsilon v \rangle = \int_{\Omega} (\varepsilon^2 \nabla u_\varepsilon \cdot \nabla v_\varepsilon + u_\varepsilon v_\varepsilon) \, dx. \quad (7.5)$$

This shows that L_ε is self-adjoint. In addition, $\langle u, L_\varepsilon u \rangle \geq 0$ and $L_\varepsilon 1 = 1$, from (7.4).

The operator \mathcal{I}_ε defined in (7.1) canonically extends to a continuous functional on $[H^1(\Omega)']^N$. A direct calculation yields for all $u, v \in [H^1(\Omega)']^N$, $\lambda \in [0, 1]$

$$\mathcal{I}_\varepsilon(\lambda u + (1-\lambda)v) - \lambda \mathcal{I}_\varepsilon(u) - (1-\lambda) \mathcal{I}_\varepsilon(v) = \frac{(\lambda-1)\lambda}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \langle u_j - v_j, L_\varepsilon(u_i - v_i) \rangle.$$

Using (7.5), denoting $q_i^k = \varepsilon \partial_k L_\varepsilon(u_i - v_i)$, $r_i = L_\varepsilon(u_i - v_i)$, we obtain

$$\mathcal{I}_\varepsilon(\lambda u + (1 - \lambda)v) - \lambda \mathcal{I}_\varepsilon(u) - (1 - \lambda) \mathcal{I}_\varepsilon(v) = \frac{(\lambda - 1)\lambda}{2\varepsilon} \int_\Omega \left(\sum_{i,j=1}^N \alpha_{ij} \left(\sum_{k=1}^d q_i^k q_j^k + r_i r_j \right) \right) dx.$$

We define the affine space

$$V = \left\{ u \in [H^1(\Omega)']^N : \sum_{i=1}^N u_i = 1 \right\}.$$

If $u, v \in V$ then $\sum_i q_i^k = \sum_i r_i = 0$. Since Q is conditionnally negative semidefinite, we infer that \mathcal{I}_ε is concave on V .

Let $\delta_V : [H^1(\Omega)']^N \rightarrow \{0, +\infty\}$ be the indicator function of V . We have that $\delta_V - \mathcal{I}_\varepsilon$ is a proper, closed, convex function on $[H^1(\Omega)']^N$. Hence the Fenchel-Moreau biconjugation theorem tells us that $(\delta_V - \mathcal{I}_\varepsilon)^{**} = \delta_V - \mathcal{I}_\varepsilon$. This leads to the following theorem.

Theorem 7.2. *Let $Q \preceq 0$, $u \in V$. We have*

$$\mathcal{I}_\varepsilon(u) = \frac{1}{\varepsilon} \inf_{\substack{v \in [H^1(\Omega)]^N \\ \sum_{i=1}^N v_i = 1}} \sum_{i,j=1}^N \alpha_{ij} \left(\langle u_i, v_j \rangle - \frac{\varepsilon^2}{2} \langle \nabla v_i, \nabla v_j \rangle - \frac{1}{2} \langle v_i, v_j \rangle \right).$$

Proof. Let $w \in H^1(\Omega)^N$. The Legendre-Fenchel transform of $\delta_V - \mathcal{I}_\varepsilon$ is defined as

$$(\delta_V - \mathcal{I}_\varepsilon)^*(w) = \sup_{u \in [H^1(\Omega)']^N} \left\{ \sum_{i=1}^N \langle u_i, w_i \rangle - \delta_V(u) + \mathcal{I}_\varepsilon(u) \right\},$$

which can be rewritten as

$$(\delta_V - \mathcal{I}_\varepsilon)^*(w) = \sup_{u \in V} \left\{ \sum_{i=1}^N \langle u_i, w_i \rangle + \frac{1}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \langle u_i, L_\varepsilon u_j \rangle \right\}. \quad (7.6)$$

By definition of L_ε and the fact that it is an isomorphism from $H^1(\Omega)'$ into $H^1(\Omega)$, we obtain with the change of variables $\hat{u}_i = L_\varepsilon u_i$

$$\begin{aligned} (\delta_V - \mathcal{I}_\varepsilon)^*(w) &= \sup_{\substack{\hat{u} \in [H^1(\Omega)]^N \\ \sum_{i=1}^N \hat{u}_i = 1}} \left\{ \sum_{i=1}^N \int_\Omega (\varepsilon^2 \nabla \hat{u}_i \cdot \nabla w_i + \hat{u}_i w_i) dx \right. \\ &\quad \left. + \frac{1}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \int_\Omega (\varepsilon^2 \nabla \hat{u}_i \cdot \nabla \hat{u}_j + \hat{u}_i \hat{u}_j) dx \right\}. \end{aligned}$$

With the notation (7.2) this reads

$$(\delta_V - \mathcal{I}_\varepsilon)^*(w) = \sup_{\substack{\hat{u} \in [H^1(\Omega)]^N \\ \sum_{i=1}^N \hat{u}_i = 1}} \left\{ \sum_{i=1}^N \langle w_i, \hat{u}_i \rangle_{H_\varepsilon^1} + \frac{1}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \langle \hat{u}_i, \hat{u}_j \rangle_{H_\varepsilon^1} \right\},$$

which we rewrite as

$$(\delta_V - \mathcal{I}_\varepsilon)^*(w) = \sup_{\substack{\psi \in [H^1(\Omega)]^N \\ \sum_{i=1}^N \psi_i = 1}} \left\{ \sum_{i=1}^N \langle w_i, \psi_i \rangle_{H_\varepsilon^1} + \frac{1}{2\varepsilon} \sum_{j=1}^N \langle (Q\psi)_j, \psi_j \rangle_{H_\varepsilon^1} \right\}.$$

From (7.3), we obtain

$$(\delta_V - \mathcal{I}_\varepsilon)^*(w) = \sup_{\substack{\psi \in [H^1(\Omega)]^N \\ \sum_{i=1}^N \psi_i = 1}} \left\{ [w, \psi] + \frac{1}{2\varepsilon} [Q\psi, \psi] \right\}. \quad (7.7)$$

Observe that, for any $\lambda \in H^1(\Omega)$,

$$(\delta_V - \mathcal{I}_\varepsilon)^*(w + \lambda \mathbf{1}) = \int_\Omega \lambda dx + (\delta_V - \mathcal{I}_\varepsilon)^*(w). \quad (7.8)$$

Call

$$H = \left\{ (\xi_1, \dots, \xi_N) \in \mathbb{R}^N : \sum_{i=1}^N \xi_i = 0 \right\},$$

and P_H the orthogonal projection of \mathbb{R}^N onto H , i.e.,

$$P_H \xi = \xi - \frac{1}{N} (\mathbf{1} \cdot \xi) \mathbf{1} = \xi - \left(\frac{1}{N} \sum_{i=1}^N \xi_i \right) \mathbf{1}.$$

Let $R = P_H \circ Q \circ P_H$ and denote

$$\bar{w}(x) = P_H \left(\left(w + \frac{1}{\varepsilon} Q \frac{1}{N} \mathbf{1} \right)(x) \right).$$

We distinguish between two cases.

- Case 1: We assume here that

$$\bar{w}(x) \in \text{Im} R \text{ for a.e. } x \in \Omega.$$

Hence there exists $v \in [H^1(\Omega)]^N$ such that $\bar{w}(x) = Rv(x)$ for a.e. $x \in \Omega$. We can write

$$w + \frac{1}{\varepsilon} Q \frac{1}{N} \mathbf{1} = \bar{w} + \mu \mathbf{1} = Rv + \mu \mathbf{1} = P_H(Q\bar{v}) + \mu \mathbf{1} = Q\bar{v} + \lambda \mathbf{1},$$

with $\bar{v} = P_H v$, $\mu, \lambda \in H^1(\Omega)$. Setting

$$\hat{v} = \bar{v} - \frac{1}{\varepsilon N} \mathbf{1} = P_H v - \frac{1}{\varepsilon N} \mathbf{1},$$

we arrive at $w = Q\hat{v} + \lambda \mathbf{1}$. Plugging this into (7.7)-(7.8) yields

$$(\delta_V - \mathcal{I}_\varepsilon)^*(w) = \int_\Omega \lambda dx - \frac{\varepsilon}{2} [Q\hat{v}, \hat{v}] + \frac{1}{2\varepsilon} \sup_{\substack{\psi \in [H^1(\Omega)]^N \\ \sum_{i=1}^N \psi_i = 1}} [Q(\psi + \varepsilon \hat{v}), \psi + \varepsilon \hat{v}]. \quad (7.9)$$

Observing that

$$\varepsilon \sum_{i=1}^N \hat{v}_i = -1 \quad (7.10)$$

and using Lemma 7.1, we conclude that

$$(\delta_V - \mathcal{I}_\varepsilon)^*(w) = \int_\Omega \lambda dx - \frac{\varepsilon}{2} [Q\hat{v}, \hat{v}]. \quad (7.11)$$

Note that conversely, if $w = Q\hat{v} + \lambda \mathbf{1}$ with \hat{v} satisfying (7.10), then

$$\bar{w}(x) = P_H \left(w(x) + \frac{1}{\varepsilon} Q \frac{1}{N} \mathbf{1} \right) = P_H \circ Q \left(\hat{v}(x) + \frac{1}{\varepsilon N} \mathbf{1} \right) \in \text{Im} R. \quad (7.12)$$

- Case 2: There exists $\mathcal{W} \subset \Omega$, $|\mathcal{W}| > 0$ such that

$$\forall x \in \mathcal{W}, \bar{w}(x) \notin \text{Im} R = (\ker R)^\perp,$$

since R is self-adjoint. Let $p(x)$ be the orthogonal projection of $\bar{w}(x)$ onto $\ker R$. By assumption we have $p(x) \neq 0 \forall x \in \mathcal{W}$. Defining

$$\psi^t = \frac{1}{N} \mathbf{1} + t P_H p, \quad (7.13)$$

we will show that

$$[w, \psi^t] + \frac{1}{2\varepsilon} [Q\psi^t, \psi^t] \rightarrow +\infty, \quad (7.14)$$

when $t \rightarrow +\infty$. To see this we proceed by

$$[w, \psi^t] + \frac{1}{2\varepsilon}[Q\psi^t, \psi^t] = [w + \frac{1}{2\varepsilon N}Q\mathbf{1}, \frac{1}{N}\mathbf{1}] + t[w + \frac{1}{\varepsilon N}Q\mathbf{1}, P_H p] + \frac{t^2}{2\varepsilon}[QP_H p, P_H p].$$

Observing that $QP_H p(x) \in H^\perp$, since $p(x) \in \ker R$, and $P_H p(x) \in H$, we infer that $QP_H p(x) \cdot P_H p(x) = 0$. In addition, writing $QP_H p(x) = \lambda(x)\mathbf{1}$, we have $\partial_k(\lambda\mathbf{1}) \cdot \partial_k P_H p = \partial_k \lambda \partial_k(\mathbf{1} \cdot P_H p) = 0$. This entails

$$[QP_H p, P_H p] = 0.$$

Now, noting that $\partial_k(P_H p) = P_H(\partial_k p)$, we have

$$[w + \frac{1}{\varepsilon N}Q\mathbf{1}, P_H p] = [P_H(w + \frac{1}{\varepsilon N}Q\mathbf{1}), p] = [\bar{w}, p] = [p, p] > 0.$$

Hence, when $t \rightarrow +\infty$, it holds

$$[w, \psi^t] + \frac{1}{2\varepsilon}[Q\psi^t, \psi^t] \rightarrow +\infty. \quad (7.15)$$

We infer from (7.7) that

$$(\delta_V - \mathcal{I}_\varepsilon)^*(w) = +\infty. \quad (7.16)$$

The biconjugate of $\delta_V - \mathcal{I}_\varepsilon$ is defined by

$$(\delta_V - \mathcal{I}_\varepsilon)^{**}(u) = \sup_{w \in [H^1(\Omega)]^N} \sum_{i=1}^N \langle u_i, w_i \rangle - (\delta_V - \mathcal{I}_\varepsilon)^*(w).$$

In view of (7.16) it is equal to

$$(\delta_V - \mathcal{I}_\varepsilon)^{**}(u) = \sup_{\substack{w \in [H^1(\Omega)]^N \\ \bar{w} \in \text{Im} R}} \sum_{i=1}^N \langle u_i, w_i \rangle - (\delta_V - \mathcal{I}_\varepsilon)^*(w).$$

We now assume that $u \in V$, which permits to write

$$\mathcal{I}_\varepsilon(u) = -(\delta_V - \mathcal{I}_\varepsilon)(u) = -(\delta_V - \mathcal{I}_\varepsilon)^{**}(u).$$

By (7.11) and (7.12), we infer

$$\mathcal{I}_\varepsilon(u) = \inf_{\substack{\hat{v} \in [H^1(\Omega)]^N, \lambda \in H^1(\Omega) \\ \varepsilon \sum_{i=1}^N \hat{v}_i = -1}} \left\{ - \sum_{i=1}^N \langle u_i, (Q\hat{v})_i + \lambda \rangle + \int_{\Omega} \lambda dx - \frac{\varepsilon}{2}[Q\hat{v}, \hat{v}] \right\} \quad (7.17)$$

$$= \inf_{\substack{\hat{v} \in [H^1(\Omega)]^N \\ \varepsilon \sum_{i=1}^N \hat{v}_i = -1}} \left\{ - \sum_{i=1}^N \langle u_i, (Q\hat{v})_i \rangle - \frac{\varepsilon}{2}[Q\hat{v}, \hat{v}] \right\}. \quad (7.18)$$

A change of variables yields

$$\mathcal{I}_\varepsilon(u) = \frac{1}{\varepsilon} \inf_{\substack{v \in [H^1(\Omega)]^N \\ \sum_{i=1}^N v_i = 1}} \left\{ \sum_{i=1}^N \langle u_i, (Qv)_i \rangle - \frac{1}{2}[Qv, v] \right\}, \quad (7.19)$$

which completes the proof. \square

Remark 7.1. For $N = 2$ the variational formulation amounts to (2.1) and has been used within alternating minimization schemes in [8] in a context of structural optimization. The multiphase case with uniform surface tensions has been considered in [7].

7.2. Case $Q \succeq 0$.

Theorem 7.3. *Given $(u_1, \dots, u_N) \in L^\infty(\Omega, [0, 1])^N$ with $\sum_i u_i = 1$ consider the approximate interface energy (7.1) with $Q = (\alpha_{ij})$ symmetric conditionally positive semi-definite. We have the expression*

$$\mathcal{I}_\varepsilon(u_1, \dots, u_N) = \frac{1}{2\varepsilon} \inf_{\substack{\tau \in [H_0^{\text{div}}(\Omega)]^N \\ \sum_{i=1}^N \tau_i = 0}} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \tau_i \cdot \tau_j dx + \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (u_i - \varepsilon \operatorname{div} \tau_i)(u_j - \varepsilon \operatorname{div} \tau_j) dx. \quad (7.20)$$

Proof. We compute a dual formulation with respect to an auxiliary perturbation variable, in order to place ourselves in an appropriate convexity framework. Therefore u is considered as fixed, as well as ε , and we set

$$I = 2\mathcal{I}_\varepsilon(u_1, \dots, u_N) = \frac{1}{\varepsilon} \langle Qu, v \rangle = \frac{1}{2\varepsilon} (\langle Qu, v \rangle + \langle Qv, u \rangle) = \frac{1}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (u_i v_j + u_j v_i) dx$$

with $v_i = L_\varepsilon u_i$. We define for all $\tau = (\tau_1, \dots, \tau_N) \in L^2(\Omega, \mathbb{R}^d)^N$

$$F(\tau) = \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (\varepsilon^2 (\nabla v_i^\tau - \tau_i) \cdot (\nabla v_j^\tau - \tau_j) + v_i^\tau v_j^\tau - u_i v_j^\tau - u_j v_i^\tau) dx$$

where $v_i^\tau \in H^1(\Omega)$ is the solution of

$$\int_{\Omega} (\varepsilon^2 (\nabla v_i^\tau - \tau_i) \cdot \nabla \varphi + v_i^\tau \varphi) dx = \int_{\Omega} u_i \varphi dx \quad \forall \varphi \in H^1(\Omega).$$

We have immediately $F(0) = -\varepsilon I$.

There exists $\Lambda \in \mathcal{L}(L^2(\Omega, \mathbb{R}^d), H^1(\Omega))$ such that $v_i^\tau = v_i^0 + \Lambda \tau_i$. Elementary differential calculus leads to

$$D^2 F(\tau)(\hat{\tau}, \hat{\tau}) = 2 \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (\varepsilon^2 (\nabla \Lambda \hat{\tau}_i - \hat{\tau}_i) \cdot (\nabla \Lambda \hat{\tau}_j - \hat{\tau}_j) + (\Lambda \hat{\tau}_i)(\Lambda \hat{\tau}_j)) dx.$$

Hence F is convex over the Hilbert space

$$H = \left\{ \tau \in L^2(\Omega, \mathbb{R}^d)^N : \sum_{i=1}^N \tau_i = 0 \right\}.$$

Let us compute the Legendre-Fenchel transform of F over H , given for any $\tau^* \in H$ by

$$F^*(\tau^*) = \sup_{\tau \in H} \sum_{i=1}^N \int_{\Omega} \tau_i^* \cdot \tau_i - F(\tau).$$

This rewrites as

$$F^*(\tau^*) = \sup_{\substack{\tau \in H \\ v \in [H^1(\Omega)]^N}} \sum_{i=1}^N \int_{\Omega} \tau_i^* \cdot \tau_i - \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (\varepsilon^2 (\nabla v_i - \tau_i) \cdot (\nabla v_j - \tau_j) + v_i v_j - u_i v_j - u_j v_i) dx \quad (7.21)$$

subject to

$$\int_{\Omega} (\varepsilon^2 (\nabla v_i - \tau_i) \cdot \nabla \varphi + v_i \varphi) dx = \int_{\Omega} u_i \varphi dx \quad \forall \varphi \in H^1(\Omega), \forall i = 1, \dots, N. \quad (7.22)$$

Assume that $F^*(\tau^*) < +\infty$. Since the functional to maximize is made of quadratic and linear terms, the supremum is attained. Call (τ, v) a maximizer. There exists Lagrange multipliers

$(w_1, \dots, w_N) \in H^1(\Omega)^N$ such that

$$\begin{aligned} & \sum_{i=1}^N \int_{\Omega} \tau_i^* \cdot \hat{\tau}_i \\ & - \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (\varepsilon^2(\nabla v_i - \tau_i) \cdot (\nabla \hat{v}_j - \hat{\tau}_j) + \varepsilon^2(\nabla \hat{v}_i - \hat{\tau}_i) \cdot (\nabla v_j - \tau_j) + v_i \hat{v}_j + \hat{v}_i v_j - u_i \hat{v}_j - u_j \hat{v}_i) dx \\ & \quad + \sum_{i=1}^N \int_{\Omega} (\varepsilon^2(\nabla \hat{v}_i - \hat{\tau}_i) \cdot \nabla w_i + \hat{v}_i w_i) dx = 0 \quad \forall (\hat{\tau}, \hat{v}) \in H \times H^1(\Omega)^N. \end{aligned} \quad (7.23)$$

Choosing $\hat{\tau} = 0$ yields

$$\begin{aligned} & - \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (\varepsilon^2(\nabla v_i - \tau_i) \cdot \nabla \hat{v}_j + \varepsilon^2 \nabla \hat{v}_i \cdot (\nabla v_j - \tau_j) + v_i \hat{v}_j + \hat{v}_i v_j - u_i \hat{v}_j - u_j \hat{v}_i) dx \\ & \quad + \sum_{i=1}^N \int_{\Omega} (\varepsilon^2 \nabla \hat{v}_i \cdot \nabla w_i + \hat{v}_i w_i) dx = 0 \quad \forall \hat{v} \in H^1(\Omega)^N. \end{aligned}$$

Due to the constraint (7.22) the first line vanishes. This entails $w_i = 0$. Choosing now $\hat{v} = 0$ yields

$$\sum_{i=1}^N \int_{\Omega} \tau_i^* \cdot \hat{\tau}_i - \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (\varepsilon^2(\nabla v_i - \tau_i) \cdot (-\hat{\tau}_j) + \varepsilon^2(-\hat{\tau}_i) \cdot (\nabla v_j - \tau_j)) dx = 0 \quad \forall \hat{\tau} \in H.$$

It follows that

$$\left(\tau_i^* + 2\varepsilon^2 \sum_{j=1}^N \alpha_{ij} (\nabla v_j - \tau_j) \right)_{1 \leq i \leq N} \in H^\perp,$$

i.e., there exists $\lambda^* \in L^2(\Omega, \mathbb{R}^d)$ such that

$$\tau_i^* + 2\varepsilon^2 \sum_{j=1}^N \alpha_{ij} (\nabla v_j - \tau_j) = \lambda^* \quad \forall i = 1, \dots, N. \quad (7.24)$$

Setting

$$\eta_j^* = -2\varepsilon^2 (\nabla v_j - \tau_j) \in H_0^{\text{div}}(\Omega), \quad (7.25)$$

by (7.22), we write (7.24) as $\tau^* = Q\eta^* + \lambda^*$. Since $\tau \in H$ and $\sum_{i=1}^N u_i = 1$, the constraint (7.22) implies $\sum_{i=1}^N v_i = 1$, whereby $\nabla v \in H$ and $\eta^* \in H$. From (7.22) and (7.24) we obtain

$$\begin{cases} -\operatorname{div}(\tau_i^* - \lambda^*) = 2 \sum_{j=1}^N \alpha_{ij} (v_j - u_j) & \text{in } \Omega \\ (\tau_i^* - \lambda^*) \cdot n = 0 & \text{on } \partial\Omega. \end{cases} \quad (7.26)$$

Choosing $\hat{v} = v$, $\hat{\tau} = \tau$ in (7.23) and recalling that $w = 0$, we obtain

$$\sum_{i=1}^N \int_{\Omega} \tau_i^* \cdot \tau_i - \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (2\varepsilon^2(\nabla v_i - \tau_i) \cdot (\nabla v_j - \tau_j) + 2v_i v_j - u_i v_j - u_j v_i) dx = 0.$$

Plugging this in (7.21) entails

$$F^*(\tau^*) = \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (\varepsilon^2(\nabla v_i - \tau_i) \cdot (\nabla v_j - \tau_j) + v_i v_j) dx.$$

This rewrites as

$$F^*(\tau^*) = \sum_{i=1}^N \int_{\Omega} \left(\varepsilon^2(\nabla v_i - \tau_i) \cdot \sum_{j=1}^N \alpha_{ij} (\nabla v_j - \tau_j) \right) dx + \sum_{i=1}^N \int_{\Omega} v_i \left(\sum_{j=1}^N \alpha_{ij} v_j \right) dx.$$

Taking into account (7.24) and (7.26) we arrive at

$$F^*(\tau^*) = -\frac{1}{2} \sum_{i=1}^N \int_{\Omega} (\nabla v_i - \tau_i) \cdot (\tau_i^* - \lambda^*) dx + \sum_{i=1}^N \int_{\Omega} v_i \left(\sum_{j=1}^N \alpha_{ij} u_j - \frac{1}{2} \operatorname{div} (\tau_i^* - \lambda^*) \right) dx.$$

This can be rearranged as

$$F^*(\tau^*) = -\frac{1}{2} \sum_{i=1}^N \int_{\Omega} (\nabla v_i - \tau_i) \cdot (\tau_i^* - \lambda^*) dx + \sum_{j=1}^N \int_{\Omega} u_j \left(\sum_{i=1}^N \alpha_{ij} v_i \right) dx - \frac{1}{2} \sum_{i=1}^N \int_{\Omega} v_i \operatorname{div} (\tau_i^* - \lambda^*) dx.$$

Using again (7.26) we obtain

$$F^*(\tau^*) = -\frac{1}{2} \sum_{i=1}^N \int_{\Omega} (\nabla v_i - \tau_i) \cdot (\tau_i^* - \lambda^*) dx + \sum_{j=1}^N \int_{\Omega} u_j \left(\sum_{i=1}^N \alpha_{ij} u_i - \frac{1}{2} \operatorname{div} (\tau_j^* - \lambda^*) \right) dx - \frac{1}{2} \sum_{i=1}^N \int_{\Omega} v_i \operatorname{div} (\tau_i^* - \lambda^*) dx.$$

With (7.24) and the notation (7.25) this leads to

$$\begin{aligned} F^*(\tau^*) &= -\frac{1}{2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (\nabla v_i - \tau_i) \cdot \eta_j^* dx + \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} u_i u_j dx \\ &\quad - \frac{1}{2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} u_j \operatorname{div} \eta_i^* dx - \frac{1}{2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} v_i \operatorname{div} \eta_j^* dx. \end{aligned}$$

Using (7.24) and (7.26) yields

$$\begin{aligned} F^*(\tau^*) &= \frac{1}{4\varepsilon^2} \sum_{j=1}^N \int_{\Omega} (\tau_j^* - \lambda^*) \cdot \eta_j^* dx + \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} u_i u_j dx - \frac{1}{2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} u_j \operatorname{div} \eta_i^* dx \\ &\quad - \frac{1}{2} \sum_{j=1}^N \int_{\Omega} \left(\sum_{i=1}^N \alpha_{ij} u_i - \frac{1}{2} \operatorname{div} (\tau_j^* - \lambda^*) \right) \operatorname{div} \eta_j^* dx. \end{aligned}$$

Expressing τ^* in terms of η^* leads to

$$\begin{aligned} F^*(\tau^*) &= \frac{1}{4\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \eta_i^* \cdot \eta_j^* dx + \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} u_i u_j dx - \frac{1}{2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} u_j \operatorname{div} \eta_i^* dx \\ &\quad - \frac{1}{2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} u_i \operatorname{div} \eta_j^* dx + \frac{1}{4} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \operatorname{div} \eta_i^* \operatorname{div} \eta_j^* dx. \end{aligned}$$

Rearranging entails

$$F^*(\tau^*) = \frac{1}{4\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \eta_i^* \cdot \eta_j^* dx + \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} (u_i - \frac{1}{2} \operatorname{div} \eta_i^*) (u_j - \frac{1}{2} \operatorname{div} \eta_j^*) dx =: \Phi(\eta^*). \quad (7.27)$$

To recapitulate, we have shown so far that

$$F^*(\tau^*) < +\infty \Rightarrow \exists (\lambda^*, \eta^*) \in L^2(\Omega, \mathbb{R}^d) \times (H \cap H_0^{\operatorname{div}}(\Omega)^N) \text{ s.t. } \begin{cases} \tau^* = Q\eta^* + \lambda^* \\ F^*(\tau^*) = \Phi(\eta^*). \end{cases}$$

Suppose now that $F^*(\tau^*) < +\infty$ and $\tau^* = Q\eta + \lambda \in H$ for some $(\lambda, \eta) \in L^2(\Omega, \mathbb{R}^d) \times (H \cap H_0^{\operatorname{div}}(\Omega)^N)$. Writing $F^*(\tau^*) = \Phi(\eta^*)$ with $\tau^* = Q\eta^* + \lambda^*$ and observing, from inspection of (7.27), that $Q(\eta - \eta^*) = \lambda^* - \lambda \Rightarrow \Phi(\eta) = \Phi(\eta^*)$, we infer that $F(Q\eta + \lambda) = \Phi(\eta)$.

We are now in position to obtain the dual formulation of F , given for any $\tau \in H$ by

$$F(\tau) = F^{**}(\tau) = \sup_{\tau^* \in H} \sum_{i=1}^N \int_{\Omega} \tau_i \cdot \tau_i^* dx - F^*(\tau^*).$$

We infer from the preceding findings that

$$F(\tau) = \sup_{\substack{\eta^* \in H \cap [H_0^{\text{div}}(\Omega)]^N \\ \lambda^* \in L^2(\Omega, \mathbb{R}^d) \\ Q\eta^* + \lambda^* \in H}} \sum_{i=1}^N \int_{\Omega} \tau_i \cdot \left(\sum_{j=1}^N \alpha_{ij} \eta_j^* + \lambda^* \right) dx - \frac{1}{4\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \eta_i^* \cdot \eta_j^* dx \\ - \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \left(u_i - \frac{1}{2} \operatorname{div} \eta_i^* \right) \left(u_j - \frac{1}{2} \operatorname{div} \eta_j^* \right) dx.$$

Since $\tau \in H$ this simplifies as

$$F(\tau) = \sup_{\eta^* \in H \cap [H_0^{\text{div}}(\Omega)]^N} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \tau_i \cdot \eta_j^* dx - \frac{1}{4\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \eta_i^* \cdot \eta_j^* dx \\ - \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \left(u_i - \frac{1}{2} \operatorname{div} \eta_i^* \right) \left(u_j - \frac{1}{2} \operatorname{div} \eta_j^* \right) dx.$$

Recalling that $I = -\frac{1}{\varepsilon} F(0)$ we arrive at

$$I = \frac{1}{\varepsilon} \inf_{\eta^* \in H \cap [H_0^{\text{div}}(\Omega)]^N} \frac{1}{4\varepsilon^2} \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \eta_i^* \cdot \eta_j^* dx + \sum_{i,j=1}^N \alpha_{ij} \int_{\Omega} \left(u_i - \frac{1}{2} \operatorname{div} \eta_i^* \right) \left(u_j - \frac{1}{2} \operatorname{div} \eta_j^* \right) dx.$$

A change of variable yields (7.20). \square

7.3. General case. Consider an arbitrary $Q \in T_N$. We see it as the matrix representation of a quadratic form q on \mathbb{R}^N . Then q can be decomposed as $q = q^- + q^+$, where q^- and q^+ are negative semi-definite and positive semi-definite, respectively, on the linear subspace $\{\xi \in \mathbb{R}^N : \sum_i \xi_i = 0\}$. This leads to the decomposition $Q = Q^- + Q^+$, where Q^- and Q^+ are conditionally negative semi-definite and conditionally positive semi-definite, respectively. The linearity of the interface energy with respect to Q allows to combine the two variational formulations. Let us recall that when $N \leq 4$ we have $Q \preceq 0$, hence it is natural to assume that $Q^+ = 0$.

8. APPLICATIONS

8.1. Algorithm. We consider the approximate minimal partition problem

$$\min_{(u_1, \dots, u_N) \in \tilde{\mathcal{E}}_N} \left\{ \sum_{i=1}^N \langle g_i, u_i \rangle + \frac{1}{\varepsilon} \sum_{1 \leq i < j \leq N} \alpha_{ij} \langle L_\varepsilon u_i, u_j \rangle \right\}. \quad (8.1)$$

Consider the decomposition $\alpha_{ij} = \alpha_{ij}^- + \alpha_{ij}^+$, with $(\alpha_{ij}^-) \preceq 0$ and $(\alpha_{ij}^+) \succeq 0$. Plugging the adequate variational formulation of each component of the approximate interface energy, (8.1) rewrites as

$$\min_{(u_1, \dots, u_N) \in \tilde{\mathcal{E}}_N} \inf_{\substack{(v_1, \dots, v_N) \in H^1(\Omega)^N \\ \sum_{i=1}^N v_i = 1}} \inf_{\substack{(\tau_1, \dots, \tau_N) \in [H_0^{\text{div}}(\Omega)]^N \\ \sum_{i=1}^N \tau_i = 0}} \left\{ \sum_{i=1}^N \langle g_i, u_i \rangle \right. \\ \left. + \frac{1}{\varepsilon} \sum_{i,j=1}^N \alpha_{ij}^- \left(\langle u_i, v_j \rangle - \frac{\varepsilon^2}{2} \langle \nabla v_i, \nabla v_j \rangle - \frac{1}{2} \langle v_i, v_j \rangle \right) \right. \\ \left. + \frac{1}{2\varepsilon} \sum_{i,j=1}^N \alpha_{ij}^+ \left(\langle \tau_i, \tau_j \rangle + \langle u_i - \varepsilon \operatorname{div} \tau_i, u_j - \varepsilon \operatorname{div} \tau_j \rangle \right) \right\}.$$

We propose an alternating minimization algorithm with respect to the three N -tuples of variables (u_1, \dots, u_N) , (v_1, \dots, v_N) and (τ_1, \dots, τ_N) .

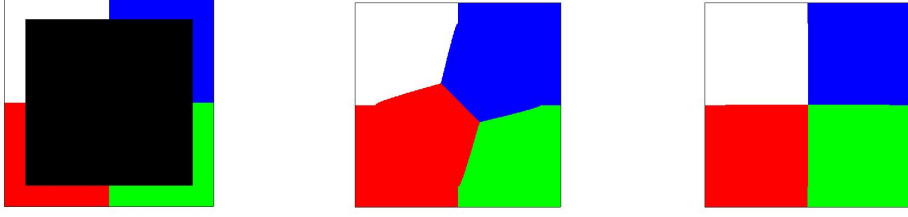


FIGURE 3. Partition with 4 phases: data E_i (left), obtained result for case (a) (middle), obtained result for case (b) (right)

- (1) Minimizing with respect to (v_1, \dots, v_N) simply amounts to setting $v_j = L_\varepsilon u_j$ for each j .
- (2) From inspection of the Euler-Lagrange equations, minimizing with respect to (τ_1, \dots, τ_N) is achieved with $\tau_j = -\varepsilon \nabla v_j$.
- (3) Minimizing with respect to (u_1, \dots, u_N) is a quadratic problem with linear constraints, spatially uncoupled. If $Q^+ = 0$, then the problem is linear. It is straightforwardly solved by

$$u_i(x) = \begin{cases} 1 & \text{if } i = k(x), \\ 0 & \text{otherwise,} \end{cases}$$

where

$$\zeta_i = g_i + \frac{1}{\varepsilon} \sum_j \alpha_{ij} v_j, \quad \zeta_{k(x)} = \min \{\zeta_1(x), \dots, \zeta_N(x)\}.$$

If $Q^+ \neq 0$, then the problem becomes more complicated. In fact, it can be simplified by performing the decomposition $Q = Q^+ + Q^-$ in such a way that Q^+ satisfies special properties. For instance, one can always choose Q^+ of the form $Q^+ = \gamma I_N$, with $\gamma > 0$ large enough. Then the minimization with respect to u amounts to performing at each point an orthogonal projection onto the simplex of \mathbb{R}^N . Note that in this case u is no longer binary-valued during the iterations, and that large values of γ tend to enhance this property.

The main computational tasks within each iteration is the numerical solution of L_ε . In the subsequent experiments we use the standard finite difference scheme with 5 points stencil combined with the Fast Fourier Transform, since the discrete system writes in terms of convolutions. In the examples under consideration the matrix Q is always chosen conditionally negative semi-definite, hence we choose $Q^- = Q$, $Q^+ = 0$.

8.2. Examples. Let E_0, E_1, \dots, E_N be a given partition of Ω . We define $g_i, i = 1, \dots, N$, by

$$g_i = \sum_{\substack{0 \leq j \leq N \\ j \neq i}} \chi_{E_j} = 1 - \chi_{E_i}.$$

This means that, in the set E_i , $i \geq 1$, the label i is favored, whereas in the set E_0 there is no preference, or, said otherwise, no information on which label to choose.

Figure 3 shows an example with four phases with two different sets of surface tensions. The domain is discretized by 512×512 pixels. We use $\varepsilon_{\max} = 512$ and $\varepsilon_{\min} = 1$, with the mesh size fixed to 1. For the initialization each u_i uniformly equals $1/4$. In case (a) we fix $\alpha_{ij} = 1$ for all i, j . We obtain a classical picture with two Fermat points. In case (b) we prescribe $\alpha_{ij} = 1$ if E_i and E_j share a common boundary and $\alpha_{ij} = 2$ otherwise.

8.3. Comments. The present algorithm shares some common features with the generalized version of the threshold dynamics presented in [19], see [24] for the seminal paper. Let us briefly point out some similarities and differences. We recall that the approximate interface energy used in [19] is based on convolutions with the heat kernel, whereas we consider instead of this latter its implicit semi-discrete counterpart. In addition, rather than convolutions, we work with the related boundary value problem which we believe more versatile regarding the geometry of the computational domain, even if both formulations are equivalent in the cases addressed here as examples. More fundamentally, our elliptic framework appears to be well-suited to develop optimization strategies, while in contrast the parabolic framework is exploited in [19] to simulate time evolutions.

9. VOLUME CONSTRAINTS

In this section we extend the previous algorithm to the minimal partition problem with constraints on the measure of each phase. Given $m_1, \dots, m_N \in \mathbb{R}_+$ such that $\sum_{i=1}^N m_i = |\Omega|$, we define the set

$$\bar{\mathcal{E}}_N = \left\{ (u_1, \dots, u_N) \in \tilde{\mathcal{E}}_N : \int_{\Omega} u_i dx = m_i \quad \forall i \right\}.$$

The approximate minimal partition problem with volume constraints and $g_i = 0$ is

$$\min_{(u_1, \dots, u_N) \in \bar{\mathcal{E}}_N} \left\{ \frac{1}{\varepsilon} \sum_{1 \leq i < j \leq N} \alpha_{ij} \langle L_{\varepsilon} u_i, u_j \rangle \right\}. \quad (9.1)$$

Theorem 7.2 yields the formulation

$$\min_{\substack{\sum_{i=1}^N u_i = 1 \\ u_i \geq 0, \int_{\Omega} u_i dx = m_i}} \inf_{\substack{v_i \in H^1(\Omega) \\ \sum_{i=1}^N v_i = 1}} \frac{1}{\varepsilon} \sum_{ij} \alpha_{ij} \left(\langle u_i, v_j \rangle - \frac{\varepsilon^2}{2} \langle \nabla v_i, \nabla v_j \rangle - \frac{1}{2} \langle v_i, v_j \rangle \right).$$

We implement the same type of alternating minimization algorithm as previously. The only difference is that the minimization with respect to u is no longer explicit due to spatial coupling. It requires solving a linear programming subproblem. Standard routines may be used, however we present a specific algorithm to take advantage of the fact that the number of volume constraints is usually very small in comparison with the number of pixels. In order to highlight this aspect we will analyze the algorithm in the continuous spatial setting.

9.1. Linear programming subproblem. Let $\zeta = (\zeta_1, \dots, \zeta_N) \in L^2(\Omega)^N$ and $m = (m_1, \dots, m_N) \in \mathbb{R}_+^N$ be given such that $\sum_{i=1}^N m_i = |\Omega|$. For $u = (u_1, \dots, u_N) \in L^2(\Omega)^N$ consider the primal criterion

$$\Lambda(u) = \sum_{i=1}^N \int_{\Omega} \zeta_i u_i dx.$$

Our goal is to solve the minimization problem

$$\min_{\substack{\sum_{i=1}^N u_i = 1 \\ u_i \geq 0, \int_{\Omega} u_i dx = m_i}} \Lambda(u). \quad (9.2)$$

In the discrete case, this kind of problem is sometimes called a semi-assignment problem, see for example [22]. As already seen, removing the volume constraints makes this problem trivial. Therefore we limit the duality treatment to those constraints. For $\lambda = (\lambda_1, \dots, \lambda_N) \in \mathbb{R}^N$ we define the Lagrangian

$$L(u, \lambda) = \Lambda(u) + \sum_{i=1}^N \lambda_i \left(\int_{\Omega} u_i dx - m_i \right).$$

By standard duality results (see e.g. [13] Theorem 3.9 and Theorem 3.4, note that Robinson's qualification holds for such linear constraints), if u is a minimizer of (9.2) then there exists $\lambda \in \mathbb{R}^N$ such that

$$L(u, \lambda) = \min_{\substack{\sum_{i=1}^N v_i = 1 \\ v_i \geq 0}} L(v, \lambda). \quad (9.3)$$

Moreover, such λ are maximizers over \mathbb{R}^N of the dual criterion

$$\mathcal{D}(\lambda) = \inf_{\substack{\sum_{i=1}^N v_i = 1 \\ v_i \geq 0}} L(v, \lambda).$$

Let us compute this dual criterion. A rearrangement yields

$$L(v, \lambda) = \sum_{i=1}^N \int_{\Omega} (\zeta_i + \lambda_i) v_i dx - \sum_{i=1}^N \lambda_i m_i. \quad (9.4)$$

It follows immediately that

$$\mathcal{D}(\lambda) = \int_{\Omega} \min\{(\zeta_i + \lambda_i)_{i=1}^N\} - \sum_{i=1}^N \lambda_i m_i.$$

Note that $\mathcal{D}(\lambda + c\mathbb{1}) = \mathcal{D}(\lambda)$ for any $c \in \mathbb{R}$, therefore the dual problem can be set over the quotient space \mathbb{R}^N/\mathbb{R} . We suggest alternating maximizations with respect to each multiplier. Since the function \mathcal{D} is not smooth some care must be taken as regards to the relevance of such a procedure. It is supported by the following equivalence.

Proposition 9.1. *The N -tuple $(\lambda_1, \dots, \lambda_N)$ is a maximizer of \mathcal{D} if and only if each λ_i is a maximizer of the partial function $\tilde{\lambda}_i \mapsto \mathcal{D}(\lambda_1, \dots, \lambda_{i-1}, \tilde{\lambda}_i, \lambda_{i+1}, \dots, \lambda_N)$. This is also equivalent to satisfying for each $i = 1, \dots, N$*

$$|\{\zeta_i + \lambda_i < \min_{j \neq i}(\zeta_j + \lambda_j)\}| \leq m_i \leq |\{\zeta_i + \lambda_i \leq \min_{j \neq i}(\zeta_j + \lambda_j)\}|. \quad (9.5)$$

Proof. Using Lemma 11.1 we obtain on the one hand the superdifferential of \mathcal{D} as

$$\begin{aligned} \partial^* \mathcal{D}(\lambda_1, \dots, \lambda_N) = & \left\{ (s_1 - m_1, \dots, s_N - m_N) \in \mathbb{R}^N : \right. \\ & \left. |\{\zeta_i + \lambda_i < \min_{j \neq i}(\zeta_j + \lambda_j)\}| \leq s_i \leq |\{\zeta_i + \lambda_i \leq \min_{j \neq i}(\zeta_j + \lambda_j)\}| \forall i, \sum_{i=1}^N s_i = |\Omega| \right\}. \end{aligned}$$

Since $\sum_i m_i = |\Omega|$ it follows

$$\begin{aligned} \partial^* \mathcal{D}(\lambda_1, \dots, \lambda_N) = & \left\{ (\tau_1, \dots, \tau_N) \in \mathbb{R}^N : \right. \\ & \left. |\{\zeta_i + \lambda_i < \min_{j \neq i}(\zeta_j + \lambda_j)\}| \leq m_i + \tau_i \leq |\{\zeta_i + \lambda_i \leq \min_{j \neq i}(\zeta_j + \lambda_j)\}| \forall i, \sum_{i=1}^N \tau_i = 0 \right\}. \end{aligned}$$

We derive the optimality condition

$$0 \in \partial^* \mathcal{D}(\lambda_1, \dots, \lambda_N) \iff |\{\zeta_i + \lambda_i < \min_{j \neq i}(\zeta_j + \lambda_j)\}| \leq m_i \leq |\{\zeta_i + \lambda_i \leq \min_{j \neq i}(\zeta_j + \lambda_j)\}| \forall i = 1, \dots, N.$$

On the other hand the partial maximization with respect to λ_i provides in a similar (simpler) way the optimality condition

$$0 \in \partial_i^* \mathcal{D}(\lambda_1, \dots, \lambda_N) \iff |\{\zeta_i + \lambda_i < \min_{j \neq i}(\zeta_j + \lambda_j)\}| \leq m_i \leq |\{\zeta_i + \lambda_i \leq \min_{j \neq i}(\zeta_j + \lambda_j)\}|.$$

This means that

$$0 \in \partial^* \mathcal{D}(\lambda_1, \dots, \lambda_N) \iff 0 \in \partial_i^* \mathcal{D}(\lambda_1, \dots, \lambda_N) \forall i = 1, \dots, N,$$

completing the proof. \square

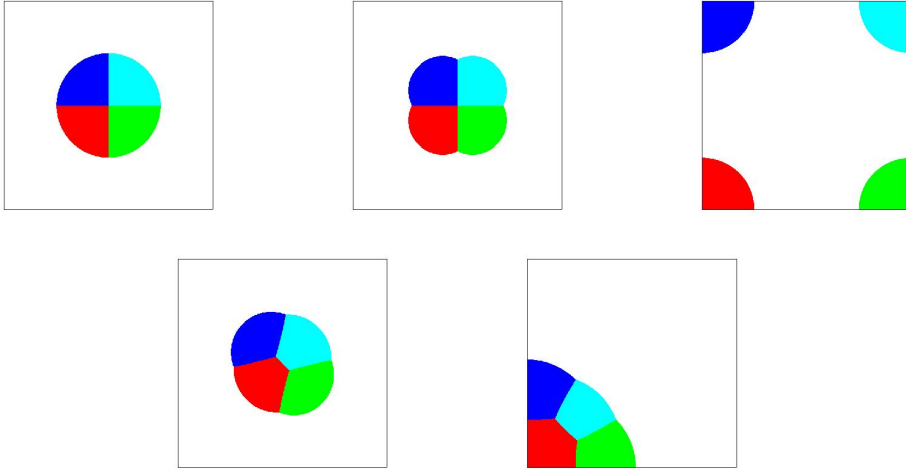


FIGURE 4. Partition with 5 phases and volume constraint: initialization (top left), obtained result in case (a) (top middle), obtained result in case (b) (top right), obtained result in case (c) (bottom left), obtained result in case (d) (bottom right).

Each iteration of the alternating procedure consists in solving (9.5), i.e., finding λ_i such that

$$|\{\lambda_i < \min_{j \neq i}(\zeta_j + \lambda_j) - \zeta_i\}| \leq m_i \leq |\{\lambda_i \leq \min_{j \neq i}(\zeta_j + \lambda_j) - \zeta_i\}|.$$

In the discrete framework this only requires sorting the values of $\min_{j \neq i}(\zeta_j + \lambda_j) - \zeta_i$ and selecting the m_i -th largest value. Once the multipliers $(\lambda_1, \dots, \lambda_N)$ have been fixed, the primal solution (u_1, \dots, u_N) is searched among the minimizers of (9.3). In view of (9.4) this minimization is straightforward, as in the unconstrained case. Note that in case of multiple solutions one that satisfies the volume constraints has to be chosen, however this situation is unlikely in practice due to numerical errors.

9.2. Examples. In figure 4 we consider 5 phases: 4 interior phases and the remaining set, called exterior phase (in white). We use the indices I to represent an arbitrary interior phase and E for the exterior phase. The computational grid is made of 512×512 pixels and we choose $\varepsilon_{\max} = 64$, $\varepsilon_{\min} = 1$. The volume constraints are given by the initialization. In case (a) we fix $\alpha_{II} = \alpha_{IE} = 1$. In case (b) we set $\alpha_{II} = 1$ and $\alpha_{IE} = 0.5$. In case (c) we choose $\alpha_{II} = 1$ and $\alpha_{IE} = 2$. Case (d) is the same as case (c) except that $\varepsilon_{\max} = 512$.

We now illustrate Herring's law at triple junction points between phases i, j, k , namely

$$\frac{\sin \theta_i}{\alpha_{jk}} = \frac{\sin \theta_j}{\alpha_{ik}} = \frac{\sin \theta_k}{\alpha_{ij}},$$

where $\theta_i, \theta_j, \theta_k$ are the opening angles of phases i, j, k , respectively. To do so we consider a four phase problem similar to the previous one, see figure 5. In case (a), the surface tensions are taken uniformly equal to 1, leading to the classical Fermat point. In the other cases we only modify a surface tension between two interior phases, chosen equal to $\sqrt{2}$ in case (b) and 0.01 in case (c). This gives rise to a right angle and a nearly flat angle, respectively.

In figure 6, we again consider 5 phases, but one of them is not subject to optimization. We use the indices L to represent the 3 first phases (liquid), S to represent the fixed phase (solid, in black), and V for the remaining set (vapor, in white). The grid contains 600×400 pixels and we use $\varepsilon_{\max} = 16$, $\varepsilon_{\min} = 1$. The surface tensions are chosen as $\alpha_{LL} = \alpha_{LS} = \alpha_{LV} = \alpha_{SV} = 1$ in case (a), $\alpha_{LL} = \alpha_{LS} = 1$, $\alpha_{LV} = \alpha_{SV} = 2$ in case (b), $\alpha_{LL} = 0.5$, $\alpha_{LS} = 1$, $\alpha_{LV} = \alpha_{SV} = 2$ in case (c).

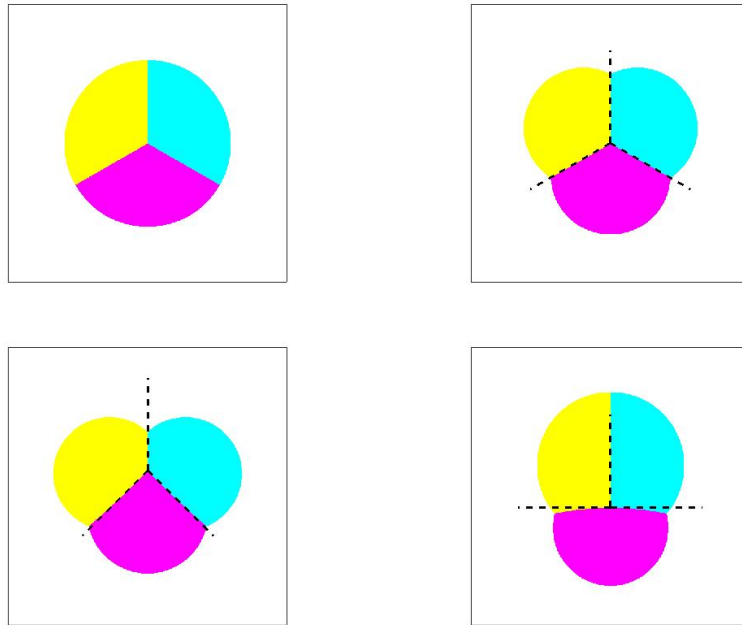


FIGURE 5. Illustration of Herring's law. Initialisation (top left), obtained result in case (a) (top right), obtained result in case (b) (bottom left), obtained result in case (c) (bottom right). The theoretical angles at the junction point are displayed in dashed line.

Finally we illustrate the lack of lower semicontinuity when the triangle inequality fails to hold in figure 7. We consider 3 phases and surface tensions given by (6.3). Phase 1 is the background medium, phases 2 and 3 are initially two half-disks. We incorporate forcing terms by functions g_i as in (8.1), while maintaining the initial volumes. These functions are chosen as $g_i = -10^{-2}u_i^{\text{ini}}$, in order to enforce u_i to stay close to its initial configuration u_i^{ini} , since for characteristic functions satisfying the constraint $-2\langle u_i, u_i^{\text{ini}} \rangle$ is equal to $\|u_i - u_i^{\text{ini}}\|_{L^2(\Omega)}^2$ up to an additive constant. The band of phase 1 appearing between phases 2 and 3, which can be theoretically arbitrarily thin, shows the lack of lower semicontinuity of the optimization problem, resulting in the absence of solution.

10. CONCLUSION

In this paper we have introduced and analyzed a Γ -convergence approximation of a class of interface energies for minimal partition problems. We have derived variational formulations of this functional that permit the implementation of alternating minimization algorithms. Our main numerical application has been the computation of equilibrium shapes of incompressible phases with surface tensions. The extension of this approach to other types of interface energies and to dynamical problems could be subjects of future research.

11. APPENDIX

Lemma 11.1. *Let $f_1, \dots, f_N \in L^1(\Omega)$ and define the function $\Phi : \mathbb{R}^N \rightarrow \mathbb{R}$ by*

$$\Phi(t_1, \dots, t_N) = \int_{\Omega} \max_{1 \leq i \leq N} (f_i(x) + t_i) dx.$$

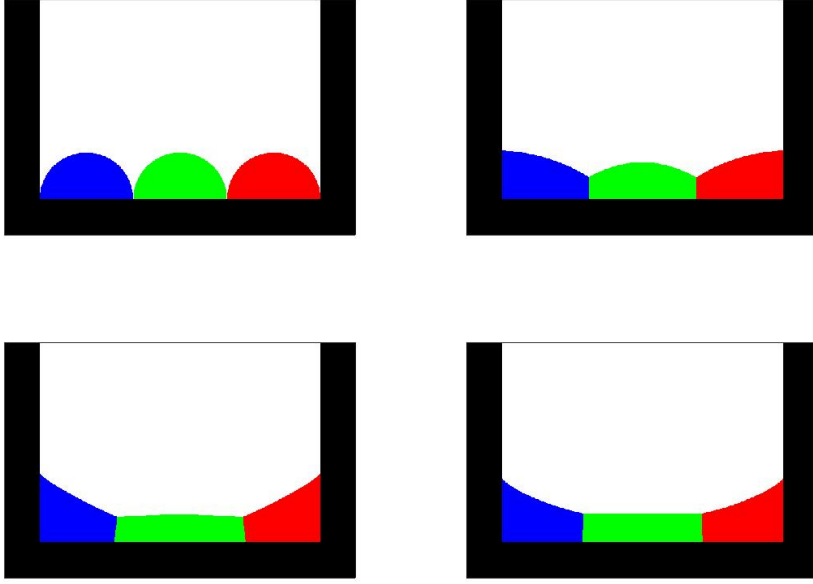


FIGURE 6. Partition with 5 phases and volume constraint: initialization (top left), obtained result in case (a) (top right), obtained result in case (b) (bottom left), obtained result in case (c) (bottom right).

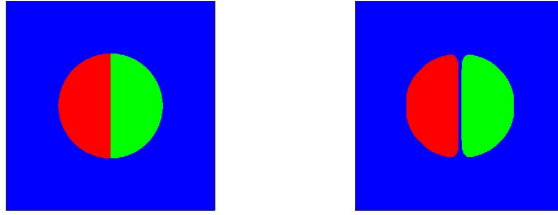


FIGURE 7. Illustration of the lack of lower semicontinuity when the triangle inequality does not hold. Initialisation (left) and obtained result (right).

Then Φ is convex and its subdifferential is

$$\partial\Phi(t_1, \dots, t_N) = \left\{ (s_1, \dots, s_N) \in \mathbb{R}^N : \right. \\ \left. |\{f_i + t_i > \max_{j \neq i} (f_j + t_j)\}| \leq s_i \leq |\{f_i + t_i \geq \max_{j \neq i} (f_j + t_j)\}| \forall i, \sum_{i=1}^N s_i = |\Omega| \right\}.$$

Proof. It is obvious that Φ is convex, since the integrand is itself convex as supremum of convex functions. Let us compute the subdifferential at 0. Then the subdifferential at $(\bar{t}_1, \dots, \bar{t}_N)$ will be inferred with the help of the change of functions $\bar{f}_i = f_i + \bar{t}_i$. We must show that

$$\partial\Phi(0, \dots, 0) = \left\{ (s_1, \dots, s_N) \in \mathbb{R}^N : |\{f_i > \max_{j \neq i} f_j\}| \leq s_i \leq |\{f_i \geq \max_{j \neq i} f_j\}| \forall i, \sum_{i=1}^N s_i = |\Omega| \right\}.$$

Assume that $(s_1, \dots, s_N) \in \partial\Phi(0, \dots, 0)$. By definition we have

$$\Phi(t_1, \dots, t_N) - \Phi(0, \dots, 0) \geq \sum_{i=1}^N s_i t_i \quad \forall (t_1, \dots, t_N) \in \mathbb{R}^N,$$

that is,

$$\int_{\Omega} \max_{1 \leq i \leq N} (f_i(x) + t_i) dx - \int_{\Omega} \max_{1 \leq i \leq N} f_i(x) dx \geq \sum_{i=1}^N s_i t_i \quad \forall (t_1, \dots, t_N) \in \mathbb{R}^N.$$

Choosing $t_i = 1$ for all i , then $t_i = -1$ for all i , yields already

$$\sum_{i=1}^N s_i = \int_{\Omega} dx = |\Omega|.$$

Fix k and take $t_k = -t$, $t > 0$, $t_i = 0$ if $i \neq k$. We have

$$s_k t \geq \int_{\Omega} \left(\max_{1 \leq i \leq N} f_i(x) - \max_{1 \leq i \leq N} (f_i(x) + t_i) \right) dx.$$

The integrand vanishes whenever $f_k(x) \leq \max_{i \neq k} f_i(x)$. Thus

$$s_k t \geq \int_{\{f_k > \max_{i \neq k} f_i\}} \left(f_k(x) - \max_{1 \leq i \leq N} (f_i(x) + t_i) \right) dx.$$

This can be rewritten as

$$s_k t \geq \int_{\{f_k > \max_{i \neq k} f_i\}} \min_{1 \leq i \leq N} (f_k(x) - f_i(x) - t_i) dx,$$

that is,

$$s_k t \geq \int_{\{f_k > \max_{i \neq k} f_i\}} \min \left(t, \min_{i \neq k} (f_k(x) - f_i(x)) \right) dx.$$

Adding and subtracting t yields

$$s_k t \geq t |\{f_k > \max_{i \neq k} f_i\}| + \int_{\{f_k > \max_{i \neq k} f_i\}} \min \left(0, \min_{i \neq k} (f_k(x) - f_i(x)) - t \right) dx.$$

Dividing by t entails

$$s_k \geq |\{f_k > \max_{i \neq k} f_i\}| + \int_{\{f_k > \max_{i \neq k} f_i\}} \min \left(0, \frac{\min_{i \neq k} (f_k(x) - f_i(x))}{t} - 1 \right) dx.$$

Letting $t \rightarrow 0^+$ yields by monotone convergence

$$s_k \geq |\{f_k > \max_{i \neq k} f_i\}|.$$

Now fix k and take $t_k = t$, $t > 0$, $t_i = 0$ if $i \neq k$. We have

$$s_k t \leq \int_{\Omega} \left(\max_{1 \leq i \leq N} (f_i(x) + t_i) - \max_{1 \leq i \leq N} f_i(x) \right) dx.$$

This entails

$$s_k t \leq t |\{f_k \geq \max_{i \neq k} f_i\}| + \int_{\{f_k < \max_{i \neq k} f_i\}} \left(\max_{1 \leq i \leq N} (f_i(x) + t_i) - \max_{1 \leq i \leq N} f_i(x) \right) dx.$$

Rearranging yields

$$s_k t \leq t |\{f_k \geq \max_{i \neq k} f_i\}| + \int_{\{f_k < \max_{i \neq k} f_i\}} \max(0, f_k(x) + t - \max_{i \neq k} f_i(x)) dx.$$

Hence

$$s_k \leq |\{f_k \geq \max_{i \neq k} f_i\}| + \int_{\{f_k < \max_{i \neq k} f_i\}} \max(0, \frac{f_k(x) - \max_{i \neq k} f_i(x)}{t} + 1) dx.$$

Letting $t \rightarrow 0^+$ yields by monotone convergence

$$s_k \leq |\{f_k \geq \max_{i \neq k} f_i\}|.$$

Assume now that

$$|\{f_i > \max_{j \neq i} f_j\}| \leq s_i \leq |\{f_i \geq \max_{j \neq i} f_j\}| \quad \forall i, \quad \sum_{i=1}^N s_i = |\Omega|.$$

Thus, there exists a partition $\Omega = \cup_{i=1}^N A_i$ such that

$$\{f_i > \max_{j \neq i} f_j\} \subset A_i \subset \{f_i \geq \max_{j \neq i} f_j\} \quad \forall i, \quad |A_i| = s_i \quad \forall i.$$

Indeed, such a construction is immediate for $N = 2$, then one proceeds by induction setting $g = \max_{1 \leq i \leq N-1} f_i$. In each A_k it holds

$$\max_{1 \leq i \leq N} (f_i(x) + t_i) - \max_{1 \leq i \leq N} f_i(x) \geq t_k.$$

It follows

$$\int_{\Omega} \max_{1 \leq i \leq N} (f_i(x) + t_i) dx - \int_{\Omega} \max_{1 \leq i \leq N} f_i(x) dx \geq \sum_{k=1}^N \int_{A_k} t_k dx = \sum_{k=1}^N t_k |A_k| = \sum_{k=1}^N t_k s_k.$$

This completes the proof. \square

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