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Modeling self-aggregation of stochastic particles: a Γ -convergence approach

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In this work, we demonstrate that a functional modeling the self-aggregation of stochastically distributed lipid molecules can be obtained as the Γ -limit of a family of discrete energies driven by a sequence of independent and identically distributed random variables. These random variables are intended to describe the asymptotic behavior of lipid molecules that satisfy an incompressibility condition. The discrete energy keeps into account the interactions between particles. We resort to transportation maps to compare functionals defined on discrete and continuous domains, and we prove that, under suitable conditions on the scaling of these maps as the number of random variables increases, the limit functional features an interfacial term with a Wasserstein-type penalization.

Keywords: Gamma-convergence; Wasserstein distance; transportation maps; self-aggregation; lipid bilayer.

AMS Subject Classification: 49J45, 74K15, 74S60

1. Introduction

Lipid bilayers are the fundamental component of cell membranes. They are composed of two layers of lipid molecules, with the hydrophilic heads facing outward and the hydrophobic tails facing inward. Lipid bilayers act as barriers, preventing

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the uncontrolled exchange of materials between the inside and outside of the cell⁹; they are dynamic and can change their shape and composition in response to various stimuli. For example, cells can regulate the fluidity of the membrane by altering the types of lipids, allowing them to respond to changes in temperature or other environmental factors.²³ Understanding the structure and functioning of lipid bilayers is essential for modeling basic biological processes such as cell signaling and membrane transport.³¹

In the last decades, a vast body of literature has been devoted to describing different mathematical settings to study the properties of biomembranes in a rigorous manner. In this regard, Canham,¹² and Helfrich,²² considered continuous models, where a lipid bilayer membrane assumes curved shapes to accommodate a spontaneous curvature which is influenced by factors such as lipid composition, temperature, and external stresses.³¹ In a similar setup, motivated by the works of Bates,⁶ and Fredrickson,¹⁶ on chains of copolymers, the authors of Ref. 9 proposed a continuous model to tackle the problem of self-aggregation of lipid molecules, which was not addressed in Helfrich's seminal paper.²² We also refer the reader to Ref. 4, 10, 13, where pattern formation of cell aggregates is analyzed by means of aggregation-diffusion equations. In the review paper 7 the dependent variable in a kinetic equation is a distribution function on the microscopic state of the interacting entities and the importance of understanding how the dynamics of the interaction produces aggregation is highlighted, whereas the paper 15 works on mechanical particles and shows how aggregation is generated by attraction-repulsion forces. More complex is the case of active particles, where the activity variable modifies the causality of mechanical interactions. In some cases, for instance in crowd dynamics, high level of stress (activity) leads to aggregation, see Ref. 8.

Lipid membranes can be studied at different length scales; in Ref. 28, the authors proposed three different models for micro-, meso-, and macroscopic scales through suitable energy functionals for idealized and rescaled head-tail densities. In the microscopic model, the state of the system is described by a probability density ψ , whose energy is the sum of two contributions, called a *non-ideal free energy* F^{nid} accounting for liquid-particle interaction, and an *ideal free energy* F^{id} accounting for a radially symmetric interaction potential; see equations (2.1) and (2.2) below for the details. In the mesoscopic model, the state of the system is described by a continuous distribution of lipid molecules (u for the hydrophilic heads and v for the hydrophobic tails) concentrated on an ε -thick interface separating the exterior of the cell from its interior; the energy functional to be minimized in this context is (2.4) below. The main result in Ref. 28 is the rigorous meso-to-macro limit in the two-dimensional setting, which recovers the Canham–Helfrich model. We highlight that in the macroscopic model the lipid bilayer is reduced to a zero-thickness membrane, whose energy is determined by its curvature; the latter is induced by the microscopic composition of the membrane, which does not enter in the model otherwise. In the same paper a formal derivation of the mesoscopic model was also proposed, from

which a series of contributions stemmed, where the nature of curved membranes was analyzed. In Ref. 26, an upper bound for the meso- to macroscopic limit is obtained in the three-dimensional setting; the optimality of this upper bound is still open, as the corresponding lower bound has been only partially proved in Ref. 27 under some restrictive technical assumptions. Finally, we mention the contribution 29, where macroscopic two-phase surfaces are analyzed. However, even though meso- and macroscopic models well describe self-aggregation of lipid molecules, they do not take into account the discrete nature of the problem. In fact, there are few works where the behavior of lipid molecules is modeled by functionals defined on discrete structures, see, e.g. Ref. 20, 32. One main reason for the lack of results in this direction is that capturing the contribution of the principal curvatures in a discrete setting is a subtle task.

In this paper, we perform the rigorous micro-to-meso derivation that was proposed in Ref. 28. To do so, we upscale (i.e., we take the limit as $n \rightarrow \infty$) discrete energies depending on a large number of molecules modeled by independent and identically distributed (according to a probability density ρ) random variables X_1, \dots, X_n ($n \in \mathbb{N}$) contained in some bounded region $D \subset \mathbb{R}^d$. Given $\delta_n > 0$, we consider a rescaled kernel $\kappa_{\delta_n}(X_i - X_j)$ that takes into account the interaction between lipid molecules at scale δ_n , for $i, j = 1, \dots, n$. As the number n of molecules increases, the interaction length-scale δ_n must vanish due to the boundedness of the container D , so that a crucial role in the identification of the mesoscopic limit will be played by the relationship between n and δ_n . We encode this interaction in a functional $GF_{n,\delta}$ defined, for a general interaction length-scale δ (see the precise definition in (3.1) below), in such a way that the amphiphilic nature of the molecules is taken into account: more precisely, the vicinity of hydrophilic heads and water or the hydrophobic tails is favored, whereas the vicinity of the hydrophobic tails and water is penalized.

A major difficulty in taking the limit as $n \rightarrow \infty$ and to recover a continuous functional is due to the stochasticity of the system; a key ingredient in performing this limit is the use of transportation maps to set the problem in a continuous framework. Our main result is Theorem 3.1 below where we show that, under a suitable rescaling of δ_n (see assumption (H4) below), the discrete GF_{n,δ_n} Γ -converges to a weighted total variation functional (originally introduced in Ref. 5). This means that, when modeling lipid bilayers using a sequence $X := \{X_i\}_{i \in \mathbb{N}}$ of random variables that interact at the scales dictated by hypothesis (H4), the resulting mesoscopic energy is a surface functional which depends on the geometric properties of the interface between the heads and the tails of the amphiphilic molecules. The remaining assumptions listed in hypotheses (H1–3) involve the geometry and regularity of the domain, structural requests on the interaction kernel κ , and properties of the random distribution of the particles. We refer the reader to Remark 3.1 for more technical details on these standing hypotheses.

As a byproduct of our Theorem 3.1, in the case of uniform distributed random variables, that is, when $\rho = |D|^{-1}$, we recover the usual perimeter functional for-

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mally derived in Ref. 28. More precisely, we consider the functional \mathcal{G}_{n,δ_n} defined in (3.8) below, given by the sum of GF_{n,δ_n} and a Wasserstein-like term and we prove in Theorem 3.2 that \mathcal{G}_{n,δ_n} Γ -converges to the same mesoscopic functional of Ref. 28. This is a significant result, which sets the ground for a derivation of the Canham–Helfrich functional starting from the more natural discrete stochastic setting.

Our result provides a rigorous approach to the micro- to mesoscopic limit for aggregation of stochastic particles. In particular, it bridges the probabilistic nature of distributions of particles at the microscopic level with the deterministic arrangement that they assume already at the mesoscopic level. This is precisely the novelty of our work and solves the main technical difficulty in performing such an upscaling. Our contribution sets the basis for a complete understanding of the direct micro- to macroscopic limit, as it selects the correct length scale for the mesoscopic intermediate passage. With our result available, the micro- to macroscopic limit would involve finding a the correct relationship between the diverging number of particles n and the vanishing layer thickness ε for the derivation of the Canham–Helfrich energy for the macroscopic membrane from the microscopic probability density ψ of particles. This is object of undergoing investigation.

The paper is organized as follows: in Section 2, we recall the derivation of the model proposed in Ref. 28 and some preliminary concepts needed later on. In Section 3, we introduce our main assumptions and state our main results, whose proofs are presented in Section 4.

2. Preliminaries

In this part, we start by recalling the derivation of the mesoscopic model to treat bilayer molecules.

2.1. Lipid models

A lipid molecule consists of a head and two tails. The head is usually charged and hydrophilic, while the tails are hydrophobic. This difference in polarity causes lipids to aggregate, and inside a cell, lipids are typically found in a bilayer structure (see Figure 1 below).

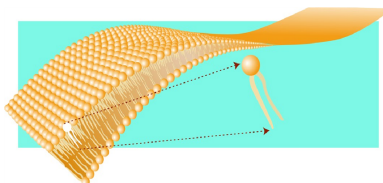


Fig. 1. A typical bilayer structure (see Figure 1 in Ref. 9).

In such a structure, the energetically unfavorable tail-water interactions are avoided by collecting the tails together in a water-free region created by the heads. Suppose that we have a system of particles composed of X_i^t , X_i^h , and X_i^w , which are the lipid tail, lipid head, and water beads, respectively, for $i = 1, \dots, n$, where $n \in \mathbb{N}$. Assuming that the beads are confined to a space $D \subset \mathbb{R}^d$, the full microscopic state space for the system is then D^{3n} . Elements $X \in D^{3n}$ are called microstates.²⁷ We describe the system in terms of probability densities on D^{3n} ; that is, the state ψ of the system is described through a probability density on D^{3n}

$$\psi \in \mathcal{E}, \quad \text{where} \quad \mathcal{E} := \left\{ \psi: D^{3n} \rightarrow \mathbb{R}_+ : \int_{D^{3n}} \psi(x) dx = 1 \right\}. \quad (2.1)$$

Moreover, suppose that X^t , X^h , and X^w are composed of independent and identically distributed random variables, which are distributed according to probability laws μ , ν , and η , respectively, and that these distributions depend on ψ . Suppose that μ , ν , and η are absolutely continuous with respect to the d -dimensional Lebesgue measure \mathcal{L}^d , and thus have densities u , v , and w , respectively. A typical assumption when modeling biomembranes is that $u + v + w = 1$. This condition is usually referred to as the incompressibility condition for particles.²⁸ It is a point-wise relation that aims to balance the portion of particles of different types stored in D . To specify the behavior of the system of particles, we consider two functionals: the *ideal* free functional $F^{\text{id}}: \mathcal{E} \rightarrow \mathbb{R}$, $\psi \mapsto F^{\text{id}}(\psi)$, which models the effects of entropy and the interaction between beads of the same type, and the *non-ideal* free energy functional $F^{\text{nid}}: \mathcal{E} \rightarrow \mathbb{R}$, $\psi \mapsto F^{\text{nid}}(\psi)$, which represents the interaction of beads of different types. The total energy of the system is then $F^{\text{nid}}(\psi) + F^{\text{id}}(\psi)$. Typical terms in the non-ideal free energy are convolution integrals in which proximity of hydrophilic beads and tail beads is penalized: up to a physical constant which we disregard, F^{nid} can be expressed as

$$F^{\text{nid}}(\psi) := \iint_{D \times D} (v(x) + w(x))u(y)\kappa(x - y) dx dy, \quad (2.2a)$$

where κ is the kernel of interaction. Since we are interested in interactions at a small scale $\delta > 0$, the kernel κ is usually rescaled to $\kappa_\delta := \delta^{-d}\kappa(\cdot/\delta)$. For the ideal free energy F^{id} , one can assume the form

$$F^{\text{id}}(\psi) = \int_{D^{3n}} \psi(x)H^{\text{id}}(x) dx, \quad (2.2b)$$

where H^{id} is a suitable interaction potential. The choice of the potential H^{id} models certain phenomena, such as attraction, repulsion, and combinations thereof. The function H^{id} is usually called the *interaction potential*, and it is in general assumed to be radially symmetric^{4,10}, i.e., $H^{\text{id}}(x) = w(|x|)$, for some $w: [0, +\infty) \rightarrow \mathbb{R}$.

In 2009, Peletier and Röger,²⁸ proposed a mesoscale model for biomembranes in the form of an energy functional for idealized and rescaled head-tail densities. Such a model is derived from the functional $F^{\text{nid}} + F^{\text{id}}$, in which heads and tails are treated as separate particles. The term F^{nid} penalizes the proximity of tails to either

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heads or water particles, and the term F^{id} implements the head-tail connection. In particular, they proposed $F^{\text{id}}(\psi) = W_p(u, v)$, the Wasserstein distance of order $p \in [1, \infty)$. From an analytic point of view, configurations of head and tail particles are modeled by suitable density functions belonging to the space of functions of bounded variation in \mathbb{R}^d , see Ref. 2. A formal upscaling procedure leads to the following model: configurations of head and tail particles are described by two rescaled density functions

$$u \in \text{BV}(\mathbb{R}^d; \{0, \epsilon^{-1}\}), \quad v \in L^1(\mathbb{R}^d; \{0, \epsilon^{-1}\}),$$

respectively, with $uv = 0$ a.e. in \mathbb{R}^d and with prescribed total mass $M > 0$, namely

$$\int_{\mathbb{R}^d} u(x) \, dx = \int_{\mathbb{R}^d} v(x) \, dx = M. \quad (2.3)$$

Here $\epsilon > 0$ is a small parameter measuring the size of the support of u . We denote by $K_\epsilon \subset L^1(\mathbb{R}^d \times \mathbb{R}^d)$ the space of such configurations, that is

$$K_\epsilon := \{(u, v) \in \text{BV}(\mathbb{R}^d, \{0, \epsilon^{-1}\}) \times L^1(\mathbb{R}^d, \{0, \epsilon^{-1}\}) : (2.3) \text{ holds and } uv = 0 \text{ a.e. in } \mathbb{R}^d\}.$$

In Ref. 28 the asymptotic behavior of the energy functional

$$F_\epsilon(u, v) := \begin{cases} \epsilon \|Du\| + \frac{1}{\epsilon} W_1(u, v) & \text{if } (u, v) \in K_\epsilon, \\ +\infty & \text{otherwise in } L^1(\mathbb{R}^d) \times L^1(\mathbb{R}^d) \end{cases} \quad (2.4)$$

is studied. The term $\|Du\|$ represents the total variation of u and it measures the boundary of the support of tails. By a rigorous analysis via Γ -convergence, it is shown in Ref. 28 that the energy (2.4) has a preference for thin structures without ends and a resistance to bending of the structure. To be precise, in the limit as $\epsilon \rightarrow 0$, the densities concentrate along families of regular curves, and a Euler-type functional appears. The result is in the two-dimensional case, whereas in the three-dimensional case one might expect convergence to a Canham–Helfrich-type functional; nonetheless, in this situation, only partial results are known.^{26,27}

2.2. Γ -convergence

In this section, we briefly review the definition of Γ -convergence of a sequence of functionals defined on a metric space, both in the deterministic and in the stochastic case. Let (Y, d_Y) be a metric space and let $F_n : Y \rightarrow [0, \infty]$ be a sequence of functionals.

Definition 2.1. The sequence $\{F_n\}_{n \in \mathbb{N}}$ Γ -converges with respect to metric d_Y to the functional $F : Y \rightarrow [0, \infty]$ if the following inequalities hold:

- i) For every $y \in Y$ and every sequence $\{y_n\}_{n \in \mathbb{N}}$ converging to y

$$F(y) \leq \liminf_{n \rightarrow \infty} F_n(y_n);$$

ii) For every $y \in Y$ there exists a sequence $\{\bar{y}_n\}_{n \in \mathbb{N}}$ converging to y such that

$$\limsup_{n \rightarrow \infty} F_n(\bar{y}_n) \leq F(y).$$

In this case, we then say that F is the Γ -limit of the sequence of functionals $\{F_n\}_{n \in \mathbb{N}}$ with respect to the metric d_Y . Since the sequence $\{\bar{y}_n\}_{n \in \mathbb{N}}$ in ii) satisfies condition i) we have $\lim_{n \rightarrow \infty} F(\bar{y}_n) = F(y)$, and the sequence $\{\bar{y}_n\}_{n \in \mathbb{N}}$ is called recovery sequence.

In the same way, we define the Γ -convergence for random functionals.

Definition 2.2. Let $(\Omega, \mathcal{T}, \mathbb{P})$ be a probability space. For a sequence of random functionals $F_n: Y \times \Omega \rightarrow [0, +\infty]$ and $F: Y \rightarrow [0, +\infty]$ a deterministic functional, we say that the sequence of functionals $\{F_n\}_{n \in \mathbb{N}}$ Γ -converges with respect to the metric d_Y to F , if for \mathbb{P} -almost every $\omega \in \Omega$, the sequence $\{F_n(\cdot, \omega)\}_{n \in \mathbb{N}}$ Γ -converges to F according to Definition 2.1.

We now recall the notion of convergence in law and convergence in probability. Let Y and Z be metric spaces. Given a probability measure $\mu \in \mathcal{P}(Y)$ and a measurable mapping $T: Y \rightarrow Z$, we denote by $\nu := T_{\#}\mu$ the push-forward of μ by T , namely the measure $\nu \in \mathcal{P}(Z)$ such that $\nu(A) = (T_{\#}\mu)(A) = \mu(T^{-1}(A))$, for any Borel set $A \subset Z$.

Definition 2.3. Let $\{F_n\}_{n \in \mathbb{N}}$ be a sequence of random functionals with F_n defined on the probability space $(\Omega_n, \mathcal{T}_n, \mathbb{P}_n)$. Let F_∞ be a random functional defined on the probability space $(\Omega_\infty, \mathcal{T}_\infty, \mathbb{P}_\infty)$. We say that $\{F_n\}_{n \in \mathbb{N}}$ converges in law to F_∞ if the sequence of measures $\mu_n := (F_n)_{\#}\mathbb{P}_n$ converges weakly-* as $n \rightarrow \infty$ to $\mu_\infty := (F_\infty)_{\#}\mathbb{P}_\infty$.

Definition 2.4. Let $\{F_n\}_{n \in \mathbb{N}}$ be a sequence of random functionals defined on a common probability space $(\Omega, \mathcal{T}, \mathbb{P})$. We say that F_n converges in probability to a random functional F_∞ if

$$\lim_{n \rightarrow \infty} \mathbb{P}(\{\omega \in \Omega : d(F_n, F_\infty) > \eta\}) = 0, \quad \text{for all } \eta > 0$$

where d is a suitable metric in the space of functionals (see Proposition 1.12 in Ref. 14).

A well-known result about the convergence of random functionals is the following one.

Proposition 2.1 (see Proposition 2.9 in Ref. 14). *Suppose that $\{F_n\}_n$ is a sequence of random functionals which converges in law to $F_\infty: Y \times \Omega \rightarrow [0, +\infty]$. If F_∞ is constant, that is, if there exists $F: Y \rightarrow [0, +\infty]$ such that $F_\infty(\omega) = F$ for \mathbb{P} -almost every $\omega \in \Omega$, then the convergence of $\{F_n\}_n$ in law and the convergence in probability are equivalent.*

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2.3. The TL^p topology and some of its properties

In this section, we recall some useful facts about the topology of measure-functions pairs spaces. This topology was introduced in Ref. 18 to treat the convergence of functionals defined on graphs. Given an open bounded subset $D \subset \mathbb{R}^d$, we define for all $p \in [1, +\infty)$

$$TL^p(D) := \{(\mu, f) : \mu \in \mathcal{P}(D), f \in L^p_\mu(D)\}.$$

This space can be endowed with a distance (see (2.7) below) and thus it is a metric space.¹⁸ The definition for the case $p = \infty$ can be presented in the usual way; we neglect it here for the sake of conciseness. Note that for a generic bounded Borel map $f: D \rightarrow \mathbb{R}$, the following change of variables

$$\int_D f(T(x)) d\mu(x) = \int_D f(y) d\nu(y),$$

holds true if and only if $\nu = T_\# \mu$, in which case we say that the Borel map $T: D \rightarrow D$ is a *transportation map* between the measures $\mu \in \mathcal{P}(D)$ and $\nu \in \mathcal{P}(D)$. In this case, we associate with T a transportation plan $\pi_T \in \Gamma(\mu, \nu)$ defined by

$$\pi_T := (\text{Id}, T)_\# \mu \tag{2.5}$$

where $(\text{Id}, T): D \rightarrow D \times D$ is given by $(\text{Id}, T)(x) = (x, T(x))$. Here, $\Gamma(\mu, \nu)$ is the set of all couplings between μ and ν , that is, the set of all Borel probability measures on $D \times D$ for which the marginal on the first variable is μ and the marginal on the second variable is ν . We notice that when μ is absolutely continuous with respect to the Lebesgue measure, the weak- $*$ convergence of μ_n to μ as $n \rightarrow \infty$ is equivalent to the existence of a sequence $\{T_n\}_{n \in \mathbb{N}}$ of transportation maps such that

$$\int_D |x - T_n(x)|^p d\mu(x) \rightarrow 0 \quad \text{as } n \rightarrow \infty. \tag{2.6}$$

This motivates the following definition.

Definition 2.5. We say that a sequence of transportation maps $\{T_n\}_{n \in \mathbb{N}}$ is *stagnating* if (2.6) holds.

Given $p \in [1, \infty)$ and $(\mu, f), (\nu, g) \in TL^p(D)$ their distance is defined by

$$d_{TL^p}((\mu, f), (\nu, g)) := \inf_{\pi \in \Gamma(\mu, \nu)} \iint_{D \times D} (|x - y|^p + |f(x) - g(x)|^p) d\pi(x, y) \tag{2.7}$$

It is well known,^{3,30} that when μ is absolutely with respect to the Lebesgue measure, problem (2.7) admits a solution. In particular, if $p > 1$ there exists a unique transport map T inducing the transport plan π_T in (2.5).

The following proposition characterized the convergence in TL^p .

Proposition 2.2 (see Proposition 3.12 in Ref. 18). *Let $(\mu, f) \in TL^p(D)$ and let $\{(\mu_n, f_n)\}_{n \in \mathbb{N}}$ be a sequence in TL^p . The following statements are equivalent:*

1. (μ_n, f_n) converges to (μ, f) in $TL^p(D)$ as $n \rightarrow \infty$, in symbols $(\mu_n, f_n) \xrightarrow{TL^p} (\mu, f)$ as $n \rightarrow \infty$.
2. $\mu_n \rightharpoonup \mu$ weakly* and for every stagnating sequence of transportation plans $\{\pi_n\}_{n \in \mathbb{N}} \subseteq \Gamma(\mu, \mu_n)$

$$\iint_{D \times D} |f(x) - f(y)|^p d\pi_n(x, y) \rightarrow 0, \quad \text{as } n \rightarrow \infty. \quad (2.8)$$

3. $\mu_n \rightharpoonup \mu$ weakly* and there exists a stagnating sequence of transportation plans $\{\pi_n\}_{n \in \mathbb{N}} \subseteq \Gamma(\mu, \mu_n)$ for which (2.8) holds.

Moreover, if the measure μ is absolutely continuous with respect to the Lebesgue measure, the following are equivalent to the previous statements:

4. $\mu_n \rightharpoonup \mu$ weakly* and there exists a stagnating sequence of transportation maps $\{T_n\}_{n \in \mathbb{N}}$ such that

$$\int_D |f(x) - f_n(T_n(x))|^p d\mu(x) \rightarrow 0, \quad \text{as } n \rightarrow \infty; \quad (2.9)$$

5. $\mu_n \rightharpoonup \mu$ weakly* and for any stagnating sequence of transportation maps $\{T_n\}_{n \in \mathbb{N}}$ (2.9) holds.

Let $\nu = \rho \mathcal{L}^d$ with the density ρ bounded from below and from above by positive constants. We consider a sequence $\{X_i\}_{i \in \mathbb{N}}$ of independent random variables which are identically distributed according to ν , and supported on a common probability space $(\Omega, \mathcal{T}, \mathbb{P})$. In the next, we make use of upper bounds on the transportation distance between ν and the empirical measure $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$. This will play an important role in the proof of our Γ -convergence results. In particular, we will use estimates of

$$d_\infty(\nu, \nu_n) := \inf \{ \| \text{Id} - T \|_\infty \text{ where } T: D \rightarrow D, T_\# \nu = \nu_n \}$$

which measures what is the least maximal distance that a transportation map T between ν and ν_n has to move the mass. Here, for a map $S: D \rightarrow D$, we denote by $\|S\|_\infty := \sup_{x \in D} |S(x)|$. In particular, we are interested in the case where ρ is a uniform probability density in D . Let us suppose that $D = (0, 1)^d$, and consider $P = \{p_1, \dots, p_n\}$ the set of n points in D where each point in P is the center of a cube contained in D with volume $\frac{1}{n}$. In Ref. 24 it is shown that, if D is connected with Lipschitz boundary, for $d \geq 3$ and ρ constant, there exist two positive constants λ, Λ such that the event

$$\frac{\lambda(\log n)^{1/d}}{n^{1/d}} \leq \min_{\sigma} \max_{i \in \{1, \dots, n\}} |p_i - X_{\sigma(i)}| \leq \frac{\Lambda(\log n)^{1/d}}{n^{1/d}}$$

has probability 1 and where σ ranges over all permutations of $\{1, \dots, n\}$. This result was further extended in Ref. 17, and we report it here.

Theorem 2.1 (see **Theorem 2.5** in Ref. 18). *Let $D \subset \mathbb{R}^d$ be an bounded connected open set with Lipschitz boundary. Let ν be a probability measure on D*

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with density ρ which is bounded from below and from above by positive constants. Let $\{X_i\}_{i \in \mathbb{N}}$ be a sequence of independent and identically distributed random variables distributed on D according to the measure ν and let $\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$. Then there exists a constant $C > 0$ such that for \mathbb{P} -almost everywhere $\omega \in \Omega$ there exists a sequence of transportation maps $\{T_n\}_{n \in \mathbb{N}}$ from ν to ν_n (i.e., $(T_n)_\# \nu = \nu_n$) and such that

$$\begin{aligned} \text{if } d = 2 \text{ then } \quad & \limsup_{n \in \mathbb{N}} \frac{n^{1/2} \|\text{Id} - T_n\|_\infty}{(\log n)^{3/4}} \leq C, \\ \text{if } d \geq 3 \text{ then } \quad & \limsup_{n \in \mathbb{N}} \frac{n^{1/d} \|\text{Id} - T_n\|_\infty}{(\log n)^{1/d}} \leq C. \end{aligned} \tag{2.10}$$

Remark 2.1. As a consequence of (2.10), we have that $\|\text{Id} - T_n\|_\infty \rightarrow 0$. In particular, the sequence $\{T_n\}_{n \in \mathbb{N}}$ is stagnating according to Definition 2.5.

2.4. Weighted BV functions

We now recall the notion of total variation and weighted total variation which will be used to state our main result. Let $\psi : D \rightarrow (0, +\infty)$ be a continuous function, and consider the measure $\nu = \psi \mathcal{L}^d$. Following Ref. 5, given $u \in L^1_\nu(D)$ we define the weighted total variation of u with respect to ψ as

$$TV(u; \psi) := \sup \left\{ \int_D u \operatorname{div} \phi \, dx : \phi \in C_c^\infty(D; \mathbb{R}^d), |\phi(x)| \leq \psi(x) \text{ for all } x \in D \right\}.$$

We denote $BV(D; \psi)$ the set of all functions $u \in L^1(D; \psi)$ for which $TV(u; \psi) < +\infty$. In particular, when $\psi \equiv 1$ we recover the usual space $BV(D)$. For a measurable set $B \subset D$, we then define the perimeter in D as the weighted total variation of the characteristic function of B , that is, $\operatorname{Per}(B; \psi) := TV(\chi_B; \psi)$.

Proposition 2.3 (see Theorem 3.3 in Ref. 5). *A function $u \in L^1(D; \psi)$ belongs to $BV(D; \psi)$ if and only if there exist a finite Radon measure $|Du|_\psi$ and a $|Du|_\psi$ -measurable function $\sigma : D \rightarrow \mathbb{R}^d$ such that $|\sigma(x)| = 1$ for $|Du|_\psi$ -almost every $x \in D$ and such that*

$$\int_D u(x) \operatorname{div} \phi(x) \, dx = - \int_D \frac{\phi(x) \cdot \sigma(x)}{\psi(x)} \, d|Du|_\psi(x). \tag{2.11}$$

The measure $|Du|_\psi$ and the function σ are uniquely determined by (2.11) and the weighted total variation $TV(u; \psi)$ is equal to $|Du|_\psi(D)$.

Note that, using (2.11), one can check that $|Du|_\psi = \psi |Du|$, so that

$$TV(u; \psi) = \int_D \psi(x) \, d|Du|(x). \tag{2.12}$$

Since the functional $TV(\cdot; \psi)$ is defined as the supremum of linear continuous functionals in $L^1(D; \psi)$, it is lower semicontinuous with respect to the $L^1(D; \psi)$ metric. The following density theorem for weighted BV functions will be used in the proof of Theorem 3.1 below.

Theorem 2.2 (see Theorem 2.4 in Ref. 17). *Let D be an open subset of \mathbb{R}^d with Lipschitz boundary and let $\rho: D \rightarrow \mathbb{R}$ be a continuous function which is bounded from below and above by positive constants. Then for every $u \in \text{BV}(D; \rho)$ there exists a sequence $\{u_n\}_{n \in \mathbb{N}} \subseteq C_c^\infty(\mathbb{R}^d)$ such that*

$$u_n \rightarrow u \quad \text{in } L^1(D) \quad \text{and} \quad \int_D |\nabla u_n| \rho \, dx \rightarrow \text{TV}(u; \rho) \quad \text{as } n \rightarrow \infty.$$

For a general statement for density of regular functions in the space $\text{BV}(D; \rho)$, we refer to Ref. 5 .

3. Setting of the problem and main results

In this section, we give a precise description of the functionals we are interested in and a precise statement of our main results. Let $X := \{X_i\}_{i \in \mathbb{N}}$ be a sequence of independent and identically distributed random variables with distribution ν which is absolutely continuous with respect to the Lebesgue measure in \mathbb{R}^d , that is there exists a function $\rho \in L^1(D)$ such that $\nu = \rho \mathcal{L}^d$. Let $\kappa: \mathbb{R}^d \rightarrow [0, +\infty)$ be a function and, for any $\delta > 0$, let $\kappa_\delta: \mathbb{R}^d \rightarrow [0, +\infty)$ be defined as

$$\kappa_\delta(x) := \frac{1}{\delta^d} \kappa\left(\frac{x}{\delta}\right).$$

For $n \in \mathbb{N}$, we consider the non-ideal free energy functional $GF_{n,\delta}: L^1_\nu(D) \rightarrow [0, +\infty]$ defined by

$$GF_{n,\delta}(u) := \begin{cases} \frac{2}{\delta n^2} \sum_{i,j=1}^n \kappa_\delta(X_i - X_j)(1 - u(X_i))u(X_j) & \text{if } 0 \leq u \leq 1, \\ +\infty & \text{otherwise.} \end{cases} \quad (3.1)$$

Our contribution in this work is to study the asymptotic behavior of GF_{n,δ_n} , for a suitable scaling δ_n depending on the number of particles n .

The factor $2/\delta$ in (3.1) comes from a modeling assumption, whereas the factor $1/n^2$ is a rescaling that keeps into account the number of particles. The scaling $\delta_n := \delta(n)$ that we are going to consider is the one that will allow us to obtain a law of large numbers as $n \rightarrow \infty$. Our main result will be to show that the Γ -limit of GF_{n,δ_n} is $|Du|_{\rho^2}$ (see Section 2.4), and we prove this in Theorem 3.1 below.

For $d > 1$, we make the following assumptions which will be valid for the remainder of the paper.

- (1) The set $D \subset \mathbb{R}^d$ is bounded, connected, and open and has Lipschitz boundary.
- (2) The kernel $\kappa: \mathbb{R}^d \rightarrow [0, +\infty)$ is isotropic and thus it can be written as $\kappa(x) = \eta(|x|)$, for a certain radial profile $\eta: [0, +\infty) \rightarrow [0, +\infty)$. We assume that η is non-increasing, continuous at 0, and that $\eta(0) > 0$, and also that

$$\int_0^{+\infty} \eta(r)r^{d+1} \, dr < +\infty. \quad (3.2)$$

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- (3) $X = \{X_i\}_{i \in \mathbb{N}}$ is a sequence of independent and identically distributed random variables, distributed according to a probability distribution $\nu = \rho \mathcal{L}^d$ with Lipschitz continuous density $\rho: D \rightarrow \mathbb{R}$ which is bounded from below and above by positive constants a and b , respectively. Associated with X , we consider the sequence of empirical measures

$$\nu_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}, \quad (3.3)$$

and by T_n the transportation maps such that $(T_n)_\# \nu = \nu_n$.

- (4) We let $\{\delta_n\}_{n \in \mathbb{N}}$ be an infinitesimal sequence of positive numbers satisfying

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{(\log n)^{3/4}}{n^{1/2} \delta_n} = 0 & \quad \text{if } d = 2, \\ \lim_{n \rightarrow \infty} \frac{(\log n)^{1/d}}{n^{1/d} \delta_n} = 0 & \quad \text{if } d \geq 3. \end{aligned} \quad (3.4)$$

Remark 3.1. Let us now give some comments about our assumptions.

- (1) Hypothesis (H2) is physically motivated and it is needed to treat, among other problems, Ising spin systems on graphs.¹ By elementary considerations, it is immediate to notice that there exists a step function $\eta_0: [0, +\infty) \rightarrow [0, +\infty)$ of the form

$$\eta_0(r) = \begin{cases} A & \text{if } r < r_0, \\ 0 & \text{if } r \geq r_0, \end{cases} \quad (3.5a)$$

where $0 < A < \eta(0)$ and $0 < r_0 < +\infty$, such that

$$\eta_0(r) \leq \eta(r) \quad \text{for all } r \in [0, +\infty). \quad (3.5b)$$

Clearly, η_0 satisfies (3.2).

- (2) Hypothesis (H3) describes how each lipid molecule moves randomly in the environment independently of all other molecules.
- (3) Hypothesis (H4) is crucial to obtain the compactness result in Lemma 3.1 below; in particular, the conditions (3.4) are quite technical and are related to upper bounds on the transportation distance between the empirical measure (3.3) and the distribution ν . It is related to the connectedness property of the limiting graph obtained starting from a random graph with edges X_1, \dots, X_n and edge weights $\kappa_{\delta_n}(X_i - X_j)$ as $n \rightarrow \infty$. That is, the conditions (3.4) guarantee that the resulting graph is connected with probability 1 as $n \rightarrow \infty$ (see Ref. 21).

Lemma 3.1. (*Compactness*) *Assume that (H1-4) hold true. Consider a sequence of functions $\{u_n\}_{n \in \mathbb{N}}$ such that $u_n \in L^1_{\nu_n}(D)$ for every $n \in \mathbb{N}$, where ν_n is given by (3.3) and suppose that*

$$\sup_{n \in \mathbb{N}} \|u_n\|_{L^1_{\nu_n}(D)} < +\infty \quad \text{and} \quad \sup_{n \in \mathbb{N}} GF_{n, \delta_n}(u_n) < +\infty. \quad (3.6)$$

Then $\{(\nu_n, u_n)\}_{n \in \mathbb{N}}$ is relatively compact in $TL^1(D)$.

We now state the main result of this paper. To this aim, we define

$$\alpha_d := \left(\int_{\mathbb{S}^{d-1}} |\langle z, e \rangle| d\mathcal{H}^{d-1}(z) \right) \cdot \left(\int_{\mathbb{R}^d} |x| \kappa(x) dx \right), \quad (3.7)$$

where $e \in \mathbb{S}^{d-1}$ any unit vector (it is not difficult to see that the averaged integral is indeed independent of e).

Theorem 3.1. *Assume that the conditions (H1-4) hold true. Then the functionals $GF_{n, \delta_n} : L^1_{\nu_n}(D) \rightarrow [0, +\infty]$ defined by (3.1) $\Gamma(TL^1(D))$ -converge to the functional $\alpha_d TV(\cdot; \rho^2) : L^1_{\nu}(D) \rightarrow [0, +\infty]$, where α_d is defined in (3.7) and where, using (2.12),*

$$TV(u; \rho^2) = \begin{cases} \int_{S_u} \rho^2(x) d\mathcal{H}^{d-1}(x) & \text{if } u \in \text{BV}(D; \rho) \\ & \text{and } u(x) \in \{0, 1\} \text{ for } \nu\text{-a.e. } x \in D, \\ +\infty & \text{otherwise in } L^1_{\nu}(D). \end{cases}$$

The next two results that we present hold in the case of constant density $\rho = |D|^{-1}$. For $D \subset \mathbb{R}^d$ such that $|D| \geq 2$, consider the class

$$\mathcal{X}(D) := \{(A, O) \in \mathcal{B}(D) \times \mathcal{B}(D) : |A| = |O| = 1, |A \cap O| = 0\}.$$

We study the asymptotic behavior as $\delta_n \rightarrow 0$ of the sequence of functionals $\mathcal{G}_{n, \delta_n} : \mathcal{B}(D) \times \mathcal{B}(D) \rightarrow [0, +\infty]$ defined as

$$\mathcal{G}_{n, \delta_n}(A, O) := \begin{cases} GF_{n, \delta_n}(\chi_A) + W_p(A, O) & \text{if } (A, O) \in \mathcal{X}(D), \\ +\infty & \text{otherwise.} \end{cases} \quad (3.8)$$

Here, we use the notation $W_p(A, O)$ to denote the p -th Wasserstein distance between the indicator functions χ_A and χ_O of two sets $A, O \in \mathcal{B}(D)$ such that $|A| = |O| = 1$.

Lemma 3.2. *Assume that (H1-4) hold true with $\rho = |D|^{-1}$. Let $\{(A_n, O_n)\}_n \subset \mathcal{X}(D)$ be a sequence such that*

$$\mathcal{G}_{n, \delta_n}(A_n, O_n) \leq \inf_{(\tilde{A}, \tilde{O}) \in \mathcal{X}(D)} \mathcal{G}_{n, \delta_n}(\tilde{A}, \tilde{O}) + \frac{1}{n}. \quad (3.9)$$

Then there exists $(A, O) \in \mathcal{X}(D)$, with A a set of finite perimeter, such that (up to subsequence)

$$\chi_{A_n} \rightarrow \chi_A \text{ in } L^1(D) \quad \text{and} \quad \chi_{O_n} \xrightarrow{*} \chi_O \text{ in } L^\infty(D) \quad \text{as } n \rightarrow \infty. \quad (3.10)$$

Finally, we will prove the following Γ -convergence result.

Theorem 3.2 (Gamma-convergence). *Assume that (H1-4) hold true with $\rho = |D|^{-1}$. Then*

$$\left(\Gamma - \lim_{n \rightarrow \infty} \mathcal{G}_{n, \delta_n} \right) (A, O) = \frac{\alpha_d}{|D|^2} \text{Per}(A; D) + W_p(A, O),$$

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where α_d is defined in (3.7), and the metric of the Γ -convergence is $(s-L^1(D)) \times (w^*-L^\infty(D))$.

Remark 3.2. In view of Proposition 2.1 we point out that both the Γ -convergence results in Theorems 3.1 and 3.2 hold also in law.

4. Proofs

We start by proving our compactness result.

Proof. [Proof of Lemma 3.1] Considering the sequence of transportation maps $\{T_n\}_{n \in \mathbb{N}}$, we have

$$GF_{n,\delta_n}(u_n) = \frac{2}{\delta_n} \iint_{D \times D} \kappa_{\delta_n}(T_n(x) - T_n(y)) u_n(T_n(x)) (1 - u_n(T_n(y))) \rho(x) \rho(y) \, dx dy, \quad (4.1)$$

and, by the second condition in (3.6), there exists $C > 0$ such that

$$\begin{aligned} +\infty &> C \\ &> GF_{n,\delta_n}(u_n) \\ &= \frac{2}{\delta_n^{d+1}} \iint_{D \times D} \eta \left(\frac{|T_n(x) - T_n(y)|}{\delta_n} \right) u_n(T_n(x)) (1 - u_n(T_n(y))) \rho(x) \rho(y) \, dx dy \\ &\geq \frac{2a^2}{\delta_n^{d+1}} \iint_{D \times D} \eta_0 \left(\frac{|T_n(x) - T_n(y)|}{\delta_n} \right) u_n(T_n(x)) (1 - u_n(T_n(y))) \, dx dy \end{aligned}$$

where we have used, in sequence, the very definition of the rescaled kernel κ_δ , hypothesis (H3), and (3.5b).

Observe now that, by the definition of $\|\cdot\|_\infty$, for almost every $x, y \in D$ the following implication holds true

$$|T_n(x) - T_n(y)| > r_0 \delta_n \quad \Rightarrow \quad |x - y| > r_0 \delta_n - 2 \|\text{Id} - T_n\|_\infty, \quad (4.2)$$

where r_0 has been introduced in (3.5a). We define the quantity

$$\tilde{\delta}_n := \delta_n - 2r_0^{-1} \|\text{Id} - T_n\|_\infty \quad (4.3)$$

and notice that, by (2.10) and (3.4),

$$\lim_{n \rightarrow \infty} \frac{\tilde{\delta}_n}{\delta_n} = 1, \quad (4.4)$$

so that, in particular, for large enough n , we have that $\tilde{\delta}_n > 0$. Moreover, for almost every $x, y \in D$, (4.2) yields

$$\eta_0 \left(\frac{|x - y|}{\tilde{\delta}_n} \right) \leq \eta_0 \left(\frac{|T_n(x) - T_n(y)|}{\delta_n} \right). \quad (4.5)$$

By (4.4) and (4.5), we can continue with the chain of inequalities above and obtain that

$$+\infty > C > \frac{1}{\widetilde{\delta}_n^{d+1}} \iint_{D \times D} \eta_0 \left(\frac{|x-y|}{\widetilde{\delta}_n} \right) u_n(T_n(x))(1-u_n(T_n(y))) \, dx dy$$

for n large enough. Then by Theorem 3.1 in Ref. 25 $\{u_n \circ T_n\}_{n \in \mathbb{N}}$ is relatively compact in $L^1_\nu(D)$ so that by Remark 2.1, condition (2.9) is satisfied with $p = 1$. Therefore, by Proposition 2.2-5, we obtain that the pair $\{(\nu_n, u_n)\}_{n \in \mathbb{N}}$ is relatively compact in $TL^1(D)$. \square

In order to prove Theorem 3.1, we define the auxiliary functional $\mathcal{F}_\delta(\cdot; \rho): L^1(D) \rightarrow [0, +\infty]$ defined as

$$\mathcal{F}_\delta(u; \rho) := \begin{cases} \frac{2}{\delta} \iint_{D \times D} \kappa_\delta(x-y)(1-u(x))u(y)\rho(x)\rho(y) \, dx dy & \text{if } 0 \leq u \leq 1, \\ +\infty & \text{otherwise in } L^1(D). \end{cases} \quad (4.6)$$

To prove the following result, our inspiration comes from the proof strategy of the main result in Ref. 25, which, in turn, relies on the main result of Ref. 1. The idea in Ref. 25 was to notice that their functional $u \mapsto F_\varepsilon(u)$ (see Section 3 in Ref. 25) could be written, up to the change of variables $v = 2u - 1$, as the functional (see formula (1.1) in Ref. 1) $v \mapsto F_\varepsilon(v) =: \text{AB}_\varepsilon(v; J, W)$ for a suitable choice of the interaction kernel J and of the potential W .

Proposition 4.1. *The sequence $\{\mathcal{F}_\delta(\cdot; \rho)\}_{\delta > 0}$ Γ -converges with respect to the $L^1(D)$ metric to $\alpha_d \text{TV}(\cdot; \rho^2)$.*

Proof. Notice that, upon defining $v := 2u - 1 \in L^1(D)$, we have

$$\mathcal{F}_\delta(u; \rho) = \Phi_\delta(v; \kappa, \rho) + \Psi_\delta(v; \kappa, \rho) =: \widetilde{\text{AB}}_\delta(v; \kappa, \rho), \quad (4.7)$$

where $\Phi_\delta(\cdot; \kappa, \rho), \Psi_\delta(\cdot; \kappa, \rho): L^1(D) \rightarrow [0, +\infty]$ are defined by

$$\Phi_\delta(v; \kappa, \rho) := \begin{cases} \frac{1}{4\delta} \iint_{D \times D} \kappa_\delta(x-y)(v(x)-v(y))^2 \rho(x)\rho(y) \, dx dy & \text{if } -1 \leq v \leq 1, \\ +\infty & \text{otherwise,} \end{cases}$$

and

$$\Psi_\delta(v; \kappa, \rho) := \begin{cases} \frac{1}{2\delta} \iint_{D \times D} \kappa_\delta(x-y)(1-v^2(x))\rho(x)\rho(y) \, dx dy & \text{if } -1 \leq v \leq 1, \\ +\infty & \text{otherwise,} \end{cases}$$

respectively. Equality (4.7) is a matter of some algebraic computations (see the proof of Theorem 3.1 in Ref. 25).

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Step 1 – liminf inequality. For fixed κ and ρ , and $v \in L^1(D; [-1, 1])$, we consider the set functions $\widetilde{\text{AB}}_\delta(v; \kappa, \rho; \cdot)$, $\Phi_\delta(v; \kappa, \rho; \cdot)$, $\Psi_\delta(v; \kappa, \rho; \cdot): \mathcal{A}(D) \rightarrow [0, \infty] \rightarrow [0, +\infty)$ defined as

$$\widetilde{\text{AB}}_\delta(v; \kappa, \rho; A) := \Phi_\delta(v; \kappa, \rho; A) + \Psi_\delta(v; \kappa, \rho; A), \quad (4.8)$$

where

$$\begin{aligned} A \mapsto \Phi_\delta(v; \kappa, \rho; A) &= \frac{1}{4\delta} \iint_{A \times A} \kappa_\delta(x-y)(v(x) - v(y))^2 \rho(x)\rho(y) dx dy, \\ A \mapsto \Psi_\delta(v; \kappa, \rho; A) &= \frac{1}{2\delta} \iint_{A \times A} \kappa_\delta(x-y)(1 - v^2(x))\rho(x)\rho(y) dx dy. \end{aligned}$$

For given $\bar{x} \in D$ a point, $r > 0$ a sufficiently small radius, and $v: D \rightarrow \mathbb{R}$ a function, we define the r -rescaling of v at \bar{x} by

$$R_{\bar{x}, r}v(x) := v(\bar{x} + rx)$$

for all $x \in r^{-1}(D - \bar{x})$.

We start by proving that for every set $A \in \mathcal{A}(D)$, $r > 0$ small enough, and $\bar{x} \in D$ we have

$$\widetilde{\text{AB}}_\delta(v; \kappa, \rho; \bar{x} + rA) \geq r^{d-1}(\rho(\bar{x}) - cr)^2 \text{AB}_{\delta/r}(R_{\bar{x}, r}v; \kappa; A) \quad (4.9)$$

for some constant $c > 0$ only depending on the Lipschitz constant of ρ . In (4.9), the functional $\text{AB}_\varepsilon(w; \kappa; A)$ is the localization of the functional defined by

$$\text{AB}_\varepsilon(w; \kappa) := \frac{1}{4\varepsilon} \iint_{D \times D} \kappa_\varepsilon(x-y)(w(x) - w(y))^2 dx dy + \frac{\tau_d}{2\varepsilon} \int_D |1 - w^2(x)| dx,$$

which is a particular case of the functional F_ε in Ref. 1, with interaction kernel $J = \kappa$ and potential $W(s) = \tau_d|1 - s^2|/2$, where $\tau_d = \int_{\mathbb{R}^d} \kappa(z) dz$.

Indeed, by the changes of variables $x' = r^{-1}(x - \bar{x})$ and $y' = r^{-1}(y - \bar{x})$, we get

$$\begin{aligned} \Phi_\delta(v; \kappa, \rho; \bar{x} + rA) &= \frac{1}{4\delta} \iint_{(\bar{x} + rA) \times (\bar{x} + rA)} \kappa_\delta(x-y)(v(x) - v(y))^2 \rho(x)\rho(y) dx dy \\ &= \frac{r^{2d}}{4\delta} \iint_{A \times A} \kappa_\delta(r(x' - y'))(v(\bar{x} + rx') - v(\bar{x} + ry'))^2 \rho(\bar{x} + rx')\rho(\bar{x} + ry') dx' dy' \\ &= \frac{r^{d-1}}{4\delta/r} \iint_{A \times A} \kappa_{\delta/r}(x' - y')(v(\bar{x} + rx') - v(\bar{x} + ry'))^2 \rho(\bar{x} + rx')\rho(\bar{x} + ry') dx' dy' \\ &\geq r^{d-1}(\rho(\bar{x}) - cr)^2 \iint_{A \times A} \kappa_{\delta/r}(x' - y')(v(\bar{x} + rx') - v(\bar{x} + ry'))^2 dx' dy' \\ &= r^{d-1}(\rho(\bar{x}) - cr)^2 \Phi_{\delta/r}(R_{\bar{x}, r}v; \kappa, 1; A), \end{aligned}$$

where we have used the Lipschitz estimate (for $z' = x', y'$)

$$|\rho(\bar{x} + rz') - \rho(\bar{x})| \leq \text{Lip}(\rho)r|z'| \leq \text{Lip}(\rho) \max_{z \in D} |z| r =: cr.$$

Notice that $\rho(\bar{x}) - cr > 0$ for $r > 0$ small enough, owing to (H3). The same reasoning can be carried out for the functional Ψ_δ , so that (4.9) follows.

Let us now take functions $u, u_\delta \in L^1(D; \nu)$ such that $u_\delta \rightarrow u$. Without loss of generality, we can assume that

$$\liminf_{\delta \rightarrow 0} \mathcal{F}_\delta(u_\delta; \rho) < +\infty \quad (4.10)$$

(otherwise the Γ -liminf inequality is trivial). Then $u_\delta(x) \in [0, 1]$ for ν -a.e. $x \in D$, so that the corresponding $v_\delta = 2u_\delta - 1 \in [-1, 1]$ for ν -a.e. $x \in D$. By (4.7) and (H3), we can write

$$\mathcal{F}_\delta(u_\delta; \rho) = \widetilde{\text{AB}}_\delta(v_\delta; \kappa, \rho) \geq a^2 \text{AB}_\delta(v_\delta; \kappa)$$

Compactness for the functional $\text{AB}_\delta(\cdot; \kappa)$ with respect to the L^1 -convergence is proved in Theorem 3.1 in Ref. 1, so that we obtain that $v = 2u - 1 \in \text{BV}(D; \{-1, 1\})$, that is $u \in \text{BV}(D; \{0, 1\})$.

Let us now consider the energy densities associated with $\widetilde{\text{AB}}_\delta(v_\delta; \kappa, \rho; A)$ and (the localization) $\text{AB}_\delta(v_\delta; \kappa, W; A)$ given, for each $x \in A$, by

$$\begin{aligned} \tilde{g}_\delta(x) &:= \frac{1}{4\delta} \int_A \kappa_\delta(x-y) (v_\delta(x) - v_\delta(y))^2 \rho(x) \rho(y) \, dy \\ &\quad + \frac{1}{2\delta} \int_A \kappa_\delta(x-y) (1 - v_\delta^2(x)) \rho(x) \rho(y) \, dy, \end{aligned}$$

$$g_\delta(x) := \frac{1}{4\delta} \int_A \kappa_\delta(x-y) (v_\delta(x) - v_\delta(y))^2 \rho(x) \rho(y) \, dy + \frac{1}{\delta} W(v_\delta(x)),$$

and the corresponding energy distributions

$$\tilde{\lambda}_\delta := \tilde{g}_\delta \mathcal{L}^d \llcorner A \quad \text{and} \quad \lambda_\delta := g_\delta \mathcal{L}^d \llcorner A.$$

By (4.10), the total variation of $\tilde{\lambda}_\delta$ is bounded uniformly with respect to δ , so that, up to a (not relabeled) subsequence, $\tilde{\lambda}_\delta \xrightarrow{*} \tilde{\lambda}$, for a certain non-negative Radon measure $\tilde{\lambda}$.

We now take a point $\bar{x} \in S_u = S_v$ where $\nu := \nu_u(\bar{x}) = \nu_v(\bar{x})$ is well defined, and we compute the Radon–Nikodým derivative of $\tilde{\lambda}$ with respect to $\mathcal{H}^{d-1} \llcorner S_v$ at \bar{x} . Letting Q_ν be a unit cube with two faces perpendicular to ν , we have, owing to (4.9),

$$\begin{aligned} \frac{d\tilde{\lambda}}{d\mathcal{H}^{d-1} \llcorner S_v}(\bar{x}) &= \lim_{r \rightarrow 0} \frac{\tilde{\lambda}(\bar{x} + rQ_\nu)}{r^{d-1}} = \lim_{r \rightarrow 0} \lim_{\delta \rightarrow 0} \frac{\tilde{\lambda}_\delta(\bar{x} + rQ_\nu)}{r^{d-1}} \\ &= \lim_{r \rightarrow 0} \lim_{\delta \rightarrow 0} \frac{\widetilde{\text{AB}}_\delta(v_\delta; \kappa, \rho; \bar{x} + rQ_\nu)}{r^{d-1}} \\ &\geq \lim_{r \rightarrow 0} \lim_{\delta \rightarrow 0} (\rho(\bar{x}) - rc)^2 \text{AB}_{\delta/r}(R_{\bar{x}, r} v_\delta; \kappa; Q_\nu). \end{aligned} \quad (4.11)$$

Arguing as in the proof of Lemma 4.3 in Ref. 1, we can use a standard diagonalization argument and find two sequences $r_n \rightarrow 0$ and $\delta_n \rightarrow 0$ such that

$$\delta_n := \delta_n / r_n \rightarrow 0, \quad \frac{d\tilde{\lambda}}{d\mathcal{H}^{d-1} \llcorner S_v}(\bar{x}) = \lim_{n \rightarrow \infty} \frac{\tilde{\lambda}(\bar{x} + r_n Q_\nu)}{r_n^{d-1}},$$

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and, letting $v_{\delta_n} := R_{\bar{x}, r_n} v_{\delta_n}$,

$$\lim_{n \rightarrow \infty} v_{\delta_n} = v \quad \text{in } L^1(Q_\nu), \quad \text{where } v(x) = v_{\bar{x}}(x) := \begin{cases} +1 & \text{if } \langle x, \nu_u(\bar{x}) \rangle > 0, \\ -1 & \text{if } \langle x, \nu_u(\bar{x}) \rangle < 0. \end{cases}$$

so that we can continue in (4.11) with

$$\begin{aligned} \frac{d\tilde{\lambda}}{d\mathcal{H}^{d-1} \llcorner S_v}(\bar{x}) &= \lim_{n \rightarrow \infty} \frac{\tilde{\lambda}(\bar{x} + r_n Q_\nu)}{r_n^{d-1}} \geq \lim_{n \rightarrow \infty} (\rho(\bar{x}) - r_n c)^2 \text{AB}_{\delta_n}(v_{\delta_n}; \kappa; Q_\nu) \\ &= \rho^2(\bar{x}) \lim_{n \rightarrow \infty} \text{AB}_{\delta_n}(v_{\delta_n}; \kappa; Q_\nu) \geq \rho^2(\bar{x}) \alpha_d, \end{aligned}$$

where the last equality follows since AB_{δ_n} is bounded and $r_n \rightarrow 0$ and the last inequality is obtained as in Lemma 4.3 in Ref. 1, for our choice of W (see Theorem 3.1 in Ref. 25 for the details).

Step 2 – limsup inequality. By standard approximation results on sets of finite perimeter (see, e.g., Theorem 1.24 in Ref. 19), it is enough to prove the limsup inequality only for polyhedral functions $u \in \text{BV}(D; \{0, 1\})$, that is, functions whose jump set S_u is a polyhedral set, i.e., a set whose faces are the essential union of finitely many affine hyperplanes (see Definition 5.1 in Ref. 1 for the details).

As a matter of fact, the proof of Theorem 5.2 in Ref. 1 can be replicated in its entirety, so we will not report it here. Two crucial steps are the covering argument and the rescaling property, both of which need care, due to the presence of the weight ρ in the functional $\mathcal{F}_\delta(\cdot; \rho)$. In particular, the translation invariance of the set functional $\widetilde{\text{AB}}_\delta(v; \kappa, \rho; \cdot)$ defined in (4.8) is not available in our case (here, as before, $v = 2u - 1$).

In what follows, we show how to adapt the chain of inequalities (5.8) of Ref. 1 to our case. Owing to the Lipschitz property of ρ , estimate (4.9) can be reversed to obtain

$$\widetilde{\text{AB}}_\delta(w; \kappa, \rho; \bar{x} + \delta A) \leq \delta^{d-1} (\rho(\bar{x}) + \delta c)^2 \text{AB}_1(R_{\bar{x}, \delta} w; \kappa; A), \quad (4.12)$$

for any function w in the domain of the functional. Let now consider a polyhedral set $A \subset D$ as in the proof of Theorem 5.2 in Ref. 1 and let $v := 2\chi_A - 1$ and let $\{v_\delta\}_{\delta>0}$ be a sequence of Lipschitz functions such that

- (1) $v_\delta \rightarrow v$ in $L^1(D)$ as $\delta \rightarrow 0$;
- (2) $\sup_{\delta>0} \int_D |\nabla v_\delta(x)| dx < +\infty$;
- (3) $\text{AB}_1(R_{\bar{x}, \delta} v_\delta; \kappa; E) \rightarrow \alpha_d$ as $\delta \rightarrow 0$, for every open set $E \subset D$ and for almost every $\bar{x} \in S_v$.

Notice that conditions (1) and (2) hold true thanks to standard BV-approximation by Lipschitz functions, while (3) is yielded by the L^1 -continuity of AB_1 .

By covering A with finitely many rescaled cubes $\{\bar{x}_i + \delta C\}_{i=1}^{h(\delta)}$, and using the subadditivity of the integral and (4.12), we have

$$\begin{aligned}
 \widetilde{\text{AB}}_\delta(v_\delta; \kappa, \rho; A) &\leq \widetilde{\text{AB}}_\delta\left(v_\delta; \kappa, \rho; \bigcup_{i=1}^{h(\delta)} (\bar{x}_i + \delta C)\right) \leq \sum_{i=1}^{h(\delta)} \widetilde{\text{AB}}_\delta(v_\delta; \kappa, \rho; \bar{x}_i + \delta C) \\
 &\leq \sum_{i=1}^{h(\delta)} \delta^{d-1} (\rho(\bar{x}_i) + \delta c)^2 \text{AB}_1(R_{\bar{x}_i, \delta} v_\delta; \kappa; C) \\
 &= \alpha_d \int_{A \cap S_u} \rho^2(x) d\mathcal{H}^{d-1}(x) + o(1),
 \end{aligned} \tag{4.13}$$

so that inequality (5.6) in Ref. 1 becomes, in our case, by choosing the recovery sequence $u_\delta = (v_\delta + 1)/2$ for every $\delta > 0$,

$$\limsup_{\delta \rightarrow 0} \mathcal{F}_\delta(u_\delta; \rho) = \limsup_{\delta \rightarrow 0} \widetilde{\text{AB}}_\delta(v_\delta; \kappa, \rho; A) \leq \alpha_d \int_{A \cap S_u} \rho^2(x) d\mathcal{H}^{d-1}(x).$$

Notice that in (4.13) we have applied (3) with $E = C$, to obtain

$$\lim_{\delta \rightarrow 0} \text{AB}_1(R_{\bar{x}_i, \delta} v; \kappa; C) = \text{AB}_1(v_{\bar{x}_i}; \kappa; Q_\nu) = \alpha_d.$$

The proposition is proved. \square

Remark 4.1. We point out that, in the proof of the limsup inequality in Proposition 4.1 above, the Lipschitz regularity of the recovery sequence $\{v_\delta\}_{\delta > 0}$ has never been used. Indeed, one could take the constant recovery sequence $v_\delta = v$ for every $\delta > 0$. We decided to require Lipschitz regularity so that the very same sequence $\{v_\delta\}_{\delta > 0}$ introduced in this proof can be used in the proof of Theorem 3.1 below.

4.1. Proof of Theorem 3.1

In this section, we prove the convergence of GF_{n, δ_n} to $\alpha_d \text{TV}(\cdot; \rho^2)$ with respect to the TL^1 topology. If $u \in L^1_\nu(D)$ and $0 \leq u \leq 1$ then $GF_{n, \delta_n}(u)$ is given by (4.1). We divide the proof into two steps.

Step 1 – liminf inequality. Let $u \in L^1_\nu(D)$ and let $u_n \in L^1_{\nu_n}(D)$ be such that $(\nu_n, u_n) \xrightarrow{TL^1} (\nu, u)$ (without loss of generality, we can assume that $0 \leq u_n \leq 1$ for every $n \in \mathbb{N}$). By Remark 3.1(1), let us consider a kernel η_0 as in (3.5). Recall that for almost every $x, y \in D$ the implication in (4.2) holds true and, defining $\tilde{\delta}_n$ as in (4.3), we have that

$$GF_{n, \delta_n}(u_n) \geq \left(\frac{\tilde{\delta}_n}{\delta_n}\right)^{d+1} \mathcal{F}_{\delta_n}(\tilde{u}_n; \rho),$$

where $\tilde{u}_n = u_n \circ T_n$ and $\mathcal{F}_{\delta_n}(\cdot; \rho)$ is defined in (4.6). By (4.4) and Proposition 4.1, we obtain that $u \in \text{BV}(D; \{0, 1\})$ and

$$\liminf_{n \rightarrow \infty} GF_{n, \delta_n}(u_n) \geq \alpha_d \text{TV}(u; \rho^2).$$

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For general kernel η as in (H2), we can find a sequence $\{\eta^m\}_{m \in \mathbb{N}}$ such that each η^m is of the form

$$\eta^m = \sum_{i=1}^m \eta_0^i$$

for some η_0^i as in (3.5), for $i = 1, \dots, m$, and $\eta^m \uparrow \eta$. Set GF_{n,δ_n}^m and $GF_{n,\delta_n}^{0,i}$ to be the functional in (3.1) defined with kernels η^m and η_0^i , respectively (keep hypothesis (H2) into account), and $\alpha_d^{0,i}$ and α_d^m the constants in (3.7) relative to the kernels η_0^i and η^m , respectively (notice that $\alpha_d^m = \sum_{i=1}^m \alpha_d^{0,i}$). By the previous argument and the superadditivity of the \liminf , we can write

$$\begin{aligned} \liminf_{n \rightarrow \infty} GF_{n,\delta_n}(u_n) &\geq \liminf_{n \rightarrow \infty} GF_{n,\delta_n}^m(u_n) \\ &\geq \sum_{i=1}^m \liminf_{n \rightarrow \infty} GF_{n,\delta_n}^{0,i}(u_n) \\ &\geq \sum_{i=1}^m \alpha_d^{0,i} TV(u; \rho^2). \end{aligned}$$

By the monotone convergence theorem, we conclude that

$$\liminf_{n \rightarrow \infty} GF_{n,\delta_n}(u_n) \geq \lim_{m \rightarrow \infty} \sum_{i=1}^m \alpha_d^{0,i} TV(u; \rho^2) = \lim_{m \rightarrow \infty} \alpha_d^m TV(u; \rho^2) = \alpha_d TV(u; \rho^2).$$

Step 2 – limsup inequality. Observe that it is not restrictive to assume that $u \in \text{BV}(D; \rho)$ with $u(x) \in \{0, 1\}$ for ν -a.e. $x \in D$, and also that u is polyhedral. Let u_δ be the recovery sequence for \mathcal{F}_δ as in the proof of the limsup inequality in Proposition 4.1; in particular, the functions u_δ are Lipschitz for every $\delta > 0$, $\sup_{\delta > 0} \int_D |\nabla u_\delta(x)| dx < +\infty$, and

$$\limsup_{\delta \rightarrow 0} \mathcal{F}_\delta(u_\delta; \rho) \leq \alpha_d TV(u; \rho^2).$$

We are going to show that the sequence $u_n = u_{\delta_n} * \nu_n$ for all $n \in \mathbb{N}$ is a recovery sequence for u .

By Remark 3.1(1), let us consider a kernel η_0 as in (3.5). Define now

$$\tilde{\delta}_n := \delta_n + 2r_0^{-1} \|\text{Id} - T_n\|_\infty$$

and let $\tilde{u}_n := u_n \circ T_n$. Notice that, whereas (4.4) still holds true for this new definition of $\tilde{\delta}_n$, inequality (4.5) is reversed, so that we have that, for almost every $(x, y) \in D \times D$,

$$\eta_0\left(\frac{|x-y|}{\tilde{\delta}_n}\right) \geq \eta_0\left(\frac{|T_n(x) - T_n(y)|}{\delta_n}\right).$$

Then, for all $n \in \mathbb{N}$,

$$\begin{aligned} & \frac{1}{\tilde{\delta}_n^{d+1}} \iint_{D \times D} \eta_0 \left(\frac{|T_n(x) - T_n(y)|}{\delta_n} \right) \tilde{u}_n(x)(1 - \tilde{u}_n(y)) \, dx dy \\ & \leq \frac{1}{\tilde{\delta}_n^{d+1}} \iint_{D \times D} \eta_0 \left(\frac{|x - y|}{\tilde{\delta}_n} \right) \tilde{u}_n(x)(1 - \tilde{u}_n(y)) \, dx dy. \end{aligned} \quad (4.14)$$

Since for $x, y \in D$

$$\begin{aligned} & u_n(x)(1 - u_n(y)) - \tilde{u}_n(x)(1 - \tilde{u}_n(y)) \\ & = (u_n(x) - \tilde{u}_n(x))(1 - u_n(y)) + \tilde{u}_n(x)(\tilde{u}_n(y) - u_n(y)) \end{aligned}$$

and $0 \leq u_n \leq 1$, recalling (H3), we have

$$\begin{aligned} & \frac{1}{\tilde{\delta}_n} \left| \iint_{D \times D} \eta_0 \left(\frac{|x - y|}{\tilde{\delta}_n} \right) (u_n(x)(1 - u_n(y)) - \tilde{u}_n(x)(1 - \tilde{u}_n(y))) \rho(x)\rho(y) \, dx dy \right| \\ & \leq \frac{b^2}{\tilde{\delta}_n} \iint_{D \times D} \eta_0 \left(\frac{|x - y|}{\tilde{\delta}_n} \right) |(u_n(x) - \tilde{u}_n(x))(1 - u_n(y)) + \tilde{u}_n(x)(\tilde{u}_n(y) - u_n(y))| \, dx dy \\ & \leq \frac{2b^2}{\tilde{\delta}_n} \iint_{D \times D} \eta_0 \left(\frac{|x - y|}{\tilde{\delta}_n} \right) |u_n(x) - u_n(T_n(x))| \, dx dy \\ & \leq \frac{C}{\tilde{\delta}_n} \int_D |u_n(x) - u_n(T_n(x))| \, dx \leq \frac{C \|\text{Id} - T_n\|_\infty}{\tilde{\delta}_n} \int_D |\nabla u_{\delta_n}(x)| \, dx \rightarrow 0 \end{aligned}$$

owing to the boundedness of the last integral and to Remark 2.1. This implies, invoking (4.4) and inequality (4.14), that

$$\begin{aligned} & \limsup_{n \rightarrow \infty} GF_{n, \delta_n}(u_n) \\ & = \limsup_{n \rightarrow \infty} \frac{2}{\tilde{\delta}_n^{d+1}} \iint_{D \times D} \eta_0 \left(\frac{|T_n(x) - T_n(y)|}{\delta_n} \right) \tilde{u}_n(x)(1 - \tilde{u}_n(y)) \rho(x)\rho(y) \, dx dy \\ & \leq \limsup_{n \rightarrow \infty} \frac{2}{\tilde{\delta}_n^{d+1}} \iint_{D \times D} \eta_0 \left(\frac{|x - y|}{\tilde{\delta}_n} \right) \tilde{u}_n(x)(1 - \tilde{u}_n(y)) \rho(x)\rho(y) \, dx dy \\ & = \limsup_{n \rightarrow \infty} \frac{2}{\tilde{\delta}_n^{d+1}} \iint_{D \times D} \eta_0 \left(\frac{|x - y|}{\tilde{\delta}_n} \right) u_n(x)(1 - u_n(y)) \rho(x)\rho(y) \, dx dy \\ & = \limsup_{n \rightarrow \infty} \mathcal{F}_{\tilde{\delta}_n}^-(u_{\tilde{\delta}_n}; \rho) \leq \alpha_d TV(u; \rho^2). \end{aligned}$$

The case of general η satisfying (H2) can now be obtained by adapting the argument of Step 2 in the proof of Theorem 4.1 in Ref. 18, which concludes the proof of our theorem. \square

4.2. Proofs of Lemma 3.2 and Theorem 3.2

Proof. [Proof of Lemma 3.2] By (3.9), we have that $GF_{n, \delta_n}(\chi_{A_n})$ is uniformly bounded with respect to n , so that, by combining Lemma 3.1 and Proposition 2.2-5, there exists a set $A \in \mathcal{B}(D)$ with finite perimeter such that $\chi_{A_n} \rightarrow \chi_A$ in $L^1(D)$, obtaining the first convergence in (3.10).

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By compactness, there exists a function $\bar{\theta} \in L^\infty(D)$ such that $\chi_{O_n} \xrightarrow{*} \bar{\theta}$ in $L^\infty(D)$. We observe that $\bar{\theta} \in \mathcal{C}(A)$, where, for any $B \in \mathcal{B}(D)$, we define

$$\mathcal{C}(B) := \left\{ \theta \in L^1(D) : 0 \leq \theta \leq 1, \int_D \theta \, dx = 1, \int_B \theta \, dx = 0 \right\}.$$

Since, for every $\tilde{O} \in \mathcal{B}(D)$ such that $\chi_{\tilde{O}} \in \mathcal{C}(A_n)$, by (3.9) we have that

$$W_p(A_n, O_n) \leq W_p(A_n, \tilde{O}) + \frac{1}{n},$$

letting $n \rightarrow \infty$, we obtain that

$$W_p(A, \bar{\theta}) \leq W_p(A, \tilde{O}) \quad \text{for every } \tilde{O} \in \mathcal{B}(D) \text{ such that } \chi_{\tilde{O}} \in \mathcal{C}(A).$$

By a relaxation argument, we deduce that

$$W_p(A, \bar{\theta}) \leq W_p(A, \theta) \quad \text{for every } \theta \in \mathcal{C}(A),$$

so that $\bar{\theta}$ solves the minimization problem

$$\min \{ W_p(A, \theta) : \theta \in \mathcal{C}(A) \} \tag{4.15}$$

By Theorem 3.10 in Ref. 11, the solution $\bar{\theta}$ to problem (4.15) is the characteristic function, $\bar{\theta} = \chi_O$, of a certain set $O \in \mathcal{B}(D)$. The second convergence in (3.10) follows and the proof is concluded. \square

We now give the proof of Theorem 3.2.

Proof. [Proof of Theorem 3.2]

We start by observing that the term $(A, O) \mapsto W_p(A, O)$ is a continuous perturbation of GF_{n, δ_n} with respect to the topology in which we compute the Γ -limit, so that it will only be necessary to prove that

$$\left(\Gamma(L^1(D)) - \lim_{n \rightarrow \infty} GF_{n, \delta_n} \right) (\cdot) = \frac{\alpha_d}{|D|^2} \text{Per}(\cdot; D).$$

The liminf inequality is a direct consequence of Theorem 3.1. We now prove the limsup inequality. The limsup inequality follows from a standard approximation result once we prove it for a polyhedral set $A \subset D$. By Remark 4.1 and Theorem 3.1, the constant sequence is a recovery sequence for A . \square

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