

# Small Volume Fraction Limit of the Diblock Copolymer Problem: I. Sharp Interface Functional

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## Abstract

We present the first of two articles on the small volume fraction limit of a nonlocal Cahn-Hilliard functional introduced to model microphase separation of diblock copolymers. Here we focus attention on the sharp-interface version of the functional and consider a limit in which the volume fraction tends to zero but the number of minority phases (called *particles*) remains  $O(1)$ . Using the language of  $\Gamma$ -convergence, we focus on two levels of this convergence, and derive first and second order *effective* energies, whose energy landscapes are simpler and more transparent. These limiting energies are only finite on weighted sums of delta functions, corresponding to the concentration of mass into ‘point particles’. At the highest level, the effective energy is entirely local and contains information about the structure of each particle but no information about their spatial distribution. At the next level we encounter a Coulomb-like interaction between the particles, which is responsible for the pattern formation. We present the results here in both three and two dimensions.

**Key words.** Nonlocal Cahn-Hilliard problem, Gamma-convergence, small volume-fraction limit, diblock copolymers.

**AMS subject classifications.** 49S05, 35K30, 35K55, 74N15

## 1 Introduction

This paper and its companion paper [13] are concerned with asymptotic properties of two energy functionals. In either case, the order parameter  $u$  is defined on the flat torus  $\mathbf{T}^n = \mathbf{R}^n/\mathbf{Z}^n$ , i.e. the square  $[-\frac{1}{2}, \frac{1}{2}]^n$  with periodic boundary conditions, and has two preferred states  $u = 0$  and  $u = 1$ . We will be concerned with both  $n = 2$  and  $n = 3$ . The nonlocal Cahn-Hilliard functional is defined on  $H^1(\mathbf{R}^n)$  and is given by

$$\mathcal{E}^\varepsilon(u) := \varepsilon \int_{\mathbf{T}^n} |\nabla u|^2 dx + \frac{1}{\varepsilon} \int_{\mathbf{T}^n} u^2(1-u^2) dx + \sigma \|u - f u\|_{H^{-1}(\mathbf{T}^n)}^2. \quad (1.1)$$

Its sharp interface limit (in the sense of  $\Gamma$ -convergence), defined on  $BV(\mathbf{T}^n; \{0, 1\})$  (characteristic functions of finite perimeter), is given by [29]

$$\mathcal{E}(u) := \int_{\mathbf{T}^n} |\nabla u| + \gamma \|u - f u\|_{H^{-1}(\mathbf{T}^n)}^2. \quad (1.2)$$

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In both cases we wish to explore the behavior of these functionals, including the structure of their minimizers, in the limit of small volume fraction  $\int_{\mathbf{T}^n} u$ . The present article addresses the sharp interface functional (1.2); the diffuse-interface functional  $\mathcal{E}^\varepsilon$  is treated in the companion article [13].

## 1.1 The diblock copolymer problem

The minimization of these nonlocal perturbations of standard perimeter problems are natural model problems for pattern formation induced by competing short and long-range interactions [35]. However, these energies have been introduced to the mathematics literature because of their connection to a model for microphase separation of diblock copolymers [6].

A diblock copolymer is a linear-chain molecule consisting of two sub-chains joined covalently to each other. One of the sub-chains is made of  $N_A$  monomers of type A and the other consists of  $N_B$  monomers of type B. Below a critical temperature, even a weak repulsion between unlike monomers A and B induces a strong repulsion between the sub-chains, causing the sub-chains to segregate. A macroscopic segregation where the sub-chains detach from one another cannot occur because the chains are chemically bonded. Rather, a phase separation on a mesoscopic scale with A and B-rich domains emerges. Depending on the material properties of the diblock macromolecules, the observed mesoscopic domains are highly regular periodic structures including lamellae, spheres, cylindrical tubes, and double-gyroids (see for example [6]).

The functional is a rescaled version of a functional (1.1) introduced by Ohta and Kawasaki [25] (see also [24]) to model microphase separation of diblock copolymers. first proposed by Ohta and Kawasaki [25]. The long-range interaction term is associated with the connectivity of the sub-chains in the diblock copolymer macromolecule:<sup>1</sup> Often this energy is minimized under a mass or volume constraint

$$\int_{\mathbf{T}^n} u = M. \quad (1.3)$$

Here  $u$  represents the relative monomer density, with  $u = 0$  corresponding to a pure-A region and  $u = 1$  to a pure-B region; the interpretation of  $M$  is therefore the relative abundance of the A-parts of the molecules, or equivalently the volume fraction of the A-region. The constraint (1.3) of fixed average  $M$  reflects that in an experiment the composition of the molecules is part of the preparation and does not change during the course of the experiment. In (1.1) the incentive for pattern formation is clear: the first term penalizes oscillation, the second term favors separation into regions of  $u = 0$  and  $u = 1$ , and the third favors rapid oscillation. Under the mass constraint (1.3) the three can not vanish simultaneously, and the net effect is to set a fine scale structure depending on  $\varepsilon, \sigma$  and  $M$ .

## 1.2 Small volume fraction regime of the diblock copolymer problem

The precise geometry of the phase distributions (i.e. the information contained in a minimizer of (1.1)) depends largely on the volume fraction  $M$ . In fact, as explained in [12], the two natural parameters controlling the phase diagram are  $\varepsilon^{3/2}\sqrt{\sigma}$  and  $M$ . When  $\varepsilon^{3/2}\sqrt{\sigma}$  is small and  $M$  is close to 0 or 1, numerical experiments [12] and experimental observations [6] reveal

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<sup>1</sup>See [14] for a derivation and the relationship to the physical material parameters and basic models for inhomogeneous polymers. Usually the wells are taken to be  $\pm 1$  representing pure phases of A and B-rich regions. For convenience, we have rescaled to wells at 0 and 1.

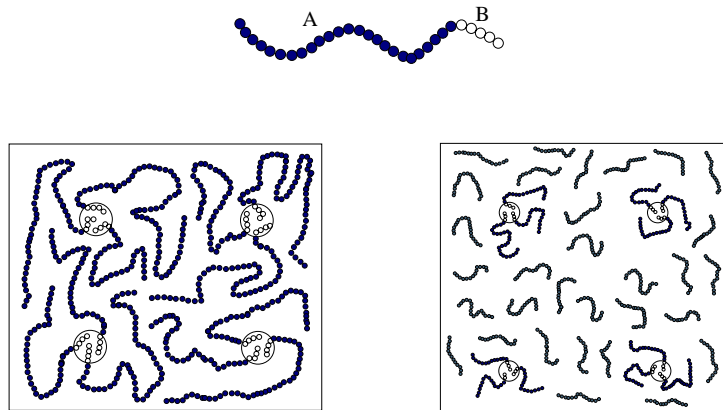


Figure 1: Top: an AB diblock copolymer macromolecule of minority A composition. Bottom: 2D schematic of two possible physical scenarios for the regime considered in this article. Left: microphase separation of *very long* diblock copolymers with minority A composition. Right: phase separation in a mixture/blend of diblock copolymers and homopolymers of another monomer species having relatively weak interactions with the A and B monomers.

structures resembling *small well-separated spherical regions of the minority phase*. We often refer to such small regions as *particles*, and they are the central objects of study of this paper.

Since we are interested in a regime of small volume fraction, it seems natural to seek asymptotic results. It is the purpose of this article and its companion article [13] to give a rigorous asymptotic description of the energy in a limit wherein the volume fraction tends to zero but where the number of particles in a minimizer remains  $O(1)$ . That is, we examine the limit where minimizers converge to weighted Dirac delta point measures and seek effective energetic descriptions for their positioning and local structure. Physically, our regime corresponds to diblock copolymers of very small molecular weight (ratio of  $B$  monomers to  $A$ ), and we envisage either a melt of such diblock copolymers (*cf.* Figure 1, bottom left) or a mixture/blend<sup>2</sup> of diblocks with homopolymers of type  $A$  (*cf.* Figure 1, bottom right).

This regime is captured by the introduction of a small parameter  $\eta$  and the appropriate rescaling of the free energy. To this end, we fix a mass parameter  $M$  reflecting the total amount of minority phase mass in the limit of delta measures. We introduce a small coefficient to  $M$ , and consider phase distributions  $u$  such that

$$\int_{\mathbf{T}^n} u = \eta^n M, \quad (1.4)$$

where  $n$  is either 2 or 3. We rescale  $u$  as follows:

$$v := \frac{u}{\eta^n}, \quad (1.5)$$

so that the new preferred values of  $v$  are 0 and  $1/\eta^n$ . We now write our free energy (either (1.1) or (1.2)) in terms of  $v$  and rescale in  $\eta$  so that the minimum of the free energy remains  $O(1)$  as  $\eta \rightarrow 0$ . In this article, we focus our attention on the sharp interface functional (1.2): that is, we assume that we have already passed to the limit as  $\varepsilon \rightarrow 0$ , and therefore consider the small-volume-fraction asymptotics of (1.2). In [13] we will show how to extend the results

<sup>2</sup>A similar nonlocal Cahn-Hilliard-like functional models a blend of diblocks and homopolymers [15].

of this paper to the diffuse-interface functional (1.1), via a diagonal argument with a suitable slaving of  $\varepsilon$  to  $\eta$ .

In Section 3, we consider a collection of small particles, determine the scaling of the  $H^{-1}$ -norm, and choose an appropriate scaling of  $\gamma$  in terms of  $\eta$  so as to capture a nontrivial limit as  $\eta$  tends to 0. This analysis yields

$$\mathcal{E}(u) = \begin{cases} \eta E_\eta^{2d}(v) & \text{if } n = 2 \\ \eta^2 E_\eta^{3d}(v) & \text{if } n = 3, \end{cases}$$

where

$$E_\eta^{2d}(v) := \eta \int_{\mathbf{T}^2} |\nabla v| + |\log \eta|^{-1} \|v - \bar{v}\|_{H^{-1}(\mathbf{T}^2)}^2 \quad \text{defined for } v \in BV(\mathbf{T}^2; \{0, 1/\eta^2\}) \quad (1.6)$$

and

$$E_\eta^{3d}(v) := \eta \int_{\mathbf{T}^3} |\nabla v| + \eta \|v - \bar{v}\|_{H^{-1}(\mathbf{T}^3)}^2 \quad \text{defined for } v \in BV(\mathbf{T}^3; \{0, 1/\eta^3\}). \quad (1.7)$$

In both cases,  $E_\eta^{2d}(v), E_\eta^{3d}(v)$  remain  $O(1)$  as  $\eta \rightarrow 0$ .

The aim of this paper is to describe the behavior of these two energies in the limit  $\eta \rightarrow 0$ . This will be done in terms of a  $\Gamma$ -*asymptotic expansion* [5] for  $E_\eta^{2d}(v)$  and  $E_\eta^{3d}(v)$ . That is, we characterize the first and second term in the expansion of, for example,  $E_\eta^{3d}$  of the form

$$E_\eta^{3d} = E_0^{3d} + \eta F_0^{3d} + \text{higher order terms.}$$

Our main results characterize these first- and second-order functionals  $E_0^{2d}, F_0^{2d}$  (respectively  $E_0^{3d}, F_0^{3d}$ ) and show that:

- At the highest level, the *effective energy* is entirely local, i.e., the energy *focuses separately* on the energy of each particle, and is blind to the spatial distribution of the particles. The effective energy contains information about the local structure of the small particles. This is presented in three and two dimensions by Theorems 4.3 and 6.1 respectively.
- At the next level, we see a Coulomb-like interaction between the particles. It is this latter part of the energy which we expect enforces a periodic array of particles.<sup>3</sup> This is presented in three and two dimensions by Theorems 4.5 and 6.4 respectively.

The paper is organized as follows. Section 2 contains some basic definitions. In Section 3 we introduce the small parameter  $\eta$ , and begin with an analysis of the small- $\eta$  behavior of the  $H^{-1}$  norm via the basic properties of the fundamental solution of the Laplacian in three and two dimensions. We then determine the correct rescalings in dimensions two and three, and arrive at (1.6) and (1.7). In Section 4 we state the  $\Gamma$ -convergence results in three dimensions, together with some properties of the  $\Gamma$ -limits. The proofs of the three-dimensional results are given in Section 5. In Section 6 we state the analogous results in two dimensions and describe the modifications in the proofs. We conclude the paper with a discussion of our results in Section 7.

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<sup>3</sup>Proving this is a non-trivial matter; see Section 7

## 2 Some definitions and notation

Throughout this article, we use  $\mathbf{T}^n = \mathbf{R}^n/\mathbf{Z}^n$  to denote the  $n$ -dimensional flat torus of unit volume. For the use of convolution we note that  $\mathbf{T}^n$  is an additive group, with neutral element  $0 \in \mathbf{T}^n$  (the ‘origin’ of  $\mathbf{T}^n$ ). For  $v \in BV(\mathbf{T}^n; \{0, 1\})$  we denote by

$$\int_{\mathbf{T}^n} |\nabla v|$$

the total variation measure evaluated on  $\mathbf{T}^n$ , i.e.  $\|\nabla v\|(\mathbf{T}^n)$  [4]. Since  $v$  is the characteristic function of some set  $A$ , it is simply a notion of its perimeter. Let  $X$  denote the space of Radon measures on  $\mathbf{T}^n$ . For  $\mu_\eta, \mu \in X$ ,  $\mu_\eta \rightharpoonup \mu$  denotes weak- $*$  measure convergence, i.e.

$$\int_{\mathbf{T}^n} f d\mu_\eta \rightarrow \int_{\mathbf{T}^n} f d\mu$$

for all  $f \in C(\mathbf{T}^n)$ . We use the same notation for functions, i.e. when writing  $v_\eta \rightharpoonup v_0$ , we interpret  $v_\eta$  and  $v_0$  as measures whenever necessary.

We introduce the Green’s function  $G_{\mathbf{T}^n}$  for  $-\Delta$  in dimension  $n$  on  $\mathbf{T}^n$ . It is the solution of

$$-\Delta G_{\mathbf{T}^n} = \delta - 1, \quad \text{with} \quad \int_{\mathbf{T}^n} G_{\mathbf{T}^n} = 0,$$

where  $\delta$  is the Dirac delta function at the origin. In two dimensions, the Green’s function  $G_{\mathbf{T}^2}$  satisfies

$$G_{\mathbf{T}^2}(x) = -\frac{1}{2\pi} \log|x| + g^{(2)}(x) \tag{2.1}$$

for all  $x = (x_1, x_2) \in \mathbf{R}^2$  with  $\max\{|x_1|, |x_2|\} \leq 1/2$ , where the function  $g^{(2)}$  is continuous on  $[-1/2, 1/2]^2$  and  $C^\infty$  in a neighborhood of the origin. In three dimensions, we have

$$G_{\mathbf{T}^3}(x) = \frac{1}{4\pi|x|} + g^{(3)}(x) \tag{2.2}$$

for all  $x = (x_1, x_2, x_3) \in \mathbf{R}^3$  with  $\max\{|x_1|, |x_2|, |x_3|\} \leq 1/2$ , where the function  $g^{(3)}$  is again continuous on  $[-1/2, 1/2]^3$  and smooth in a neighbourhood of the origin.

For  $\mu \in X$  such that  $\mu(\mathbf{T}^n) = 0$ , we may solve

$$-\Delta v = \mu,$$

in the sense of distributions on  $\mathbf{T}^n$ . If  $v \in H^1(\mathbf{T}^n)$ , then  $\mu \in H^{-1}(\mathbf{T}^n)$ , and

$$\|\mu\|_{H^{-1}(\mathbf{T}^n)}^2 := \int_{\mathbf{T}^n} |\nabla v|^2 dx.$$

In particular, if  $u \in L^2(\mathbf{T}^n)$  then  $(u - f u) \in H^{-1}(\mathbf{T}^n)$  and

$$\|u - f u\|_{H^{-1}(\mathbf{T}^n)}^2 = \int_{\mathbf{T}^n} \int_{\mathbf{T}^n} u(x)u(y) G_{\mathbf{T}^n}(x - y) dx dy.$$

Note that on the right-hand side we may write the function  $u$  rather than its zero-average version  $u - f u$ , since the function  $G_{\mathbf{T}^n}$  itself is chosen to have zero average.

We will also need an expression for the  $H^{-1}$  norm of the characteristic function of a set of finite perimeter on all of  $\mathbf{R}^3$ . To this end, let  $f$  be such a function and define

$$\|f\|_{H^{-1}(\mathbf{R}^3)}^2 = \int_{\mathbf{R}^3} |\nabla v|^2 dx,$$

where  $-\Delta v = f$  on  $\mathbf{R}^3$  with  $|v| \rightarrow 0$  as  $|x| \rightarrow \infty$ .

### 3 The small parameter $\eta$ , degeneration of the $H^{-1}$ -norm, and the rescaling of (1.2)

We introduce a new parameter  $\eta$  controlling the vanishing volume. That is, we consider the total mass to be  $\eta^n M$ , for some fixed  $M$ , and rescale as

$$v_\eta = \frac{u}{\eta^n}.$$

This will facilitate the convergence to Dirac delta measures of total mass  $M$  and will lead to functionals defined over functions  $v_\eta : \mathbf{T}^n \rightarrow \{0, 1/\eta^n\}$ . Note that this transforms the characteristic function  $u$  of mass  $\eta^n M$  to a function  $v_\eta$  with mass  $M$ , i.e.,

$$\int_{\mathbf{T}^n} u = \eta^n M \quad \text{while} \quad \int_{\mathbf{T}^n} v_\eta = M.$$

On the other hand, throughout our analysis with functions taking on two values  $\{0, 1/\eta^n\}$ , we will often need to rescale back to characteristic functions in a way such that *the mass is conserved*. To this end, let us fix some notation which we will use throughout the sequel. Consider a collection  $v_\eta : \mathbf{T}^n \rightarrow \{0, 1/\eta^n\}$  of components of the form

$$v_\eta = \sum_i v_\eta^i, \quad v_\eta^i = \frac{1}{\eta^n} \chi_{A_i}, \quad (3.1)$$

where the  $A_i$  are disjoint, connected subsets of  $\mathbf{T}^n$ . Moreover, we will always be able to assume<sup>4</sup> without loss of generality that the  $A_i$  have a diameter<sup>5</sup> less than  $1/2$ . Thus by associating the torus  $\mathbf{T}^n$  with  $[-1/2, 1/2]^n$ , we may assume that the  $A_i$  do not intersect the boundary  $\partial[-1/2, 1/2]^n$  and hence we may trivially extend  $v_\eta^i$  to  $\mathbf{R}^n$  by defining it to be zero for  $x \notin A_i$ . In this extension the total variation of  $v_\eta^i$  calculated on the torus is preserved when calculated over all of  $\mathbf{R}^n$ . We may then transform the components  $v_\eta^i$  to functions  $z_\eta^i : \mathbf{R}^n \rightarrow \mathbf{R}$  by a mass-conservative rescaling that maps their amplitude to 1, i.e., set

$$z_\eta^i(x) := \eta^n v_\eta^i(\eta x). \quad (3.2)$$

We first consider the case  $n = 3$ . Consider a sequence of functions  $v_\eta$  of the form (3.1). The norm  $\|v_\eta - f v_\eta\|_{H^{-1}}^2$  can be split up as

$$\begin{aligned} \|v_\eta - f v_\eta\|_{H^{-1}(\mathbf{T}^3)}^2 &= \sum_{i=1}^{\infty} \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) G_{\mathbf{T}^3}(x-y) dx dy \\ &\quad + \sum_{\substack{i,j=1 \\ i \neq j}}^{\infty} \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^j(y) G_{\mathbf{T}^3}(x-y) dx dy. \end{aligned} \quad (3.3)$$

<sup>4</sup>We will show in the course of the proofs that this basic *Ansatz* of separated connected sets of small diameter is in fact generic for a sequence of bounded mass and energy (cf. Lemma 5.2).

<sup>5</sup>For the definition of *diameter*, we first note that the torus  $\mathbf{T}^n$  has an induced metric

$$d(x, y) := \min\{|x - y - k| : k \in \mathbf{Z}^n\} \quad \text{for } x, y \in \mathbf{T}^n.$$

The diameter of a set is then defined in the usual way,

$$\text{diam } A := \sup\{d(x, y) : x, y \in A\}.$$

As we shall see (*cf.* the proof of Theorem 4.3), in the limit  $\eta \rightarrow 0$  it is the first sum, containing the diagonal terms, that dominates. For these terms we have

$$\begin{aligned}
\|v_\eta^i - f v_\eta^i\|_{H^{-1}(\mathbf{T}^3)}^2 &= \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) G_{\mathbf{T}^3}(x-y) dx dy \\
&= \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) \frac{1}{4\pi} |x-y|^{-1} dx dy + \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy \\
&= \eta^{-6} \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} z_\eta^i(x/\eta) z_\eta^i(y/\eta) \frac{1}{4\pi} |x-y|^{-1} dx dy + \\
&\quad + \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy \\
&= \eta^{-1} \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} z_\eta^i(\xi) z_\eta^i(\zeta) \frac{1}{4\pi} |\xi-\zeta|^{-1} d\xi d\zeta + \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy \\
&= \eta^{-1} \|z_\eta^i\|_{H^{-1}(\mathbf{R}^3)}^2 + \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy. \tag{3.4}
\end{aligned}$$

This calculation shows that if the transformed components  $z_\eta^i$  converge in a ‘reasonable’ sense, then the dominant behavior of the  $H^{-1}$ -norm of the original sequence  $v$  is given by the term

$$\frac{1}{\eta} \sum_i \|z_\eta^i\|_{H^{-1}(\mathbf{R}^3)}^2 = O\left(\frac{1}{\eta}\right).$$

This argument shows how in the leading-order term only information about the local behavior of each of the separate components enters. The position information is lost, at this level; we will recover this in the study of the next level of approximation.

Turning to the energy, we calculate

$$\begin{aligned}
\mathcal{E}(u) &= \int_{\mathbf{T}^3} |\nabla u| + \gamma \|u - f u\|_{H^{-1}(\mathbf{T}^3)}^2 \\
&= \eta^3 \int_{\mathbf{T}^3} |\nabla v| + \gamma \eta^6 \|v - f v\|_{H^{-1}(\mathbf{T}^3)}^2 \\
&= \eta^2 \left( \eta \int_{\mathbf{T}^3} |\nabla v| + \gamma \eta^4 \|v - f v\|_{H^{-1}(\mathbf{T}^3)}^2 \right). \tag{3.5}
\end{aligned}$$

Note that if  $v_\eta$  consists of  $N = O(1)$  particles of typical size  $O(\eta)$ , then

$$\eta \int_{\mathbf{T}^3} |\nabla v| \sim O(1).$$

Prompted by (3.4), we expect to make both terms in (3.5) of the same order by setting

$$\gamma = \frac{1}{\eta^3}.$$

Therefore we define

$$\mathbb{E}_\eta^{3d}(v) := \frac{1}{\eta^2} \mathcal{E}(u) = \begin{cases} \eta \int_{\mathbf{T}^3} |\nabla v| + \eta \|v - f v\|_{H^{-1}(\mathbf{T}^3)}^2 & \text{if } v \in BV(\mathbf{T}^3; \{0, 1/\eta^3\}) \\ \infty & \text{otherwise.} \end{cases}$$

We now switch to the case  $n = 2$ . Here the critical scaling of the  $H^{-1}$  in two dimensions causes a different behavior:

$$\begin{aligned}
& \int_{\mathbf{T}^2} \int_{\mathbf{T}^2} v_\eta^i(x) v_\eta^i(y) G_{\mathbf{T}^2}(x-y) dx dy = \\
&= -\frac{1}{2\pi} \int_{\mathbf{T}^2} \int_{\mathbf{T}^2} v_\eta^i(x) v_\eta^i(y) \log|x-y| dx dy + \int_{\mathbf{T}^2} \int_{\mathbf{T}^2} v_\eta^i(x) v_\eta^i(y) g^{(2)}(x-y) dx dy \\
&= -\frac{1}{2\pi} \int_{\mathbf{R}^2} \int_{\mathbf{R}^2} z_\eta^i(x) z_\eta^i(y) \log|\eta(x-y)| dx dy + \int_{\mathbf{T}^2} \int_{\mathbf{T}^2} v_\eta^i(x) v_\eta^i(y) g^{(2)}(x-y) dx dy \\
&= -\frac{1}{2\pi} \left( \int_{\mathbf{R}^2} z_\eta^i \right)^2 \log \eta - \frac{1}{2\pi} \int_{\mathbf{R}^2} \int_{\mathbf{R}^2} z_\eta^i(x) z_\eta^i(y) \log|x-y| dx dy \\
&\quad + \int_{\mathbf{T}^2} \int_{\mathbf{T}^2} v_\eta^i(x) v_\eta^i(y) g^{(2)}(x-y) dx dy \\
&= \frac{1}{2\pi} \left( \int_{\mathbf{R}^2} z_\eta^i \right)^2 |\log \eta| - \frac{1}{2\pi} \int_{\mathbf{R}^2} \int_{\mathbf{R}^2} z_\eta^i(x) z_\eta^i(y) \log|x-y| dx dy \\
&\quad + \int_{\mathbf{T}^2} \int_{\mathbf{T}^2} v_\eta^i(x) v_\eta^i(y) g^{(2)}(x-y) dx dy. \tag{3.6}
\end{aligned}$$

By this calculation we expect that the dominant behavior of the  $H^{-1}$ -norm of the original sequence  $v$  is given by the term

$$\sum_i \frac{1}{2\pi} \left( \int_{\mathbf{R}^2} z_\eta^i \right)^2 |\log \eta| = \frac{|\log \eta|}{2\pi} \sum_i \left( \int_{\mathbf{T}^2} v_\eta^i \right)^2. \tag{3.7}$$

Note how, in contrast to the three-dimensional case, only the distribution of the mass of  $v$  over the different components enters in the limit behavior. Note also that the critical scaling here is  $|\log \eta|$ .

Following the same line as for the three-dimensional case, and setting

$$v = \frac{u}{\eta^2}, \tag{3.8}$$

we calculate

$$\begin{aligned}
\mathcal{E}(u) &= \int_{\mathbf{T}^2} |\nabla u| + \gamma \|u - f u\|_{H^{-1}(\mathbf{T}^2)}^2 \\
&= \eta^2 \int_{\mathbf{T}^2} |\nabla v| + \gamma \eta^4 \|v - f v\|_{H^{-1}(\mathbf{T}^2)}^2 \\
&= \eta \left( \eta \int_{\mathbf{T}^2} |\nabla v| + \gamma \eta^3 \|v - f v\|_{H^{-1}(\mathbf{T}^2)}^2 \right).
\end{aligned}$$

Following (3.6), (3.7), in order to capture a nontrivial limit we must choose

$$\gamma = \frac{1}{|\log \eta| \eta^3}.$$

With this choice of  $\gamma$ , we define

$$\mathbf{E}_\eta^{2d}(v) := \frac{1}{\eta} \mathcal{E}(u) = \begin{cases} \eta \int_{\mathbf{T}^2} |\nabla v| + |\log \eta|^{-1} \|v - f v\|_{H^{-1}(\mathbf{T}^2)}^2 & \text{if } v \in BV(\mathbf{T}^2; \{0, 1/\eta^2\}) \\ \infty & \text{otherwise.} \end{cases}$$



## 4 Statement of the main results in three dimensions

We now state precisely the  $\Gamma$ -convergence results for  $E_\eta^{3d}$  in three dimensions. Both our  $\Gamma$ -limits will be defined over countable sums of weighted Dirac delta measures  $\sum_{i=1}^\infty m^i \delta_{x^i}$ . We start with the first-order limit. To this end, let us introduce the function

$$e_0^{3d}(m) := \inf \left\{ \int_{\mathbf{R}^3} |\nabla z| + \|z\|_{H^{-1}(\mathbf{R}^3)}^2 : z \in BV(\mathbf{R}^3; \{0, 1\}), \int_{\mathbf{R}^3} z = m \right\}. \quad (4.1)$$

We also define the limit functional<sup>6</sup>

$$E_0^{3d}(v) := \begin{cases} \sum_{i=1}^\infty e_0^{3d}(m^i) & \text{if } v = \sum_{i=1}^\infty m^i \delta_{x^i}, \{x^i\} \text{ distinct, and } m^i \geq 0 \\ \infty & \text{otherwise.} \end{cases}$$

**Remark 4.1.** Under weak convergence multiple point masses may join to form a single point mass. The functional  $E_0^{3d}$  is lower-semicontinuous under such a change if and only if the function  $e_0^{3d}$  satisfies the related inequality

$$e_0^{3d}\left(\sum_{i=1}^\infty m^i\right) \leq \sum_{i=1}^\infty e_0^{3d}(m^i). \quad (4.2)$$

The function  $e_0^{3d}$  does satisfy this property, as can be recognized by taking approximating functions  $z^i$  with bounded support, and translating them far from each other; the sum  $\sum_i z^i$  is admissible and its limiting energy, in the limit of large separation, is the sum of the individual energies.

**Remark 4.2.** The minimization problem of  $e_0^{3d}$  need not have a solution: if the mass  $m$  is too large, we expect that for any minimizing sequence the mass will divide into small particles that spread out over  $\mathbf{R}^3$  — but we have no proof yet for this statement. Also the exact structure of mass-constrained minimizers of  $E_0^{3d}$ , when they *do* exist, is a subtle question. We briefly discuss these issues in the last section.

Having introduced the limit functional  $E_0^{3d}$ , we are now in a position to state the first main result of this paper.

**Theorem 4.3.** *Within the space  $X$ , we have*

$$E_\eta^{3d} \xrightarrow{\Gamma} E_0^{3d} \quad \text{as } \eta \rightarrow 0.$$

*That is,*

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<sup>6</sup>The definition of  $E_0^{3d}$  requires the point mass positions  $x^i$  to be distinct, and the reader might wonder why this is necessary. Consider the following functional, which might be seen as an alternative,

$$\widetilde{E}_0^{3d}(v) := \begin{cases} \sum_{i=1}^\infty e_0^{3d}(m^i) & \text{if } v = \sum_{i=1}^\infty m^i \delta_{x^i} \text{ with } m^i \geq 0, \\ \infty & \text{otherwise.} \end{cases}$$

This functional is actually not well defined: the function  $v$  will have many representations (of the type  $\delta = a\delta + (1-a)\delta$ , for any  $a \in (0, 1)$ ) that will not give rise to the same value of the functional. Therefore the functional  $\widetilde{E}_0^{3d}$  is a functional of the representation, not of the limit measure  $v$ . The restriction to distinct  $x^i$  eliminates this dependence on representation.

- (Condition 1 – the lower bound and compactness) Let  $v_\eta$  be a sequence such that the sequence of energies  $E_\eta^{3d}(v_\eta)$  is bounded. Then (up to a subsequence)  $v_\eta \rightharpoonup v_0$ ,  $\text{supp } v_0$  is countable, and

$$\liminf_{\eta \rightarrow 0} E_\eta^{3d}(v_\eta) \geq E_0^{3d}(v_0). \quad (4.3)$$

- (Condition 2 – the upper bound) Let  $E_0^{3d}(v_0) < \infty$ . Then there exists a sequence  $v_\eta \rightharpoonup v_0$  such that

$$\limsup_{\eta \rightarrow 0} E_\eta^{3d}(v_\eta) \leq E_0^{3d}(v_0).$$

Note that the compactness condition which usually accompanies a Gamma-convergence result has been built into Condition 1 (the lower bound). The fact that sequences with bounded energy  $E_\eta^{3d}$  converge to a collection of delta functions is partly so by construction: the functions  $v_\eta$  are positive, have uniformly bounded mass, and only take values either 0 or  $1/\eta^3$ . Since  $\eta \rightarrow 0$ , the size of the support of  $v_\eta$  shrinks to zero, and along a subsequence  $v_\eta$  converges in the sense of measures to a limit measure; in line with the discussion above, this limit measure is shown to be a sum of Dirac delta measures (Lemma 5.1).

We have the following properties of  $e_0^{3d}$  whose proofs are presented in Section 5.4.

**Lemma 4.4.** 1. For every  $a > 0$ ,  $e_0^{3d}$  is non-negative and bounded from above on  $[a, \infty)$ .

2.  $e_0^{3d}$  is strictly concave on  $[0, 2\pi]$ .

3. If  $\{m^i\}_{i \in \mathbf{N}}$  with  $\sum_i m^i < \infty$  satisfies

$$\sum_{i=1}^{\infty} e_0^{3d}(m^i) = e_0^{3d}\left(\sum_{i=1}^{\infty} m^i\right), \quad (4.4)$$

then only a finite number of  $m^i$  are non-zero.

4. If  $z$  achieves the infimum in the definition (4.1) of  $e_0^{3d}$ , then  $\text{supp } z$  is bounded.

The value of  $E_0^{3d}$  is independent of the positions  $x^i$  of the point masses. In order to capture this positional information, we consider the next level of approximation, by subtracting the minimum of  $E_0^{3d}$  and renormalizing the result. To this end, note that among all measures of mass  $M$ , the global minimizer of  $E_0^{3d}$  is given by

$$\min \left\{ E_0^{3d}(v) : \int_{\mathbf{T}^3} v = M \right\} = e_0^{3d}(M).$$

We recover the next term in the expansion as the limit of  $E_\eta^{3d} - e_0^{3d}$ , appropriately rescaled, that is of the functional

$$F_\eta^{3d}(v_\eta) := \eta^{-1} \left[ E_\eta^{3d}(v_\eta) - e_0^{3d} \left( \int_{\mathbf{T}^3} v_\eta \right) \right].$$

If this second-order energy remains bounded in the limit  $\eta \rightarrow 0$ , then the limiting object  $v_0 = \sum_i m^i \delta_{x^i}$  necessarily has two properties:

1. The limiting mass weights  $\{m^i\}$  satisfy (4.4);

2. For each  $m^i$ , the minimization problem defining  $e_0^{3d}(m^i)$  has a minimizer.

The first property above arises from the condition that  $E_\eta^{3d}(v_\eta)$  converges to its minimal value as  $\eta \rightarrow 0$ . The second is slightly more subtle, and can be understood by the following formal scaling argument.

In the course of the proof we construct truncated versions of  $v_\eta$ , called  $v_\eta^i$ , each of which is localized around the corresponding limiting point  $x^i$  and rescaled as in (3.2) to a function  $z_\eta^i$ . For each  $i$  the sequence  $z_\eta^i$  is a minimizing sequence for the minimization problem  $e_0^{3d}(m^i)$ , and the scaling of  $F_\eta^{3d}$  implies that the energy  $E_\eta^{3d}(v_\eta)$  converges to the limiting value at a rate of at least  $O(\eta)$ . In addition, since  $v_\eta^i$  converges to a delta function, the typical spatial extent of  $\text{supp } v_\eta^i$  is of order  $o(1)$ , and therefore the spatial extent of  $\text{supp } z_\eta^i$  is of order  $o(1/\eta)$ . If the sequence  $z_\eta^i$  does not converge, however, then it splits up into separate parts; the interaction between these parts is penalized by the  $H^{-1}$ -norm at the rate of  $1/d$ , where  $d$  is the distance between the separating parts. Since  $d = o(1/\eta)$ , the energy penalty associated with separation scales larger than  $O(\eta)$ , which contradicts the convergence rate mentioned above.

This is no coincidence; the scaling of  $F_\eta^{3d}$  has been chosen just so that the interaction between objects that are separated by  $O(1)$ -distances in the original variable  $x$  contributes an  $O(1)$  amount to this second-level energy. If they are asymptotically closer, then the interaction blows up. Motivated by these remarks we define the set of admissible limit sequences

$$\mathcal{M} := \left\{ \{m^i\}_{i \in \mathbf{N}} : m^i \geq 0, \text{ satisfying (4.4), such that } e_0^{3d}(m^i) \text{ admits a minimizer for each } i \right\}.$$

The limiting energy functional  $F_0^{3d}$  can already be recognized in the decomposition given by (3.3) and (3.4). We show in the proof in Section 5 that the interfacial term in the energy  $E_\eta^{3d}$  is completely cancelled by the corresponding term in  $e_0^{3d}$ , as is the highest-order term in the expansion of  $\|v_\eta - f v_\eta\|_{H^{-1}}^2$ . What remains is a combination of cross terms,

$$\sum_{\substack{i,j=1 \\ i \neq j}}^{\infty} \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^j(y) G_{\mathbf{T}^3}(x-y) dx dy,$$

and lower-order self-interaction parts of the  $H^{-1}$ -norm.

$$\sum_{i=1}^{\infty} \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy.$$

With these remarks we define

$$F_0^{3d}(v) := \begin{cases} \sum_{i=1}^{\infty} g^{(3)}(0) (m^i)^2 + \\ \quad \sum_{i \neq j} m^i m^j G_{\mathbf{T}^3}(x^i - x^j) & \text{if } v = \sum_{i=1}^n m^i \delta_{x^i} \text{ with } \{x^i\} \text{ distinct, } \{m^i\} \in \mathcal{M} \\ \infty & \text{otherwise.} \end{cases}$$

We have:

**Theorem 4.5.** *Within the space  $X$ , we have*

$$F_\eta^{3d} \xrightarrow{\Gamma} F_0^{3d} \quad \text{as } \eta \rightarrow 0.$$

*That is, Conditions 1 and 2 of Theorem 4.3 hold with  $E_\eta^{3d}$  and  $E_0^{3d}$  replaced with  $F_\eta^{3d}$  and  $F_0^{3d}$ .*

The interesting aspects of this limit functional  $F_0^{3d}$  are

- In contrast to  $E_0^{3d}$ , the functional  $F_0^{3d}$  is only finite on *finite* collections of point masses, which in addition satisfy two constraints: the collection should satisfy (4.4), and each weight  $m^i$  should be such that the corresponding minimization problem (4.1) is achieved. In Section 7 we discuss these properties further.
- The main component of  $F_0^{3d}$  is the two-point interaction energy

$$\sum_{i,j: i \neq j} m^i m^j G_{\mathbf{T}^3}(x^i - x^j).$$

This two-point interaction energy is known as a Coulomb interaction energy, by reference to electrostatics. A similar limit functional also appeared in [31].

## 5 Proofs of Theorems 4.3 and 4.5

### 5.1 Concentration into point measures

**Lemma 5.1** (Compactness). *Let  $v_\eta$  be a sequence in  $BV(\mathbf{T}^3; \{0, 1/\eta^3\})$  such that both  $\int_{\mathbf{T}^3} v_\eta$  and  $E_\eta^{3d}(v_\eta)$  are uniformly bounded. Then there exists a subsequence such that  $v_\eta \rightharpoonup v_0$  as measures, where*

$$v_0 := \sum_{i=1}^{\infty} m^i \delta_{x^i}, \quad (5.1)$$

with  $m^i \geq 0$  and  $x^i \in \mathbf{T}^3$  distinct.

Note that we often write “a sequence  $v_\eta$ ” instead of “a sequence  $\eta_n \rightarrow 0$  and a sequence  $v_n$ ” whenever this does not lead to confusion. The essential tool to prove convergence to delta measures is the *Second Concentration Compactness Lemma* of Lions [21].

*Proof.* The functions  $w_\eta := \eta v_\eta$  satisfy  $w_\eta \rightarrow 0$  in  $L^1(\mathbf{T}^3)$ , and  $|\nabla w_\eta| = \eta |\nabla v_\eta|$  bounded in  $L^1(\mathbf{T}^3)$ . On the other hand, since  $w_\eta$  and  $v_\eta$  are essentially characteristic functions with equal support, one has  $w_\eta^{3/2} = v_\eta$  which is bounded in  $L^1(\mathbf{T}^3)$ . Hence we extract a subsequence such that  $v_\eta \rightharpoonup v_0$  as measures. Lemma I.1 (i) of [21] (with  $m = p = 1, q = 3/2$ ) then implies that  $v_0$  has the structure (5.1).  $\square$

The proof of the two lower-bound inequalities uses a partition of  $\text{supp } v_\eta$  into disjoint sets with positive pairwise distance. This division implies the equality

$$\int_{\mathbf{T}^3} |\nabla v_\eta| = \sum_i \int_{\mathbf{T}^3} |\nabla v_\eta^i|,$$

and is a crucial step towards the separation of local and global effects in the functionals. The following lemma provides this partition into disjoint particles. It states that for the lower bounds, it suffices to assume that a sequence with bounded energy and mass satisfies the ansatz of well-separated small inclusions assumed in our calculations of Section 3.

**Lemma 5.2.** (i) *Suppose that for every sequence  $v_\eta$  satisfying:*

1.  $E_\eta^{3d}(v_\eta)$  and  $\int_{\mathbf{T}^3} v_\eta$  are bounded;
2. for some  $n \in \mathbf{N}$ ,  $v_\eta = \sum_{i=1}^n v_\eta^i$  with  $w\text{-}\liminf_{\eta \rightarrow 0} v_\eta^i \geq m^i \delta_{x^i}$  as measures,  $\text{dist}(\text{supp } v_\eta^i, \text{supp } v_\eta^j) > 0$  for all  $i \neq j$ , and  $\text{diam supp } v_\eta^i < 1/4$ ;

we have

$$\liminf_{\eta \rightarrow 0} E_\eta^{3d}(v_\eta) \geq E_0^{3d} \left( \sum_{i=1}^n m^i \delta_{x^i} \right).$$

Then for every sequence  $v_\eta$  satisfying 1. with  $v_\eta \rightharpoonup v_0$ , we have

$$\liminf_{\eta \rightarrow 0} E_\eta^{3d}(v_\eta) \geq E_0^{3d}(v_0).$$

(ii) Suppose that for every sequence  $v_\eta$  satisfying:

1.  $F_\eta^{3d}(v_\eta)$  and  $\int_{\mathbf{T}^3} v_\eta$  are bounded;
2. for some  $n \in \mathbf{N}$ ,  $v_\eta = \sum_{i=1}^n v_\eta^i$  with  $v_\eta^i \rightharpoonup m^i \delta_{x^i}$ ,  $\text{dist}(\text{supp } v_\eta^i, \text{supp } v_\eta^j) > 0$  for all  $i \neq j$ , and  $\text{diam supp } v_\eta^i < 1/4$ ;
3. there exist  $\xi_\eta^i \in \mathbf{T}^3$  and a constant  $C^i > 0$  such that

$$\int_{\mathbf{T}^3} |x - \xi_\eta^i|^2 v_\eta^i(x) dx \leq C^i \eta^2; \quad (5.2)$$

we have

$$\liminf_{\eta \rightarrow 0} F_\eta^{3d}(v_\eta) \geq F_0^{3d} \left( \sum_{i=1}^n m^i \delta_{x^i} \right).$$

Then for every sequence  $v_\eta$  satisfying 1. with  $v_\eta \rightharpoonup v_0$ , we have

$$\liminf_{\eta \rightarrow 0} F_\eta^{3d}(v_\eta) \geq F_0^{3d}(v_0).$$

The proof of Lemma 5.2 is given in detail in Section 5.4. A central ingredient is the following truncation lemma. Here  $\Omega$  is either the torus  $\mathbf{T}^3$  or an open bounded subset of  $\mathbf{R}^3$ .

**Lemma 5.3.** *Let  $n \in \mathbf{N}$  be fixed, let  $a_k \rightarrow \infty$ , and let  $u_k \in BV(\Omega; \{0, a_k\})$  satisfy*

$$\int_{\Omega} |\nabla u_k| = o(a_k), \quad (5.3)$$

and converges weakly in  $X$  to a weighted sum

$$\sum_{i=1}^{\infty} m^i \delta_{x^i},$$

where  $m^i \geq 0$  and the  $x^i \in \Omega$  are distinct. Then there exist components  $u_k^i \in BV(\Omega; \{0, a_k\})$ ,  $i = 1 \dots n$ , satisfying  $\text{diam supp } u_k^i \leq 1/4$ ,  $\inf_k \inf_{i \neq j} \text{dist}(\text{supp } u_k^i, \text{supp } u_k^j) > 0$ , and

$$w\text{-}\liminf_{k \rightarrow \infty} u_k^i \geq m^i \delta_{x^i}, \quad (5.4)$$

in the sense of distributions. In addition, the modified sequence  $\tilde{u}_k = \sum_i u_k^i$  satisfies

1.  $\tilde{u}_k \leq u_k$  for all  $k$ ;
2.  $\limsup_{k \rightarrow \infty} \int (u_k - \tilde{u}_k) \leq \sum_{i=n+1}^{\infty} m^i$ ;
3. There exists a constant  $C = C(n) > 0$  such that for all  $k$

$$\int |\nabla \tilde{u}_k| \leq \int |\nabla u_k| - C \|u_k - \tilde{u}_k\|_{L^{3/2}(\Omega)}. \quad (5.5)$$

The essential aspects of this lemma are the construction of a new sequence which again lies in  $BV(\Omega; \{0, a_k\})$ , and the quantitative inequality (5.5) relating the perimeters.

## 5.2 Proof of Theorem 4.3

*Proof. (Lower bound)* Let  $v_\eta$  be a sequence such that the sequences of energies  $E_\eta^{3d}(v_\eta)$  and masses  $\int_{\mathbf{T}^3} v_\eta$  are bounded. By Lemma 5.1, a subsequence converges to a limit  $v_0$  of the form (5.1). By Lemma 5.2 it is sufficient to consider a sequence (again called  $v_\eta$ ) such that  $v_\eta = \sum_{i=1}^n v_\eta^i$  with  $w\text{-}\liminf_{\eta \rightarrow 0} v_\eta^i \geq m_0^i \delta_{x^i}$ ,  $\text{supp } v_\eta^i \subset B(x^i, 1/4)$ , and  $\text{dist}(\text{supp } v_\eta^i, \text{supp } v_\eta^j) > 0$  for all  $i \neq j$ . Then, writing

$$z_\eta^i(y) := \eta^3 v_\eta^i(x^i + \eta y), \quad (5.6)$$

we have

$$\int_{\mathbf{T}^3} v_\eta^i = \int_{\mathbf{R}^3} z_\eta^i \quad \text{and} \quad \int_{\mathbf{T}^3} |\nabla v_\eta^i| = \eta^{-1} \int_{\mathbf{R}^3} |\nabla z_\eta^i|,$$

and by (3.4)

$$\|v_\eta^i - f v_\eta^i\|_{H^{-1}(\mathbf{T}^3)}^2 = \eta^{-1} \|z_\eta^i\|_{H^{-1}(\mathbf{R}^3)}^2 + \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy.$$

For future use we introduce the shorthand

$$m_\eta^i := \int_{\mathbf{T}^3} v_\eta^i = \int_{\mathbf{R}^3} z_\eta^i.$$

Then

$$\begin{aligned} E_\eta^{3d}(v_\eta) &= \sum_{i=1}^n E_\eta^{3d}(v_\eta^i) + \eta \sum_{\substack{i,j=1 \\ i \neq j}}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^j(y) G_{\mathbf{T}^3}(x-y) dx dy \\ &= \sum_{i=1}^n \left[ \int_{\mathbf{R}^3} |\nabla z_\eta^i| + \|z_\eta^i\|_{H^{-1}(\mathbf{R}^3)}^2 \right] \\ &\quad + \eta \sum_{i=1}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy + \eta \sum_{\substack{i,j=1 \\ i \neq j}}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^j(y) G_{\mathbf{T}^3}(x-y) dx dy \\ &\geq \sum_{i=1}^n e_0^{3d}(m_\eta^i) + \eta \inf g^{(3)} \sum_{i=1}^n (m_\eta^i)^2 + \eta \inf G_{\mathbf{T}^3} \sum_{\substack{i,j=1 \\ i \neq j}}^n m_\eta^i m_\eta^j. \end{aligned} \quad (5.7)$$

Since the last two terms vanish in the limit, the continuity and monotonicity of  $e_0^{3d}$  (a consequence of Lemma 4.4) imply that

$$\liminf_{\eta \rightarrow 0} \mathbf{E}_\eta^{3d}(v_\eta) \geq \sum_{i=1}^n e_0^{3d} \left( \liminf_{\eta \rightarrow 0} m_\eta^i \right) \geq \sum_{i=1}^n e_0^{3d}(m^i) \geq \mathbf{E}_0^{3d}(v_0).$$

**(Upper bound)** Let  $v_0$  satisfy  $\mathbf{E}_0^{3d}(v_0) < \infty$ . It is sufficient to prove the statement for finite sums

$$v_0 = \sum_{i=1}^n m^i \delta_{x^i},$$

since an infinite sum  $v_0 = \sum_{i=1}^\infty m^i \delta_{x^i}$  can trivially be approximated by finite sums, and in that case

$$\mathbf{E}_0^{3d} \left( \sum_{i=1}^n m^i \delta_{x^i} \right) = \sum_{i=1}^n e_0^{3d}(m^i) \leq \sum_{i=1}^\infty e_0^{3d}(m^i) = \mathbf{E}_0^{3d}(v_0).$$

To construct the appropriate sequence  $v_\eta \rightharpoonup v_0$ , let  $\epsilon > 0$  and let  $z^i$  be near-optimal in the definition of  $e_0^{3d}(m^i)$ , i.e.,

$$\int_{\mathbf{R}^3} |\nabla z^i| + \|z^i\|_{H^{-1}(\mathbf{R}^3)}^2 \leq e_0^{3d}(m^i) + \frac{\epsilon}{n}. \quad (5.8)$$

By an approximation argument we can assume that the support of  $z^i$  is bounded. We then set

$$v_\eta^i(x) := \eta^{-3} z^i(\eta^{-1}(x - x^i)), \quad (5.9)$$

so that

$$\int_{\mathbf{T}^3} v_\eta^i = m^i \quad \text{and} \quad v_\eta^i \rightharpoonup m^i \delta_{x^i}.$$

Since the diameters of the supports of the  $v_\eta^i$  tend to zero, and since the  $x^i$  are distinct,  $v_\eta := \sum_i v_\eta^i$  is admissible for  $\mathbf{E}_\eta^{3d}$  when  $\eta$  is sufficiently small.

Following the argument of (5.7), we have

$$\begin{aligned} \mathbf{E}_\eta^{3d}(v_\eta) &= \sum_{i=1}^n \left[ \int_{\mathbf{R}^3} |\nabla z^i| + \|z^i\|_{H^{-1}(\mathbf{R}^3)}^2 \right] \\ &\quad + \eta \sum_{i=1}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy + \eta \sum_{\substack{i,j=1 \\ i \neq j}}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^j(y) G_{\mathbf{T}^3}(x-y) dx dy \end{aligned}$$

and thus

$$\limsup_{\eta \rightarrow 0} \mathbf{E}_\eta^{3d}(v_\eta) \leq \mathbf{E}_0^{3d}(v_0) + \epsilon.$$

The result now follows by taking a diagonal sequence with respect to  $\epsilon \rightarrow 0$ .  $\square$

### 5.3 Proof of Theorem 4.5

*Proof. (Lower bound)* Let  $v_\eta = \sum_{i=1}^n v_\eta^i$  be a sequence with bounded energy  $\mathbb{F}_\eta^{3d}(v_\eta)$  as given by Lemma 5.2, converging to a  $v_0$  of the form

$$v_0 = \sum_{i=1}^n m^i \delta_{x^i},$$

where  $m_0^i \geq 0$  and the  $x^i$  are distinct. Again we use the rescaling (5.6) and we set

$$m_\eta^i := \int_{\mathbf{T}^3} v_\eta^i = \int_{\mathbf{R}^3} z_\eta^i.$$

Following the second line of (5.7) we have

$$\begin{aligned} \mathbb{F}_\eta^{3d}(v_\eta) &= \eta^{-1} \left[ \mathbb{E}_\eta^{3d}(v_\eta) - e_0^{3d} \left( \int_{\mathbf{T}^3} v_\eta \right) \right] \\ &= \frac{1}{\eta} \sum_{i=1}^n \left[ \int_{\mathbf{R}^3} |\nabla z_\eta^i| + \|z_\eta^i\|_{H^{-1}(\mathbf{R}^3)}^2 - e_0^{3d}(m_\eta^i) \right] + \frac{1}{\eta} \left[ \sum_{i=1}^n e_0^{3d}(m_\eta^i) - e_0^{3d} \left( \sum_{i=1}^n m_\eta^i \right) \right] \\ &\quad + \sum_{i=1}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy + \sum_{\substack{i,j=1 \\ i \neq j}}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^j(y) G_{\mathbf{T}^3}(x-y) dx dy. \end{aligned} \tag{5.10}$$

Since the first two terms are both non-negative, the boundedness of  $\mathbb{F}_\eta^{3d}(v_\eta)$  and continuity of  $e_0^{3d}$  imply that

$$0 \leq \sum_{i=1}^n e_0^{3d}(m^i) - e_0^{3d} \left( \sum_{i=1}^n m^i \right) = \lim_{\eta \rightarrow 0} \left[ \sum_{i=1}^n e_0^{3d}(m_\eta^i) - e_0^{3d} \left( \int_{\mathbf{T}^3} v_\eta \right) \right] \leq 0,$$

and therefore the sequence  $\{m^i\}$  satisfies (4.4).

By the condition (5.2) the sequence  $z_\eta^i$  is tight, and since it is bounded in  $BV(\mathbf{R}^3; \{0, 1\})$ , a subsequence converges in  $L^1(\mathbf{R}^3)$  to a limit  $z_0^i$  (see for instance Corollary IV.26 of [8]). We then have

$$\begin{aligned} 0 &\leq \int_{\mathbf{R}^3} |\nabla z_0^i| + \|z_0^i\|_{H^{-1}(\mathbf{R}^3)}^2 - e_0^{3d}(m^i) \\ &\leq \liminf_{\eta \rightarrow 0} \left[ \int_{\mathbf{R}^3} |\nabla z_\eta^i| + \|z_\eta^i\|_{H^{-1}(\mathbf{R}^3)}^2 \right] - \lim_{\eta \rightarrow 0} e_0^{3d}(m_\eta^i) \stackrel{(5.10)}{=} 0, \end{aligned}$$

which implies that  $z_0^i$  is a minimizer for  $e_0^{3d}(m^i)$ .

Finally we conclude that

$$\begin{aligned} \liminf_{\eta \rightarrow 0} \mathbb{F}_\eta^{3d}(v_\eta) &\geq \liminf_{\eta \rightarrow 0} \left( \sum_{i=1}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^i(y) g^{(3)}(x-y) dx dy \right. \\ &\quad \left. + \sum_{\substack{i,j=1 \\ i \neq j}}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^j(y) G_{\mathbf{T}^3}(x-y) dx dy \right) \\ &= g^{(3)}(0) \sum_{i=1}^n (m^i)^2 + \sum_{\substack{i,j=1 \\ i \neq j}}^n m^i m^j G_{\mathbf{T}^3}(x^i - x^j) = \mathbb{F}_0^{3d}(v_0). \end{aligned}$$



(Upper bound) Let

$$v_0 = \sum_{i=1}^n m^i \delta_{x^i},$$

with the  $x^i$  distinct and  $\{m^i\} \in \mathcal{M}$ . By the definition of  $\mathcal{M}$  we may choose  $z^i$  that achieve the minimum in the minimization problem defining  $e_0^{3d}(m^i)$ ; by part 4 of Lemma 4.4 the support of  $z^i$  is bounded.

Setting  $v_\eta^i$  by (5.9), for  $\eta$  sufficiently small the function  $v_\eta := \sum_{i=1}^n v_\eta^i$  is admissible for  $F_\eta^{3d}$ , and  $v_\eta \rightharpoonup v_0$ . Then following (5.10) we have

$$\lim_{\eta \rightarrow 0} F_\eta^{3d}(v_\eta) = F_0^{3d}(v_0).$$

□

#### 5.4 Proofs of Lemmas 5.2 and 5.3

For the proof of Lemma 5.2 we first state and prove two lemmas. Throughout this section, if  $B$  is a ball in  $R^3$  and  $\lambda > 0$ , then  $\lambda B$  is the ball in  $\mathbf{R}^3$  obtained by multiplying  $B$  by  $\lambda$  with respect to the center of  $B$ ;  $B$  and  $\lambda B$  therefore have the same center.

**Lemma 5.4.** *Let  $w \in BV(B_R; \{0, 1\})$ . Choose  $0 < r < R$ , and set  $A := B_R \setminus \overline{B_r}$ . Then for any  $r \leq \rho \leq R$  we have*

$$\frac{\mathcal{H}^2(\partial B_\rho \cap \text{supp } w)}{\mathcal{H}^2(\partial B_\rho)} \leq \frac{1}{\mathcal{H}^2(\partial B_r)} \int_A |\nabla w| + \int_A w$$

*Proof.* Let  $P$  be the projection of  $\mathbf{R}^3$  onto  $B_r$ . For any closed set  $D \subset \mathbf{R}^3$  with finite perimeter, the projected set  $P(A \cap D)$  is included in  $E_b \cup E_r$ , where the two set are:

- The projected boundary  $E_b := P(A \cap \partial D)$ ; since  $P$  is a contraction,  $\mathcal{H}^2(E_b) \leq \mathcal{H}^2(A \cap \partial D)$ ;
- The set of projections of full radii  $E_r := \{x \in \partial B_r : \lambda x \in D \text{ for all } 1 \leq \lambda \leq R/r\}$ , for which

$$\mathcal{H}^2(E_r) = \frac{\mathcal{H}^2(\partial B_r)}{\mathcal{L}^3(A)} \mathcal{L}^3(\{\lambda x : x \in E_r, 1 \leq \lambda \leq R/r\}) \leq \frac{\mathcal{H}^2(\partial B_r)}{\mathcal{L}^3(A)} \mathcal{L}^3(D \cap A).$$

Applying these estimates to  $D = \text{supp } w$  we find

$$\begin{aligned} \frac{\mathcal{H}^2(\partial B_\rho \cap \text{supp } w)}{\mathcal{H}^2(\partial B_\rho)} &= \frac{\mathcal{H}^2(P(\partial B_\rho \cap \text{supp } w))}{\mathcal{H}^2(\partial B_r)} \\ &\leq \frac{\mathcal{H}^2(P(A \cap \text{supp } w))}{\mathcal{H}^2(\partial B_r)} \\ &\leq \frac{1}{\mathcal{H}^2(\partial B_r)} \left\{ \mathcal{H}^2(A \cap \partial \text{supp } w) + \frac{\mathcal{H}^2(\partial B_r)}{\mathcal{L}^3(A)} \mathcal{L}^3(A \cap \text{supp } w) \right\}, \end{aligned}$$

and this last expression implies the assertion. □

**Lemma 5.5.** *There exists  $0 < \alpha < 1$  with the following property. For any  $w \in BV(B_R; \{0, 1\})$  with*

$$\frac{1}{\mathcal{H}^2(\partial B_{\alpha R})} \int_{B_R \setminus B_{\alpha R}} |\nabla w| + \int_{B_R \setminus B_{\alpha R}} w \leq \frac{1}{2}, \quad (5.11)$$

*there exists  $\alpha \leq \beta < 1$  such that*

$$2\|\partial B_{\beta R}\|(\text{supp } w) \leq \int_{B_R \setminus B_{\beta R}} |\nabla w|. \quad (5.12)$$

*Proof.* By approximating (see for example Theorem 3.42 of [4]) and scaling we can assume that  $w$  has smooth support and that  $R = 1$ . Set  $0 < \alpha < 1$  to be such that

$$\frac{(1 - \alpha)^2}{16C} = \mathcal{H}^2(\partial B_\alpha), \quad (5.13)$$

where  $C$  is the constant in the relative isoperimetric inequality on the sphere  $S^2$  [16, 4.4.2]:

$$\min\{\mathcal{H}^2(D \cap S^2), \mathcal{H}^2(S^2 \setminus D)\} \leq C(\mathcal{H}^1(\partial D \cap S^2))^2.$$

We note that the combination of the assumption (5.11) and Lemma 5.4 implies that when applying this inequality to  $D = \text{supp } w$ , with  $S^2$  replaced by  $B_{1-s}$ , the minimum is attained by the first argument, i.e. we have

$$\mathcal{H}^2(D \cap \partial B_{1-s}) \leq C(\mathcal{H}^1(\partial D \cap \partial B_{1-s}))^2.$$

We now assume that the assertion of the Lemma is false, i.e. that for all  $\alpha < r < 1$

$$0 < 2\|\partial B_r\|(D) - \|\partial D\|(B_1 \setminus B_r). \quad (5.14)$$

Setting  $f(s) := \mathcal{H}^1(\partial D \cap \partial B_{1-s})$  we have

$$\int_0^s f(\sigma) d\sigma = \int_{1-s}^1 \mathcal{H}^1(\partial D \cap \partial B_r) dr \leq \int_{B_1 \setminus B_{1-s}} |\nabla w| \stackrel{(5.14)}{<} 2\|\partial B_{1-s}\|(D). \quad (5.15)$$

By the relative isoperimetric inequality we find

$$\int_0^s f(\sigma) d\sigma < 2\|\partial B_{1-s}\|(D) \leq 2C(\mathcal{H}^1(\partial D \cap \partial B_{1-s}))^2 = 2Cf(s)^2.$$

Note that this inequality implies that  $f$  is strictly positive for all  $s$ . Solving this inequality for positive functions  $f$  we find

$$\int_0^{1-\alpha} f(\sigma) d\sigma > \frac{(1 - \alpha)^2}{8C} \stackrel{(5.13)}{=} 2\mathcal{H}^2(\partial B_\alpha) \geq 2\|\partial B_\alpha\|(D) \stackrel{(5.15)}{>} \int_0^{1-\alpha} f(\sigma) d\sigma,$$

a contradiction. Therefore there exists an  $r =: \beta R$  satisfying (5.12), and the result follows as remarked above.  $\square$

**Proof of Lemma 5.3:** Let  $\alpha$  be as in Lemma 5.5. Choose  $n$  balls  $B^i$ , of radius less than  $1/8$ , centered at  $\{x^i\}_{i=1}^n$ , and such that the family  $\{2B^i\}$  is disjoint. Set  $w_k := a_k^{-1}u_k$ , and note that for each  $i$ ,

$$\frac{1}{\mathcal{H}^2(\partial \alpha B^i)} \int_{B^i \setminus \alpha B^i} |\nabla w_k| + \int_{B^i \setminus \alpha B^i} w_k \leq \frac{C}{a_k} \left\{ \int_{\Omega} |\nabla u_k| + \int_{\Omega} u_k \right\},$$

and this number tends to zero by (5.3), implying that the function  $w_k$  on  $B^i$  is admissible for Lemma 5.5. For each  $i$  and each  $k$ , let  $\beta_k^i$  be given by Lemma 5.5, so that

$$2\|\partial\beta_k^i B^i\|(\text{supp } u_k) \leq a_k^{-1}\|\nabla u_k\|(B^i \setminus \beta_k^i B^i). \quad (5.16)$$

Now set  $\tilde{u}_k^i := u_k \chi_{\beta_k^i B^i}$  and  $\tilde{u}_k := \sum_{i=1}^n \tilde{u}_k^i$ . Then for any open  $A \subset \Omega$  such that  $x^i \in A$ ,

$$\liminf_{k \rightarrow \infty} \int_A \tilde{u}_k^i = \liminf_{k \rightarrow \infty} \int_{A \cap \beta_k^i B^i} u_k \geq \liminf_{k \rightarrow \infty} \int_{A \cap \alpha B^i} u_k \geq \sum_{j=1}^{\infty} m^j \delta_{x^j}(A \cap \alpha B^i) \geq m^i,$$

which proves (5.4); property 2 follows from this by remarking that

$$\limsup_{k \rightarrow \infty} \int_{\Omega} (u_k - \tilde{u}_k) = \lim_{k \rightarrow \infty} \int_{\Omega} u_k - \liminf_{k \rightarrow \infty} \int_{\Omega} \tilde{u}_k \leq \sum_{j=1}^{\infty} m^j - \sum_{j=1}^n m^j.$$

The uniform separation of the supports is guaranteed by the condition that the family  $\{2B^i\}$  is disjoint, and property 1 follows by construction; it only remains to prove (5.5).

For this we calculate

$$\begin{aligned} \int_{\Omega} |\nabla \tilde{u}_k| &= \|\nabla u_k\| \left( \bigcup_{i=1}^n \beta_k^i B^i \right) + a_k \sum_{i=1}^n \|\partial\beta_k^i B^i\|(\text{supp } u_k) \\ &\stackrel{(5.16)}{\leq} \int_{\Omega} |\nabla u_k| - \|\nabla u_k\| \left( \Omega \setminus \bigcup_{i=1}^n \beta_k^i B^i \right) + \frac{1}{2} \sum_{i=1}^n \|\nabla u_k\|(B^i \setminus \beta_k^i B^i) \\ &\leq \int_{\Omega} |\nabla u_k| - \frac{1}{2} \|\nabla u_k\| \left( \Omega \setminus \bigcup_{i=1}^n \beta_k^i B^i \right) \\ &\leq \int_{\Omega} |\nabla u_k| - C_k \|u_k - f_{A_k} u_k\|_{L^{3/2}(A_k)} \end{aligned} \quad (5.17)$$

Here the constant  $C_k$  is the constant in the Sobolev inequality on the domain  $A_k := \Omega \setminus \cup_i \beta_k^i B^i$ ,

$$C_k \|u - f_{A_k} u\|_{L^{3/2}(A_k)} \leq \frac{1}{2} \int_{A_k} |\nabla u|.$$

The number  $C_k > 0$  depends on  $k$  through the geometry of the domain  $A_k$ . Note that the size of the holes  $\beta_k^i B^i$  is bounded from above by  $B^i$  and from below by  $\alpha B^i$ . Consequently, for each  $k_1$  and  $k_2$  there exists a smooth diffeomorphism mapping  $A_{k_1}$  into  $A_{k_2}$ , and the first and second derivatives of this mapping are bounded uniformly in  $k_1$  and  $k_2$ . Therefore we can replace in (5.17) the  $k$ -dependent constant  $C_k$  by a  $k$ -independent (but  $n$ -dependent) constant  $C > 0$ .

Note that since  $u_k$  is bounded in  $L^1$ ,

$$a_k^{-3/2} \|u_k\|_{L^{3/2}(A_k)}^{3/2} = a_k^{-1} \|u_k\|_{L^1(A_k)} \rightarrow 0 \quad \text{as } k \rightarrow \infty. \quad (5.18)$$

Continuing from (5.17) we then estimate by the inverse triangle inequality

$$\begin{aligned}
\int_{\Omega} |\nabla \tilde{u}_k| &\leq \int_{\Omega} |\nabla u_k| - C \|u_k\|_{L^{3/2}(A_k)} + \frac{C}{|A_k|^{1/3}} \|u_k\|_{L^1(A_k)} \\
&= \int_{\Omega} |\nabla u_k| - C \|u_k\|_{L^{3/2}(A_k)} + \frac{C}{|A_k|^{1/3} a_k^{1/2}} \|u_k\|_{L^{3/2}(A_k)}^{3/2} \\
&= \int_{\Omega} |\nabla u_k| - C \|u_k\|_{L^{3/2}(A_k)} \left\{ 1 - \frac{1}{|A_k|^{1/3} a_k^{1/2}} \|u_k\|_{L^{3/2}(A_k)}^{1/2} \right\} \\
&\stackrel{(5.18)}{\leq} \int_{\Omega} |\nabla u_k| - C' \|u_k\|_{L^{3/2}(A_k)} = \int_{\Omega} |\nabla u_k| - C' \|u_k - \tilde{u}_k\|_{L^{3/2}(\Omega)}.
\end{aligned}$$

This proves the inequality (5.5).  $\square$

**Proof of Lemma 5.2:** By Lemma 5.1 and by passing to a subsequence we can assume that  $v_\eta$  converges as measures to  $v_0$ . We first concentrate on the lower bound for  $\mathbf{E}_\eta^{3d}$ .

Fix  $n \in \mathbf{N}$  for the moment. We apply Lemma 5.3 to the sequence  $v_\eta$  and find a collection of components  $v_\eta^i$ ,  $i = 1 \dots n$ , and  $\tilde{v}_\eta = \sum_i v_\eta^i$ , such that

$$\text{w-liminf}_{\eta \rightarrow 0} v_\eta^i \geq \sum_{i=1}^n m^i \delta_{x^i},$$

and

$$\int_{\mathbf{T}^3} |\nabla \tilde{v}_\eta| \leq \int_{\mathbf{T}^3} |\nabla v_\eta| - C \|v_\eta - \tilde{v}_\eta\|_{L^{3/2}(\mathbf{T}^3)}.$$

Setting  $r_\eta := v_\eta - \tilde{v}_\eta$  we also have

$$\begin{aligned}
\|\tilde{v}_\eta - f \tilde{v}_\eta\|_{H^{-1}(\mathbf{T}^3)}^2 &= \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta(x) v_\eta(y) G_{\mathbf{T}^3}(x-y) dx dy - 2 \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} r_\eta(x) \tilde{v}_\eta(y) G_{\mathbf{T}^3}(x-y) dx dy \\
&\quad - \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} r_\eta(x) r_\eta(y) G_{\mathbf{T}^3}(x-y) dx dy \\
&\leq \|v_\eta - f v_\eta\|_{H^{-1}(\mathbf{T}^3)}^2 - 2 \inf G_{\mathbf{T}^3} \|r_\eta\|_{L^1(\mathbf{T}^3)} \|\tilde{v}_\eta\|_{L^1(\mathbf{T}^3)}.
\end{aligned}$$

Therefore

$$\mathbf{E}_\eta^{3d}(\tilde{v}_\eta) \leq \mathbf{E}_\eta^{3d}(v_\eta) - C \eta \|r_\eta\|_{L^{3/2}(\mathbf{T}^3)} + C' \|r_\eta\|_{L^1(\mathbf{T}^3)}. \quad (5.19)$$

Assuming the lower bound has been proved for  $\tilde{v}_\eta$ , we then find

$$\begin{aligned}
\liminf_{\eta \rightarrow 0} \mathbf{E}_\eta^{3d}(v_\eta) &\geq \liminf_{\eta \rightarrow 0} \left[ \mathbf{E}_\eta^{3d}(\tilde{v}_\eta) - C' \|r_\eta\|_{L^1(\mathbf{T}^3)} \right] \\
&\geq \mathbf{E}_0^{3d} \left( \text{w-liminf}_{\eta \rightarrow 0} \tilde{v}_\eta \right) - C' \lim_{\eta \rightarrow 0} \int_{\mathbf{T}^3} v_\eta + C' \liminf_{\eta \rightarrow 0} \int_{\mathbf{T}^3} \tilde{v}_\eta \\
&\geq \mathbf{E}_0^{3d} \left( \sum_{i=1}^n m^i \delta_{x^i} \right) - C' \sum_{i=n+1}^{\infty} m^i.
\end{aligned}$$

Taking the supremum over  $n$  the lower bound inequality for  $v_\eta$  follows.

Turning to a lower bound for  $F_\eta^{3d}$ , we remark that by Lemma 4.4 the number of  $x^i$  in (5.1) with non-zero weight  $m^i$  is finite. Choosing  $n$  equal to this number and adapting the same modified sequence  $\tilde{v}_\eta$  as in the first part, we have

$$\lim_{\eta \rightarrow 0} \int_{\mathbf{T}^3} v_\eta \geq \liminf_{\eta \rightarrow 0} \int_{\mathbf{T}^3} \tilde{v}_\eta \geq \sum_{i=1}^n \liminf_{\eta \rightarrow 0} \int_{\mathbf{T}^3} v_\eta^i \geq \sum_{i=1}^n m^i = \lim_{\eta \rightarrow 0} \int_{\mathbf{T}^3} v_\eta,$$

and therefore  $v_\eta^i \rightharpoonup m_0^i \delta_{x^i}$ , and  $\int_{\mathbf{T}^3} r_\eta \rightarrow 0$ . Then

$$\begin{aligned} F_\eta^{3d}(\tilde{v}_\eta) &= \frac{1}{\eta} \left[ \mathbb{E}_\eta^{3d}(\tilde{v}_\eta) - e_0^{3d} \left( \int_{\mathbf{T}^3} \tilde{v}_\eta \right) \right] \\ &\stackrel{(5.19)}{\leq} \frac{1}{\eta} \left[ \mathbb{E}_\eta^{3d}(v_\eta) - e_0^{3d} \left( \int_{\mathbf{T}^3} v_\eta \right) \right] - C \|r_\eta\|_{L^{3/2}(\mathbf{T}^3)} + \frac{C'}{\eta} \|r_\eta\|_{L^1(\mathbf{T}^3)} \\ &\quad + \frac{1}{\eta} \left[ e_0^{3d} \left( \int_{\mathbf{T}^3} v_\eta \right) - e_0^{3d} \left( \int_{\mathbf{T}^3} \tilde{v}_\eta \right) \right] \\ &\leq F_\eta^{3d}(v_\eta) - \frac{C}{\eta} \left( \int_{\mathbf{T}^3} r_\eta \right)^{2/3} + \frac{L + C'}{\eta} \int_{\mathbf{T}^3} r_\eta. \end{aligned} \tag{5.20}$$

Here  $L$  is an upper bound for  $e_0^{3d'}$  on the set  $[\inf_\eta \int \tilde{v}_\eta, \infty)$  (see Lemma 4.4) and in the passage to the last inequality we used the triangle inequality for  $\|\cdot\|_{L^{3/2}}$  and the fact that by construction,  $r_\eta$  takes on only two values. For sufficiently small  $\eta$ , the last two terms add up to a negative value, and therefore we again have  $F_\eta^{3d}(\tilde{v}_\eta) \leq F_\eta^{3d}(v_\eta)$ . Because of the choice of  $n$  we have  $\tilde{v}_\eta \rightharpoonup v_0$ . Let us assume for the moment we can establish property 3. Then if we assume, in the same way as above, that the lower bound has been proved for  $\tilde{v}_\eta$ , we then find that

$$\liminf_{\eta \rightarrow 0} F_\eta^{3d}(v_\eta) \geq \liminf_{\eta \rightarrow 0} F_\eta^{3d}(\tilde{v}_\eta) \geq F_0^{3d}(v_0).$$

We must now show that property 3. holds. To this end, we will need to modify yet again the sequence  $\tilde{v}_\eta$ , preserving all the previous properties 1 – 2. For use below we note that

$$\begin{aligned} F_\eta^{3d}(v_\eta) &\geq F_\eta^{3d}(\tilde{v}_\eta) = \frac{1}{\eta} \left[ \mathbb{E}_\eta^{3d}(\tilde{v}_\eta) - e_0^{3d} \left( \int_{\mathbf{T}^3} \tilde{v}_\eta \right) \right] \\ &\stackrel{(4.2)}{\geq} \sum_{i=1}^n \left[ \int_{\mathbf{T}^3} |\nabla v_\eta^i| + \|v_\eta^i\|_{H^{-1}(\mathbf{T}^3)}^2 - \frac{1}{\eta} e_0^{3d} \left( \int_{\mathbf{T}^3} v_\eta^i \right) \right] + 2 \sum_{\substack{i,j=1 \\ i \neq j}}^n \int_{\mathbf{T}^3} \int_{\mathbf{T}^3} v_\eta^i(x) v_\eta^j(y) G_{\mathbf{T}^3}(x-y) dx dy \\ &\geq \sum_{i=1}^n \left[ \int_{\mathbf{R}^3} |\nabla v_\eta^i| + \|v_\eta^i\|_{H^{-1}(\mathbf{R}^3)}^2 - \frac{1}{\eta} e_0^{3d} \left( \int_{\mathbf{R}^3} v_\eta^i \right) \right] + \inf_{\mathbf{T}^3} g^{(3)} \sum_{i=1}^n \left( \int_{\mathbf{R}^3} v_\eta^i \right)^2 \\ &\quad + 2 \inf_{\mathbf{T}^3} G_{\mathbf{T}^3} \sum_{\substack{i,j=1 \\ i \neq j}}^n \int_{\mathbf{R}^3} v_\eta^i \int_{\mathbf{R}^3} v_\eta^j \end{aligned} \tag{5.21}$$

In the calculation above, and in the remainder of the proof, we switch to considering  $v_\eta^i$  defined on  $\mathbf{R}^3$  instead of  $\mathbf{T}^3$ . Since the terms in the first sum above are non-negative, boundedness of  $F_\eta^{3d}(v_\eta)$  as  $\eta \rightarrow 0$  implies the boundedness of each of the terms in the sum independently.

We now show that when  $F_\eta^{3d}(v_\eta)$  is bounded, then for each  $i$

$$\exists \xi_\eta^i \in \mathbf{R}^3 : \quad \int_{\mathbf{R}^3} |x - \xi_\eta^i|^2 v_\eta^i(x) dx = O(\eta^2) \quad \text{as } \eta \rightarrow 0. \tag{5.22}$$

Suppose that this is not the case for some  $i$ ; fix this  $i$ . We choose for  $\xi_\eta$  the barycenter of  $v_\eta^i$ , i.e.

$$\xi_\eta = \frac{\int_{\mathbf{R}^3} x v_\eta^i(x) dx}{\int_{\mathbf{R}^3} v_\eta^i}. \quad (5.23)$$

Since we assume the negation of (5.22), we find that

$$\rho_\eta^2 := \int_{\mathbf{R}^3} |x - \xi_\eta|^2 v_\eta^i(x) dx \gg \eta^2. \quad (5.24)$$

Note that by (5.23) and the fact that  $v_\eta^i \rightharpoonup m^i \delta_{x^i}$ ,

$$\lim_{\eta \rightarrow 0} \rho_\eta = 0. \quad (5.25)$$

Now rescale  $v_\eta^i$  by defining  $\zeta_\eta(x) := \rho_\eta^3 v_\eta^i(\xi_\eta + \rho_\eta x)$ . The sequence  $\zeta_\eta$  satisfies

1.  $\zeta_\eta \in BV(\mathbf{R}^3, \{0, \rho_\eta^3 \eta^{-3}\})$ ;
2.  $\int_{\mathbf{R}^3} \zeta_\eta = \int_{\mathbf{R}^3} v_\eta^i$ ;
3.  $\frac{\eta}{\rho_\eta} \left( \int_{\mathbf{R}^3} |\nabla \zeta_\eta| + \|\zeta_\eta\|_{H^{-1}(\mathbf{R}^3)}^2 \right) = \eta \int_{\mathbf{R}^3} |\nabla v_\eta^i| + \eta \|v_\eta^i\|_{H^{-1}(\mathbf{R}^3)}^2$ , and
4.  $\int_{\mathbf{R}^3} |x|^2 \zeta_\eta(x) dx = 1$ .

The first three properties imply that the sequence  $\zeta_\eta$  is of the same type as the sequence  $v_\eta$  in the rest of this paper, provided one replaces the small parameter  $\eta$  by the small parameter  $\tilde{\eta} := \eta/\rho_\eta$ . The fourth property implies that the sequence is tight. By the third property above, (5.21), and (5.25), the boundedness of  $F_\eta^{3d}$  translates into the vanishing of the analogous expression for  $\zeta_\eta$ :

$$\limsup_{\eta \rightarrow 0} \left\{ \int_{\mathbf{R}^3} |\nabla \zeta_\eta| + \|\zeta_\eta\|_{H^{-1}(\mathbf{R}^3)}^2 - \frac{\rho_\eta}{\eta} e_0^{3d} \left( \int_{\mathbf{R}^3} \zeta_\eta \right) \right\} = 0. \quad (5.26)$$

We now construct a contradiction with this limiting behavior, and therefore prove (5.22).

Following the same arguments as for  $v_\eta$  we apply the concentration-compactness lemma of Lions [21] to find that the sequence  $\zeta_\eta$  converges to (yet another) weighted sum of delta functions

$$\mu := \sum_{j=1}^{\infty} \mathbf{m}^j \delta_{y^j} \quad \text{with} \quad \mu(\mathbf{R}^3) = m^i,$$

where  $\mathbf{m}^j \geq 0$  and  $y^j \in \mathbf{R}^3$  are distinct. Since

$$\int x d\mu(x) = \lim_{\eta \rightarrow 0} \int_{\mathbf{R}^3} x \zeta_\eta(x) dx = 0 \quad \text{and} \quad \int |x|^2 d\mu(x) = \lim_{\eta \rightarrow 0} \int_{\mathbf{R}^3} |x|^2 \zeta_\eta(x) dx = 1,$$

at least two different  $\mathbf{m}^j$  are non-zero; we assume those to be  $j = 1$  and  $j = 2$ .

We will need to show that the number of non-zero  $\mathbf{m}^j$  is finite. Assuming the opposite for the moment, choose  $n \in \mathbf{N}$  so large that

$$\sum_{j=1}^n e_0^{3d}(\mathbf{m}^j) > e_0^{3d}(m^i);$$

this is possible since there exist no minimizers for  $e_0^{3d}(m^i)$  with infinitely many non-zero components (Lemma 4.4). We apply Lemma 5.3 to find a new sequence  $\tilde{\zeta}_\eta = \sum_{j=1}^n \zeta_\eta^j$ , where  $\zeta_\eta^j \rightharpoonup \mathbf{m}^j \delta_{y^j}$ . Then

$$\begin{aligned} \liminf_{\eta \rightarrow 0} \frac{\eta}{\rho_\eta} \left\{ \int_{\mathbf{R}^3} |\nabla \zeta_\eta| + \|\zeta_\eta\|_{H^{-1}(\mathbf{R}^3)}^2 \right\} &\geq \liminf_{\eta \rightarrow 0} \sum_{j=1}^n \frac{\eta}{\rho_\eta} \left\{ \int_{\mathbf{R}^3} |\nabla \zeta_\eta^j| + \|\zeta_\eta^j\|_{H^{-1}(\mathbf{R}^3)}^2 \right\} \\ &\geq \liminf_{\eta \rightarrow 0} \sum_{j=1}^n e_0^{3d} \left( \int_{\mathbf{R}^3} \zeta_\eta^j \right) > e_0^{3d}(m^i), \end{aligned}$$

which contradicts (5.26); therefore the number of non-zero components  $\mathbf{m}^j$  is finite, and we can choose  $n$  such that  $m^i = \sum_{j=1}^n \mathbf{m}^j$  and  $\int (\zeta_\eta - \tilde{\zeta}_\eta) \rightarrow 0$ .

To conclude the proof we now note that

$$\begin{aligned} &\int_{\mathbf{R}^3} |\nabla \zeta_\eta| + \|\zeta_\eta\|_{H^{-1}(\mathbf{R}^3)}^2 - \frac{\rho_\eta}{\eta} e_0^{3d} \left( \int_{\mathbf{R}^3} \zeta_\eta \right) \\ &\geq \sum_{j=1}^n \left\{ \int_{\mathbf{R}^3} |\nabla \zeta_\eta^j| + \|\zeta_\eta^j\|_{H^{-1}(\mathbf{R}^3)}^2 \right\} + 2(\zeta_\eta^1, \zeta_\eta^2)_{H^{-1}(\mathbf{R}^3)} + C\|\zeta_\eta - \tilde{\zeta}_\eta\|_{L^{3/2}(\mathbf{R}^3)} \\ &\quad - \frac{\rho_\eta}{\eta} e_0^{3d} \left( \int_{\mathbf{R}^3} \zeta_\eta \right) \\ &\geq \frac{\rho_\eta}{\eta} \left[ \sum_{j=1}^n e_0^{3d} \left( \int_{\mathbf{R}^3} \zeta_\eta^j \right) - e_0^{3d} \left( \int_{\mathbf{R}^3} \tilde{\zeta}_\eta \right) \right] + \frac{\rho_\eta}{\eta} \left[ e_0^{3d} \left( \int_{\mathbf{R}^3} \tilde{\zeta}_\eta \right) - e_0^{3d} \left( \int_{\mathbf{R}^3} \zeta_\eta \right) \right] \\ &\quad + 2(\zeta_\eta^1, \zeta_\eta^2)_{H^{-1}(\mathbf{R}^3)} + C\|\zeta_\eta - \tilde{\zeta}_\eta\|_{L^{3/2}(\mathbf{R}^3)} \\ &\geq -\frac{L\rho_\eta}{\eta} \int_{\mathbf{R}^3} (\zeta_\eta - \tilde{\zeta}_\eta) + \frac{C\rho_\eta}{\eta} \left( \int_{\mathbf{R}^3} (\zeta_\eta - \tilde{\zeta}_\eta) \right)^{2/3} + \frac{1}{2\pi} \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} \frac{\zeta_\eta^1(x)\zeta_\eta^2(y)}{|x-y|} dx dy. \end{aligned}$$

Since  $\lim_{\eta \rightarrow 0} \int_{\mathbf{R}^3} (\zeta_\eta - \tilde{\zeta}_\eta) = 0$ , the first two terms in the last line above eventually become positive; the final term converges to  $(2\pi)^{-1} \mathbf{m}^1 \mathbf{m}^2 |y^1 - y^2|^{-1} > 0$ . This contradicts (5.26).  $\square$

## 5.5 Proof of Lemma 4.4

Let  $z_n$  be a minimizing sequence for  $e_0^{3d}(m)$ . The functions

$$z_n^\varepsilon(x) := z_n \left( \frac{x}{(1 + \varepsilon/m)^{1/3}} \right)$$

are admissible for  $e_0^{3d}(m + \varepsilon)$  for all  $\varepsilon > -m$ . Since the functions

$$f_n(\varepsilon) := \int_{\mathbf{R}^3} |\nabla z_n^\varepsilon| + \|z_n^\varepsilon\|_{H^{-1}(\mathbf{R}^3)}^2 = (1 + \varepsilon/m)^{2/3} \int_{\mathbf{R}^3} |\nabla z_n| + (1 + \varepsilon/m)^{5/3} \|z_n\|_{H^{-1}(\mathbf{R}^3)}^2$$

satisfy

$$f_n(\varepsilon) = f_n(0) + \frac{\varepsilon}{m} \left( \frac{2}{3} \int_{\mathbf{R}^3} |\nabla z_n| + \frac{5}{3} \|z_n\|_{H^{-1}(\mathbf{R}^3)}^2 \right) + \frac{\varepsilon^2}{2m^2} \left( -\frac{2}{9} \int_{\mathbf{R}^3} |\nabla z_n| + \frac{10}{9} \|z_n\|_{H^{-1}(\mathbf{R}^3)}^2 \right) + O\left(\frac{\varepsilon}{m}\right)^3, \quad (5.27)$$

uniformly in  $n$ , we have for all  $\varepsilon \geq 0$ ,

$$e_0^{3d}(m + \varepsilon) \leq \inf_n f_n(\varepsilon) \leq e_0^{3d}(m) + \frac{5}{3} e_0^{3d}(m) \frac{\varepsilon}{m} + \frac{5}{9} e_0^{3d}(m) \left(\frac{\varepsilon}{m}\right)^2 + O\left(\frac{\varepsilon}{m}\right)^3, \quad (5.28)$$

We deduce that

$$e_0^{3d}(m + \varepsilon) - e_0^{3d}(m) \leq \frac{5}{3m} e_0^{3d}(m) \varepsilon + O(\varepsilon^2). \quad (5.29)$$

By (4.2), we find that for any  $m \geq 1$  and any positive integer  $n$ , we have

$$e_0^{3d}(m) \leq e_0^{3d}(1) + n e_0^{3d} \left( \frac{m-1}{n} \right).$$

By taking  $n$  such that  $\frac{m-1}{n} \in [1, 2]$ , we have

$$e_0^{3d}(m) \leq e_0^{3d}(1) + Cn$$

where  $C$  denotes a uniform bound for  $e_0^{3d}$  on the interval  $[1, 2]$ . By choice of  $n$  we have for some constant  $C'$ ,  $e_0^{3d}(m) \leq e_0^{3d}(1) + C'm$ . Combining this with (5.29), we find that  $e_0^{3d'}$  is bounded from above on sets of the form  $[a, \infty)$  with  $a > 0$ .

For the concaveness of  $e_0^{3d}$ , note that under a constant-mass constraint  $\int |\nabla z|$  is minimal for balls and  $\|z\|_{H^{-1}(\mathbf{R}^3)}$  is maximal for balls (see e.g. [9] for the latter). Setting  $m = \int z$  and  $r^3 = 3m/4\pi$ , we therefore have

$$-\frac{2}{9} \int_{\mathbf{R}^3} |\nabla z_n| + \frac{10}{9} \|z_n\|_{H^{-1}(\mathbf{R}^3)}^2 \leq -\frac{2}{9} \int_{\mathbf{R}^3} |\nabla \chi_{B_r}| + \frac{10}{9} \|\chi_{B_r}\|_{H^{-1}(\mathbf{R}^3)}^2,$$

and an explicit calculation shows that the right-hand side is negative iff  $m < 2\pi$ . From (5.27) we therefore have for all  $m < 2\pi$  and all  $\varepsilon > -m$ ,

$$e_0^{3d}(m + \varepsilon) \leq e_0^{3d}(m) + \inf_n \left[ a_n \varepsilon - b\varepsilon^2 + c\varepsilon^3 \right],$$

where  $a_n$  is a sequence of real numbers, and  $b, c > 0$ . Writing this as

$$e_0^{3d}(m) \leq \inf_{m_0 \in (0, 2\pi)} \left\{ e_0^{3d}(m_0) + \inf_n \left[ a_n(m - m_0) - b(m - m_0)^2 + c(m - m_0)^3 \right] \right\},$$

we note that for each  $m_0$  the expression in braces is strictly concave in  $m$  for  $|m - m_0| < b/3c$ ; since the infimum of a set of concave functions is concave, it follows that the right-hand side is a concave function of  $m$ . Since equality holds for  $m_0 = m$ ,  $e_0^{3d}$  is therefore concave for  $m \leq 2\pi$ , and  $e_0^{3d''}(m) < 0$  for  $m < 2\pi$ .

Part 3 follows from remarking that if (say)  $m^1, m^2 \in (0, 2\pi)$ , then

$$\frac{d^2}{d\varepsilon^2} \left( e_0^{3d}(m^1 + \varepsilon) + e_0^{3d}(m^2 - \varepsilon) \right) \Big|_{\varepsilon=0} = e_0^{3d''}(m^1) + e_0^{3d''}(m^2) < 0.$$



Therefore the sequence  $(m^1, m^2, \dots)$  is not optimal, a contradiction. It follows that there can be at most one  $m^i$  in the region  $(0, 2\pi)$ , and since the total sum is finite, the number of non-zero  $m^i$  is finite.

For part 4 we assume that  $z$  achieves the infimum in the definition (4.1) of  $e_0^{3d}(m)$ , for some  $m > 0$ . By the relative isoperimetric equality on the exterior domain of a sphere (see for example [10]), there exists a  $C > 0$  such that

$$\forall R > 0 : \quad \int_{\mathbf{R}^3 \setminus B_R} z \leq C \left( \int_{\mathbf{R}^3 \setminus B_R} |\nabla z| \right)^{3/2}.$$

For sufficiently large  $R$ ,  $z$  satisfies (5.11). Fix such an  $R$  which we may assume additionally insures that  $\int_{B_{\alpha R}} z \geq m/2$ . Let  $0 < \alpha \leq \beta < 1$  be given by Lemma 5.5. We then calculate

$$\begin{aligned} e_0^{3d}(m) &= \int_{\mathbf{R}^3} |\nabla z| + \|z\|_{H^{-1}(\mathbf{R}^3)}^2 \\ &\geq \int_{B_{\beta R}} |\nabla z| + \int_{\mathbf{R}^3 \setminus B_{\beta R}} |\nabla z| + \|z\chi_{B_{\beta R}}\|_{H^{-1}(\mathbf{R}^3)}^2 \\ &\geq e_0^{3d} \left( \int_{B_{\beta R}} z \right) - \|\partial B_{\beta R}\|(\text{supp } z) + \int_{\mathbf{R}^3 \setminus B_{\beta R}} |\nabla z| \\ &\geq e_0^{3d}(m) - \|e_0^{3d'}\|_{L^\infty(m/2, \infty)} \left( m - \int_{B_{\beta R}} z \right) - \frac{1}{2} \int_{B_R \setminus B_{\beta R}} |\nabla z| + \int_{\mathbf{R}^3 \setminus B_{\beta R}} |\nabla z| \\ &\geq e_0^{3d}(m) - \|e_0^{3d'}\|_{L^\infty(m/2, \infty)} \int_{\mathbf{R}^3 \setminus B_{\beta R}} z + \frac{1}{2} \int_{\mathbf{R}^3 \setminus B_{\beta R}} |\nabla z| \\ &\geq e_0^{3d}(m) - \|e_0^{3d'}\|_{L^\infty(m/2, \infty)} C \left( \int_{\mathbf{R}^3 \setminus B_R} |\nabla z| \right)^{3/2} + \frac{1}{2} \int_{\mathbf{R}^3 \setminus B_{\beta R}} |\nabla z|. \end{aligned} \quad (5.30)$$

To pass to the fourth line, we used Lemma 5.5 and part 1 of Lemma 4.4. Inequality (5.30) holds for all  $R$  sufficiently large. Since  $\int_{\mathbf{R}^3 \setminus B_{\beta R}} |\nabla z| \rightarrow 0$  as  $R \rightarrow \infty$ , the sum of the last two terms in (5.30) becomes strictly positive if the integrals are positive. Since strict positivity is a contradiction, it follows that the support of  $z$  is bounded.  $\square$

## 6 Two dimensions

All differences between the two- and three-dimensional case arise from a single fact: the scaling of the  $H^{-1}$  is critical in two dimensions, making the two-dimensional case special.

### 6.1 Leading-order convergence

The first difference is encountered in the leading-order limiting behavior. As we discussed in Section 3, the leading-order contribution to the  $H^{-1}$ -norm involves the masses of the particles instead of their localized  $H^{-1}$ -norm (see (3.7)). For the local problem in two dimensions we

therefore introduce the function

$$\begin{aligned} e_0^{2d}(m) &:= \frac{m^2}{2\pi} + \inf \left\{ \int_{\mathbf{R}^2} |\nabla z| : z \in BV(\mathbf{R}^2; \{0, 1\}), \int_{\mathbf{R}^2} z = m \right\} \\ &= \frac{m^2}{2\pi} + 2\sqrt{\pi m}. \end{aligned} \quad (6.1)$$

Note that the minimization problem in (6.1) is simply to minimize perimeter for a given area, and a disc of the appropriate area is the only solution. Thus the value of  $e_0^{2d}(m)$  can be determined explicitly.

The function  $e_0^{2d}$  does not satisfy the lower-semicontinuity condition (4.2) (*cf.* Remark 4.1). We therefore introduce the lower-semicontinuous envelope function

$$\overline{e_0^{2d}}(m) := \inf \left\{ \sum_{j=1}^{\infty} e_0^{2d}(m^j) : m^j \geq 0, \sum_{j=1}^{\infty} m^j = m \right\}. \quad (6.2)$$

The limit functional is defined in terms of this envelope function:

$$\mathbb{E}_0^{2d}(v) := \begin{cases} \sum_{i=1}^{\infty} \overline{e_0^{2d}}(m^i) & \text{if } v = \sum_{i=1}^{\infty} m^i \delta_{x^i} \text{ with } \{x^i\} \text{ distinct and } m^i \geq 0 \\ \infty & \text{otherwise.} \end{cases}$$

**Theorem 6.1.** *Within the space  $X$ , we have*

$$\mathbb{E}_\eta^{2d} \xrightarrow{\Gamma} \mathbb{E}_0^{2d} \quad \text{as } \eta \rightarrow 0.$$

*That is, conditions 1 and 2 of Theorem 4.3 hold with  $\mathbb{E}_\eta^{3d}$  and  $\mathbb{E}_0^{3d}$  replaced by  $\mathbb{E}_\eta^{2d}$  and  $\mathbb{E}_0^{2d}$ .*

The proof follows along exactly the same lines as the proof of Theorem 4.3. In fact, for the lower bound it is simpler since one can bypass the technicalities associated with Lemma 5.2. Indeed, a standard result on the approximation for sets of finite perimeter (see for example Theorem 3.42 of [4]) implies that, without loss of generality, we may assume that a sequence  $v_\eta$  with bounded energy (for  $\eta$  sufficiently small) satisfies

$$v_\eta = \sum_{i=1}^{\infty} v_\eta^i \quad \text{with} \quad v_\eta^i = \frac{1}{\eta^2} \chi_{A_\eta^i}, \quad (6.3)$$

where the sets  $A_\eta^i$  are connected, disjoint, smooth, and with diameters which tend to zero as  $\eta \rightarrow 0$ . Then the following estimate holds true in two dimensions:

$$\sum_{i=1}^{\infty} \text{diam}(\text{supp } v_\eta^i) \leq \eta^2 \sum_{i=1}^{\infty} \int_{\mathbf{T}^2} |\nabla v_\eta^i| \leq \eta \mathbb{E}_\eta^{2d}(v_\eta) = O(\eta), \quad (6.4)$$

which can be used to bypass Lemma 5.2.

The upper bound again follows the argument in three space dimensions. In the construction, one can now choose optimal two-dimensional balls for the minimizer of  $e_0^{2d}$ . The only small technicality is that one needs to relate the limiting energy of these balls to  $\overline{e_0^{2d}}$ . However one can argue as follows. It is sufficient to prove the statement for finite sums

$$v_0 = \sum_{i=1}^n m^i \delta_{x^i},$$

since an infinite sum  $v_0 = \sum_{i=1}^{\infty} m^i \delta_{x^i}$  can trivially be approximated by finite sums, and in that case

$$\mathbb{E}_0^{2d} \left( \sum_{i=1}^n m^i \delta_{x^i} \right) = \sum_{i=1}^n \overline{e_0^{2d}}(m^i) \leq \sum_{i=1}^{\infty} \overline{e_0^{2d}}(m^i) = \mathbb{E}_0^{2d}(v_0).$$

Finally, taking for  $v_0$  now a finite sum,  $\mathbb{E}_0^{2d}(v_0) = \sum_{i=1}^n \overline{e_0^{2d}}(m^i)$  can be approximated to arbitrary precision by

$$\sum_{i=1}^n \sum_{j=1}^{k_i} e_0^{2d}(m^{ij})$$

where  $\sum_j m^{ij} = m^i$ . Therefore it is sufficient to construct a sequence  $v_\eta \rightharpoonup v_0$  such that

$$\limsup_{\eta \rightarrow 0} \mathbb{E}_\eta^{2d}(v_\eta) \leq \sum_{i=1}^n e_0^{2d}(m^i) \quad \text{for} \quad v_0 = \sum_{i=1}^n m^i \delta_{x^i}. \quad (6.5)$$

By slightly perturbing the positions the  $x^i$  can still be assumed to be distinct.

## 6.2 Next-order behavior

Turning to the next-order behavior, note that among all measures of mass  $M$ , the global minimizer of  $\mathbb{E}_0^{2d}$  is given by

$$\min \left\{ \mathbb{E}_0^{2d}(v) : \int_{\mathbf{T}^2} v = M \right\} = \overline{e_0^{2d}}(M).$$

We recover the next term in the expansion as the limit of  $\mathbb{E}_\eta^{2d} - \overline{e_0^{2d}}$ , appropriately rescaled, that is of the functional

$$\mathbb{F}_\eta^{2d}(v) := |\log \eta| \left[ \mathbb{E}_\eta^{2d}(v) - \overline{e_0^{2d}} \left( \int_{\mathbf{T}^2} v \right) \right].$$

Here the situation is similar to the three-dimensional case in that for boundedness of the sequence  $\mathbb{F}_\eta^{2d}$  the limiting weights  $m^i$  should satisfy two requirements: a minimality condition and a compactness condition. The compactness condition is most simply written as the condition that

$$\overline{e_0^{2d}}(m^i) = e_0^{2d}(m^i) \quad (6.6)$$

and corresponds to the condition in three dimensions that there exist a minimizer of the minimization problem (4.1).

In two dimensions, the minimality condition (6.7) provides a characterization that is stronger than the in three dimensions:

**Lemma 6.2.** *Let  $\{m^i\}_{i \in \mathbf{N}}$  be a solution of the minimization problem*

$$\min \left\{ \sum_{i=1}^{\infty} e_0^{2d}(m^i) : m^i \geq 0, \sum_{i=1}^{\infty} m^i = M. \right\}. \quad (6.7)$$

*Then only a finite number of the terms  $m^i$  are non-zero and all the non-zero terms are equal. In addition, if one  $m^i$  is less than  $2^{-2/3}\pi$ , then it is the only non-zero term.*

The proof is presented in Section 6.3. We will also need the following corollary on the stability of  $E_0^{2d}$  under perturbation of mass:

**Corollary 6.3.** *The function  $\overline{e_0^{2d}}$  is Lipschitz continuous on  $[\delta, 1/\delta]$  for any  $0 < \delta < 1$ .*

The limit as  $\eta \rightarrow 0$  of the functional  $F_\eta^{2d}$  has one additional term in comparison to the three-dimensional case, which arises from the second term in (3.6),

$$-\frac{1}{2\pi} \sum_{i=1}^{\infty} \int_{\mathbf{R}^2} \int_{\mathbf{R}^2} z_\eta^i(x) z_\eta^i(y) \log|x-y| dx dy. \quad (6.8)$$

To motivate the limit of this term, recall that  $z_\eta^i$  appears in the minimization problem (6.1), which has only balls as solutions. Assuming  $z_\eta^i$  to be a characteristic function of a ball of mass  $m^i$ , we calculate that (6.8) has the value  $f_0(m^i)$ , where

$$f_0(m) := \frac{m^2}{8\pi} \left( 3 - 2 \log \frac{m}{\pi} \right).$$

We therefore define the intended  $\Gamma$ -limit  $F_0^{2d}$  of  $F_\eta^{2d}$  as follows. First let us introduce some notation: for  $n \in \mathbf{N}$  and  $m > 0$  the sequence  $n \otimes m$  is defined by

$$(n \otimes m)^i := \begin{cases} m & 1 \leq i \leq n \\ 0 & n+1 \leq i < \infty. \end{cases}$$

Let  $\widetilde{\mathcal{M}}$  be the set of optimal sequences for the problem (6.7):

$$\widetilde{\mathcal{M}} := \left\{ n \otimes m : n \otimes m \text{ minimizes (6.7) for } M = nm, \text{ and } \overline{e_0^{2d}}(m) = e_0^{2d}(m) \right\}.$$

Then define

$$F_0^{2d}(v) := \begin{cases} n \left\{ f_0(m) + m^2 g^{(2)}(0) \right\} + \\ \quad \frac{m^2}{2} \sum_{\substack{i,j \geq 1 \\ i \neq j}} G_{\mathbf{T}^2}(x^i - x^j) & \text{if } v = m \sum_{i=1}^n \delta_{x^i}, \{x^i\} \text{ distinct, } n \otimes m \in \widetilde{\mathcal{M}}, \\ \infty & \text{otherwise.} \end{cases} \quad (6.9)$$

**Theorem 6.4.** *Within the space  $X$ , we have*

$$F_\eta^{2d} \xrightarrow{\Gamma} F_0^{2d} \quad \text{as } \eta \rightarrow 0.$$

*That is, Conditions 1 and 2 of Theorem 6.1 hold with  $E_\eta^{2d}$  and  $E_0^{2d}$  replaced with  $F_\eta^{2d}$  and  $F_0^{2d}$  respectively.*

The proof of this theorem again closely follows that of Theorem 4.5. The compactness property (6.6) in the lower bound follows by a simpler argument than in three dimensions, however. Using the division into components with connected support (6.3), we have

$$\begin{aligned} \mathbb{F}_\eta^{2d}(v_\eta) &= |\log \eta| \left[ \mathbb{E}_\eta^{2d}(v_\eta) - \overline{e_0^{2d}} \left( \int_{\mathbf{T}^2} v_\eta \right) \right] \\ &= |\log \eta| \sum_{i=1}^{\infty} \left[ \int_{\mathbf{R}^2} |\nabla z_\eta^i| + \frac{1}{2\pi} \left( \int_{\mathbf{R}^2} z_\eta^i \right)^2 - e_0^{2d} \left( \int_{\mathbf{R}^2} z_\eta^i \right) \right] \\ &\quad + |\log \eta| \sum_{i=1}^{\infty} \left[ e_0^{2d} \left( \int_{\mathbf{R}^2} z_\eta^i \right) - \overline{e_0^{2d}} \left( \int_{\mathbf{R}^2} z_\eta^i \right) \right] \end{aligned} \tag{6.10}$$

$$+ |\log \eta| \left[ \sum_{i=1}^{\infty} \overline{e_0^{2d}} \left( \int_{\mathbf{R}^2} z_\eta^i \right) - \overline{e_0^{2d}} \left( \int_{\mathbf{T}^2} v_\eta \right) \right] \tag{6.11}$$

$$+ \sum_{i=1}^{\infty} \left\{ -\frac{1}{2\pi} \int_{\mathbf{R}^2} \int_{\mathbf{R}^2} z_\eta^i(x) z_\eta^i(y) \log |x-y| dx dy + \int_{\mathbf{T}^2} \int_{\mathbf{T}^2} v_\eta^i(x) v_\eta^i(y) g^{(2)}(x-y) dx dy \right\} \tag{6.12}$$

$$+ \sum_{\substack{i,j=1 \\ i \neq j}}^{\infty} \int_{\mathbf{T}^2} \int_{\mathbf{T}^2} v_\eta^i(x) v_\eta^j(y) G_{\mathbf{T}^2}(x-y) dx dy. \tag{6.13}$$

The last two lines in the development above are uniformly bounded from below. Since  $\mathbb{F}_\eta^{2d}(v_\eta)$  is bounded from above, it follows that the terms in square brackets, which are non-negative, tend to zero. In combination with the continuity of  $e_0^{2d}$  and  $\overline{e_0^{2d}}$  this implies the compactness property (6.6). We also remark that because the contents of the square brackets in (6.10) and (6.11) is zero in the limit, we find with the aid of Lemma 6.2 that the number of concentration points  $x^i$  in the weak limit of  $v_\eta$  is finite with equal coefficient weights. Moreover, we may assume that there are a finite number of different components of  $v_\eta$ , and each must converge to a different  $x^i$ ; otherwise, the last term (6.13) would tend to  $\infty$  as  $\eta$  tends to 0.

Letting  $\eta \rightarrow 0$  and using the the definition (6.8) of  $f_0$ , one readily sees that the terms (6.12) and (6.13) directly correspond to the respective three terms of (6.9). The upper bound directly follows the arguments in three dimensions, now taking optimal two-dimensional balls for the sequence.

### 6.3 Proofs of Lemma 6.2 and Corollary 6.3

The proof of Lemma 6.2 contains two elements. The first element is general, and only uses the property that  $e_0^{2d}$  is concave on  $\left[0, \frac{\pi}{\sqrt[3]{4}}\right]$  and convex on  $\left[\frac{\pi}{\sqrt[3]{4}}, \infty\right)$ . This property reduces the possibilities to a combination of (a) a finite number of equal  $m^i$  in the convex region with possibly (b) one  $m^i$  in the concave region (see [20, Section 5.4] for a similar reasoning). The second part, in which possibility (b) above is excluded, depends heavily on the exact form of  $e_0^{2d}$ , and is an uninspiring exercise in estimation.

**Proof of Lemma 6.2:** For this proof only, let us abuse notation and use  $x, x^i, y, z$  to denote positive real numbers. We note that

$$e_0^{2d}(m) = 2^{5/3} \pi f\left(\frac{m}{\pi 2^{4/3}}\right) \quad \text{with} \quad f(x) = x^2 + \sqrt{x}.$$

We therefore continue with  $f$  instead of  $e_0^{\text{d}}$ . Since  $f$  is concave on  $(0, \frac{1}{4}]$  and convex on  $[\frac{1}{4}, \infty)$ , the following hold true:

- There is at most one  $x^i \in (0, \frac{1}{4})$ ; for if  $x^i, x^j \in (0, \frac{1}{4})$ , then

$$\left. \frac{d^2}{d\varepsilon^2} (f(x^i + \varepsilon) + f(x^j - \varepsilon)) \right|_{\varepsilon=0} = f''(x^i) + f''(x^j) < 0,$$

contradicting minimality. Therefore only one non-zero element is less than  $\frac{1}{4}$ , which also implies that the number of non-zero elements is finite.

- The set of elements  $\{x^i : x^i \geq \frac{1}{4}\}$  is a singleton, since the function is convex on  $[\frac{1}{4}, \infty)$ .

Therefore the lemma is proved if we can show the following. Take any sequence of the form

$$x^i = \begin{cases} x & i = 1 \\ y & i = 2, \dots, n+1 \\ 0 & i \geq n+2, \end{cases} \quad (6.14)$$

with  $x < 1/4 \leq y$ ; then this sequence can *not* be a solution of the minimization problem (6.7).

To this end, we first note that

$$(n+1)f\left(\frac{n}{n+1}y\right) - nf(y) = \frac{n}{n+1}\sqrt{y} \left( -y^{3/2} + (n+1) \left( \sqrt{\frac{n+1}{n}} - 1 \right) \right).$$

If this expression is negative, then by replacing the  $n$  copies of  $y$  in (6.14) by  $n+1$  copies of  $ny/(n+1)$  we decrease the value in (6.7). Therefore we can assume that

$$\frac{1}{4} \leq y \leq y_m(n) := (n+1)^{2/3} \left( \sqrt{\frac{n+1}{n}} - 1 \right)^{2/3}.$$

We distinguish two cases. **Case one:** If  $y + x/n < y_m(n)$ , then we compare our sequence (6.14) with  $n$  copies of  $z := y + x/n$ :

$$\begin{aligned} f(x) + nf(y) - nf(y + x/n) &= f(x) + nf(z - x/n) - nf(z) \\ &= x^2 \left( 1 + \frac{1}{n} \right) - 2xz + \sqrt{x} + n\sqrt{z - \frac{x}{n}} - n\sqrt{z} \\ &=: g(x, z). \end{aligned}$$

We now show that  $g$  is strictly positive for all relevant values of  $x$  and  $z$ , i.e. for  $0 < x < 1/4$  and  $1/4 + 1/n < z < y_m(n)$ .

Differentiating  $g(x, z)/x$  we find that

$$\frac{\partial}{\partial x} \frac{g(x, z)}{x} = 1 + \frac{1}{n} - \frac{1}{2x^{3/2}} - \frac{n}{x^2} \left( \sqrt{z - \frac{x}{n}} - \sqrt{z} \right) - \frac{1}{2x\sqrt{z - \frac{x}{n}}}. \quad (6.15)$$

This expression is negative:  $x < 1/4$  implies that

$$1 + \frac{1}{n} - \frac{1}{2x^{3/2}} < 0,$$

and by concavity of the square root function we have

$$\sqrt{z} \leq \sqrt{z - \frac{x}{n}} + \frac{1}{2\sqrt{z - \frac{x}{n}}} \frac{x}{n},$$

so that the last two terms in (6.15) together are also negative.

Since  $g(x, z)/x$  is decreasing in  $x$ , it is bounded from below by

$$4g(1/4, z) = \frac{1}{4} \left(1 + \frac{1}{n}\right) - 2z + 2 + 4n \left(\sqrt{z - \frac{1}{4n}} - \sqrt{z}\right).$$

The right-hand side of this expression is concave in  $z$ , and therefore bounded from below by the values at  $z = (1 + 1/n)/4$  and at  $z = y_m(n)$ . The first of these is

$$-\frac{1}{4} \left(1 + \frac{1}{n}\right) + 2 + 2n \left(1 - \sqrt{1 + \frac{1}{n}}\right) \geq -\frac{1}{2} + 2 + 2n(1 - (1 - 1/2n)) = \frac{1}{2}.$$

For the second, the expression

$$4g(1/4, y_m(n)) = \frac{1}{4} \left(1 + \frac{1}{n}\right) - 2y_m(n) + 2 + 4n \left(\sqrt{y_m(n) - \frac{1}{4n}} - \sqrt{y_m(n)}\right)$$

is positive for  $n = 1, 2$ , as can be checked explicitly; for  $n \geq 3$ , we estimate  $2^{-2/3} \leq y_m(n) \leq ((n+1)/2n)^{2/3}$  and therefore

$$\begin{aligned} & \frac{1}{4} \left(1 + \frac{1}{n}\right) - 2y_m(n) + 2 + 4n \left(\sqrt{y_m(n) - \frac{1}{4n}} - \sqrt{y_m(n)}\right) \\ & \geq \frac{1}{4} - 2 \left(\frac{n+1}{2n}\right)^{2/3} + 2 - \frac{1}{2\sqrt{y_m(n) - \frac{1}{4n}}} \\ & \geq \frac{9}{4} - 2 \left(\frac{n+1}{2n}\right)^{2/3} - \frac{1}{2\sqrt{2^{-2/3} - \frac{1}{12}}} \end{aligned}$$

The right-hand side of this expression is strictly positive for all  $n \geq 3$ . This concludes the proof of case one.

For **case two** we assume that  $y + x/n \geq y_m(n)$ , set

$$z := \frac{ny + x}{n+1},$$

and compare the original structure with  $n+1$  copies of  $z$ :

$$\begin{aligned} f(x) + nf(y) - (n+1)f(z) &= f(x) + nf\left(\frac{n+1}{n}z - \frac{x}{n}\right) - (n+1)f(z) \\ &= \frac{n+1}{n}(z-x)^2 + \sqrt{x} + \sqrt{n}\sqrt{(n+1)z-x} - (n+1)\sqrt{z} \\ &=: h(x, z). \end{aligned}$$

Note that the admissible values for  $z$  are

$$\frac{n}{n+1}y_m(n) \leq z \leq \frac{ny_m(n) + x}{n+1} \leq y_m(n). \quad (6.16)$$

We first restrict ourselves to  $n \geq 2$ , and state an intermediary lemma:

**Lemma 6.5.** *Let  $n \geq 2$ . Then for all  $0 < x < 1/4$  and for all  $z$  satisfying (6.16),*

$$h(x, z) > \min\{h(0, z), h(1/4, z)\}.$$

Assuming this lemma for the moment, we first remark that  $h(0, z) \geq 0$  by the bound  $z \geq ny_m(n)/(n+1)$  and the definition of  $y_m$ . For the other case we remark that the function

$$n \mapsto \sqrt{n}\sqrt{(n+1)z-x} - (n+1)\sqrt{z}$$

is increasing in  $n$  for fixed  $z$ . Keeping in mind that  $n \geq 2$  we therefore have

$$h(1/4, z) \geq \frac{3}{2}\left(z - \frac{1}{4}\right)^2 + \frac{1}{2} + \sqrt{2}\sqrt{3z - \frac{1}{4}} - 3\sqrt{z},$$

and this function is positive for all  $z \geq 2y_m(2)/3 \approx 0.51$ . This concludes the proof for  $n \geq 2$ .

Before we prove Lemma 6.5 we first discuss the case  $n = 1$ , for which

$$h(x, z) = 2(z-x)^2 + \sqrt{x} + \sqrt{2z-x} - 2\sqrt{z}.$$

The domain of definition of  $z$  is

$$\left[\frac{1}{2}y_m(1), y_m(1)\right] \subset [0.4410, 0.8821].$$

The mixed derivative  $h_{zx}$  is negative on the domain of  $x$  and  $z$ , so that

$$h_z(x, z) \geq h_z(1/4, z) = 4z - 1 + \frac{1}{\sqrt{2z - 1/4}} - \frac{1}{\sqrt{z}}.$$

This expression is again positive for the admissible values of  $z$ , and we find

$$h(x, z) \geq h\left(x, \frac{1}{2}y_m(1)\right) = 2\left(\frac{1}{2}y_m(1) - x\right)^2 + \sqrt{x} + \sqrt{y_m(1) - x} - 2\sqrt{\frac{1}{2}y_m(1)}.$$

Similarly this expression is non-negative for all  $0 \leq x \leq 1/4$ , which concludes the proof for the case  $n = 1$ .  $\square$

**Proof of Corollary 6.3:** Fix  $0 < \delta < 2^{-2/3}\pi$  and  $M \in [\delta, 1/\delta]$ ; by Lemma 6.2 there exist  $n, m$  with  $M = nm$  such that  $\overline{e_0^{2d}}(M) = n e_0^{2d}(m)$ . Note that if  $n = 1$  then  $m = M \geq \delta$ , and if  $n > 1$  then by Lemma 6.2  $m \geq 2^{-2/3}\pi > \delta$ ; therefore we have  $m \geq \delta$  and  $n \leq M/\delta$ . Since  $\overline{e_0^{2d}}$  is the pointwise minimum of a collection of functions  $e_0^{2d}$ , local Lipschitz continuity of  $\overline{e_0^{2d}}$  now follows from the same property for the functions  $e_0^{2d}$  on the domain  $[\delta, 1/\delta]$ .  $\square$

We still owe the reader the proof of Lemma 6.5.

**Proof of Lemma 6.5:** We first show that if  $4/25 \leq x \leq 1/4$ , then  $h_x(x, z) < 0$ . We estimate the derivative by using the bounds on  $z$  and  $x$ :

$$\begin{aligned} h_x(x, z) &= -2\frac{n+1}{n}(z-x) - \frac{\sqrt{n}}{2\sqrt{(n+1)z-x}} + \frac{1}{2\sqrt{x}} \\ &\leq -2y_m(n) + \frac{n+1}{2n} - \frac{\sqrt{n}}{2\sqrt{ny_m(n)}} + \frac{5}{4}. \end{aligned}$$



Note that  $y_m$  is monotonically decreasing in  $n$ , and that we can estimate  $y_m$  from below by

$$y_m(n)^{3/2} = (n+1) \left( \sqrt{1 + \frac{1}{n}} - 1 \right) \geq (n+1) \frac{1}{2\sqrt{\frac{n+1}{n}}} \frac{1}{n} = \frac{1}{2} \sqrt{\frac{n+1}{n}}.$$

Using  $n \geq 2$  we find

$$h_x(x, z) \leq -2 \cdot 2^{-2/3} \left( \frac{n+1}{n} \right)^{1/3} + \frac{n+1}{2n} - \frac{1}{2\sqrt{y_m(2)}} + \frac{5}{4} =: \ell \left( \frac{n+1}{n} \right).$$

The function  $\ell$  is increasing on  $[1, \infty)$ , and we have

$$\ell \left( \frac{n+1}{n} \right) \leq \ell \left( \frac{3}{2} \right) < 0.$$

On the remaining region  $0 < x < 4/25$  the second derivative  $h_{xx}$  is negative:

$$\begin{aligned} h_{xx}(x, z) &= 2 \frac{n+1}{n} - \frac{\sqrt{n}}{4((n+1)z - x)^{3/2}} - \frac{1}{4x^{3/2}} \\ &\leq 3 - \frac{1}{4} \frac{125}{8} < 0. \end{aligned}$$

For any fixed  $z$ , therefore, the function  $x \mapsto h(x, z)$  takes its minimum on the boundary, that is in one of the two points  $x = 0$  and  $x = 1/4$ . Since the first derivative is non-zero on  $[4/25, 1/4]$ , and since the second derivative is non-zero on  $(0, 4/25]$ , the minimum is only attained on the boundary. This concludes the proof of Lemma 6.2.  $\square$

## 7 Discussion

The results of this work provide a rigorous connection between the detailed, micro-scale model defined by  $\mathcal{E}$  in (1.2) and the macroscopic, upscaled models given by the limiting energies  $E_0^{2d}$ ,  $F_0^{2d}$ ,  $E_0^{3d}$ , and  $F_0^{3d}$ . We now discuss some related aspects.

*Differences between the two- and three-dimensional cases: scaling.* The consequences of the difference between two and three dimensions in the scaling of the  $H^{-1}$ -norm are best appreciated in the Green's functions in the whole space: if we replace  $x$  by  $\eta x$ , then

$$\log \eta x = \log \eta + \log x \quad \text{in 2D, and} \quad \frac{1}{|\eta x|} = \frac{1}{\eta} \cdot \frac{1}{|x|} \quad \text{in 3D.}$$

The difference between the additive effects in two dimensions and the multiplicative effect in three dimensions is responsible for the difference between the two limiting problems:

$$\int |\nabla z| + \left( \int z \right)^2 \quad \text{in two dimensions, and} \quad \int |\nabla z| + \|z\|_{H^{-1}}^2 \quad \text{in three.}$$

*Differences between the two- and three-dimensional cases: local problems.* Because of this difference in scaling, the local energy contributions  $e_0^{2d}$  (and  $\overline{e_0^{2d}}$ ) and  $e_0^{3d}$  are necessarily different, and since the two-dimensional local problem is the isoperimetric problem, its solution

can be calculated explicitly in terms of  $m$ . For the three-dimensional local problem we can only conjecture on the structure of minimizers (see below).

In addition to this, there is a difference in the handling of the lower semicontinuity in two and three dimensions. This comes from the fact that the definition of  $e_0^{2d}$  presupposes that the mass of  $z$  remains localized (does not escape to infinity) while the definition of  $e_0^{3d}$  does not. As a result, the function  $e_0^{3d}$  already has the right lower semi-continuity properties, while for  $e_0^{2d}$  we need to explicitly construct the lower-semicontinuous envelope function  $\overline{e_0^{2d}}$ .

Some of the other differences are only apparent. For instance, the requirement, in the definition of  $F_0^{3d}$ , that for each  $m^i$  the minimization problem  $e_0^{3d}(m^i)$  admits a minimizer, is mirrored in two dimensions by the compactness property  $\overline{e_0^{2d}}(m^i) = e_0^{2d}(m^i)$ . The reduction to ‘blobs’ of bounded and separated support (Lemma 5.2) is immediate in two dimensions, since it follows from the vanishing of the perimeter.

*Minimizers of the local problem in three dimensions.* For the three-dimensional minimization problem (4.1) one can show a number of properties. For instance, the concaveness of  $e_0^{3d}$  for small  $m$  implies that for small  $m$  minimizing sequences are compact, and the minimizers are balls. One can also show that for sufficiently large  $m$ , a ball with volume  $m$  will be unstable with respect to symmetry-breaking perturbations; Ren and Wei have documented this phenomenon in two space dimensions [32]. For the three-dimensional case, however, one can show that balls become unstable with respect to splitting into two balls of half the volume before they become unstable with respect to small symmetry-breaking perturbations. This leads us to postulate that *All global minimizers of the problem (4.1) are balls.* We will discuss this variational problem further in [13].

*Limiting structures.* In both two and three dimensions, the limiting energies ‘at the next level’  $F_0^{2d}$  and  $F_0^{3d}$  penalize proximity of particles as if they were electrically charged. In two dimensions Lemma 6.2 guarantees that the masses  $m^i$ , which play the role of the charges of the particles, are all the same; in three dimensions we conjecture that the same holds, although currently we are not able to exclude the possibility of  $(n - 1)$  equal masses and one different mass.

The question whether minimizers of these Coulomb energies are necessarily periodic is a subtle one. It is easy to construct numerical examples of bounded domains on which minimizers *can not* be periodic; see e.g. [30] for examples on discs in  $\mathbf{R}^2$ . At the same time, the examples with many particles do show a tendency to a triangular packing away from the boundary. In the physical literature such structures are known as *Wigner crystals*, and in that field it is generally assumed that periodic structures have lowest energy. As far as we know, there are no rigorous results that show periodicity without any *a priori* assumptions on the geometry. Turning to what can be proved, the closest related results we know of are: (i) a novel application of the modular function to show that among periodic structures, spot patterns on a hexagonal lattice have minimal energy [11]; (ii) for the two-dimensional, Leonard-Jones crystallization result of [36]. Moreover, for the full problem (1.2), the only *periodicity-like* results we know of, in dimension larger than one, a statement concerning the uniformity of the energy distribution on large boxes [3], and for finite-size structures in  $\mathbf{R}^n$  a scaling result bounding the energy in terms of lower-dimensional energies [17].

*The role of the mass constraint.* Note that in the main theorems (6.1, 6.4, 4.3, and 4.5) there is no mass constraint, as in (1.3), but only the weaker requirement that  $\int v$  is bounded. This merits some remarks:

- Free minimization of the limiting functionals  $E_0^{2d}$ ,  $F_0^{2d}$ ,  $E_0^{3d}$ , and  $F_0^{3d}$  simply yields the zero function with zero energy. In order to have a non-trivial object in the limit some additional restriction is therefore necessary. Typically one expects to have a sequence  $v_\eta$  for which the mass either is fixed or converges to a positive value.
- The fact that only boundedness of  $\int v$  is required also implies that this scaling of mass is the smallest one to give (for this scaling of the energies) non-trivial results; if  $\int v$  converges to zero, then the limiting energies are also zero, and no structure can be determined. This conclusion resonates with the fact that in the formal phase diagram of the Ohta-Kawasaki functional (1.1) the phase at the extreme ends of the volume fraction range is the spherical phase [12].

*Related work.* Our results are consistent with and complementary to three other recent studies in the regime of small volume fraction. In [31] Ren and Wei prove the existence of sphere-like solutions to the Euler-Lagrange equation of (1.1), and further investigate their stability. They also show that the centers of sphere-like solutions are close to global minimizers of an effective energy defined over delta measures which includes both a local energy defined over each point measure, and a Green's function interaction term which sets their location. While their results are similar in spirit to ours, they are based upon completely different techniques which are local rather than global.

Very recently, Muratov [22] proves a strong and rather striking result for the sharp interface problem in two dimensions. In an analogous small volume fraction regime, he proves that the global minimizers are *close* to being identical circular droplets of a small size separated by large distances. While this result does not precisely determine the placement of the droplets – ideally proving periodicity of the ground state, to our knowledge it presents the first rigorous work characterizing some *geometric* properties of the ground state (global minimizer).

In [18, 23] the authors explore the dynamics of small spherical phases for a gradient flow for (1.2) with small volume fraction. Here one finds a separation of time scales for the dynamics: Small particles both exchange material as in usual Ostwald ripening, and migrate because of an effectively repulsive nonlocal energetic term. Coarsening via mass diffusion only occurs while particle radii are small, and they eventually approach a finite equilibrium size. Migration, on the other hand, is responsible for producing self-organized patterns. By constructing approximations based upon an Ansatz of spherical particles similar to the classical LSW (Lifshitz-Slyozov-Wagner) theory, one derives a finite dimensional dynamics for particle positions and radii. For large systems, kinetic-type equations which describe the evolution of a probability density are constructed. A separation of time scales between particle growth and migration allows for a variational characterization of spatially inhomogeneous quasi-equilibrium states. Heuristically this matches our findings of (a) a first order energy which is local and essentially driven by perimeter reduction, and (b) a Coulomb-like interaction energy, at the next level, responsible for placement and self organization of the pattern. It would be interesting if one could make these statements precise via the calculation of gradient flows and their connection with  $\Gamma$ -convergence [33].

We further note that this asymptotic study has much in common with the asymptotic analysis of the well-known *Ginzburg-Landau functional* for the study of magnetic vortices (*cf.* [34, 19, 2]). However our problem is much more direct as it pertains to the asymptotics of the support of minimizers. This is in strong contrast to the Ginzburg-Landau functional

wherein one is concerned with an intrinsic vorticity quantity which is captured via a certain gauge-invariant Jacobian determinant of the order parameter.

Although the energy functional (1.1) provides a relatively simple, and mathematically accessible, description of patterns in this block copolymer system, rigorous results characterizing minimal-energy patterns in higher dimensions are few and far between. We also mention the comparison of large, localized structures in multiple dimensions with extended lower-dimensional structures [17]. For a slightly different model for block copolymer behavior additional results are available. In [26, 27, 28] the authors study an energy functional consisting of two terms as in  $\mathcal{E}$  in (1.2), but with the  $H^{-1}$ -norm replaced by the  $W^{-1,1}$ -norm, or equivalently by the Wasserstein distance of order 1. For this functional the authors study the symmetric regime, in which  $A$  and  $B$  appear in equal amounts; a parameter  $\varepsilon$  characterizes the small length scale of the patterns. They prove that low-energy structures in two dimensions become increasingly stripe-like as  $\varepsilon \rightarrow 0$ , that the stripe width approaches  $\varepsilon$ , and that the Gamma-limit of the rescaled energy measures the square of the local stripe curvature.

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