Emergence of non-trivial minimizers for the three-dimensional Ohta-Kawasaki energy

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November 6, 2018

Abstract

This paper is concerned with the diffuse interface Ohta-Kawasaki energy in three space dimensions, in a periodic setting, in the parameter regime corresponding to the onset of non-trivial minimizers. We identify the scaling in which a sharp transition from asymptotically trivial to non-trivial minimizers takes place as the small parameter characterizing the width of the interfaces between the two phases goes to zero, while the volume fraction of the minority phases vanishes at an appropriate rate. The value of the threshold is shown to be related to the optimal binding energy solution of Gamow's liquid drop model of the atomic nucleus. Beyond the threshold the average volume fraction of the minority phase is demonstrated to grow linearly with the distance to the threshold. In addition to these results, we establish a number of properties of the minimizers of the sharp interface screened Ohta-Kawasaki energy in the considered parameter regime. We also establish rather tight upper and lower bounds on the value of the transition threshold.

Contents

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1 Introduction and main results

The Ohta-Kawasaki energy is a prototypical energy functional in the studies of spatially modulated phases that appear as a result of the competition of short-range attractive and long-range repulsive forces in physical systems of very different nature. Although it was originally introduced in the context of microphase separation in diblock copolymer melts [25], Ohta-Kawasaki energy is relevant to a wide range of both soft and hard condensed matter systems (for a discussion of the specific physical systems see, e.g., [23] and references therein), as well as to dense nuclear matter at the other extreme of energy and spatial scales [16, 20]. From the mathematical point of view, Ohta-Kawasaki energy functional, together with the closely related Thomas-Fermi-Dirac-von Weizsäcker energy [14, 17, 18, 29], serve as a paradigm for energy-driven pattern forming systems with competing interactions [4], which is why the associated variational problem has received an increasing amount of attention in recent years [3, 5, 6, 12, 13, 19, 24, 28].

In the macroscopic setting, one considers the Ohta-Kawasaki energy functional defined on a sufficiently large box with periodic boundary conditions, i.e., for $u \in H^1(\mathbb{T}_\ell)$ one sets

$$\mathcal{E}_\varepsilon(u) := \int_{\mathbb{T}_\ell} \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + \frac{1}{4}(1-u^2)^2 + \frac{1}{2}(u - \bar{u}_\varepsilon)(-\Delta)^{-1}(u - \bar{u}_\varepsilon) \right) dx, \tag{1.1}$$

where $\mathbb{T}_\ell$ is the flat d-dimensional torus with sidelength $\ell > 0$, $\varepsilon > 0$ is the parameter characterizing interfacial thickness and assumed to be sufficiently small, and $\bar{u}_\varepsilon \in (-1, 1)$ is the parameter equal to the constant background charge density. In the sequel will investigate the limit $\varepsilon \to 0$, assuming that u_ε depends on ε suitably. Of course, the physical dimension of the underlying spatial domain is $d = 3$. The definition in (1.1) needs to be supplemented with the "electroneutrality" constraint in order to make sense of the last term in (1.1):

$$\frac{1}{\ell^d} \int_{\mathbb{T}_\ell} u \, dx = \bar{u}_\varepsilon. \tag{1.2}$$

One then wishes to characterize global energy minimizers of the energy in (2.1) for all ℓ sufficiently large. These global energy minimizers are expected to determine the ground states of the corresponding physical system in a macroscopically large sample.

It is widely believed that as the value of ℓ is increased with all other parameters fixed, the global energy minimizer of $\mathcal{E}_\varepsilon$ should be either constant or spatially periodic, with period approaching a constant independent of ℓ as $\ell \to \infty$. Proving such a *crystallization* result would be one of the main challenges in the theory of energy-driven pattern formation and is currently out of reach (for a recent review, see [1]), except for the case $d = 1$, $\bar{u}_\varepsilon \in (-1, 1)$ fixed and $\varepsilon > 0$ sufficiently small [2, 22, 26] (for a very recent result in that direction in higher dimensions, see [7]). On the other hand, it is known that for $\bar{u}_\varepsilon \in (-1,1)$ fixed, global energy minimizers are not constant as soon as $\varepsilon \ll 1$ and $\ell \gtrsim 1$ [3, 24]. This is in contrast with the case $\bar{u}_\varepsilon \notin (-1,1)$, for which by direct inspection $u = \bar{u}_\varepsilon$ is the unique global minimizer of the energy. Thus, a transition from the trivial minimizer $u = \bar{u}_\varepsilon$ to a non-trivial, spatially non-uniform minimizer of $\mathcal{E}_\varepsilon$ must occur for $\varepsilon \ll 1$ and $\ell \gtrsim 1$ fixed as the value of $\bar{u}_\varepsilon$ increases from $\bar{u}_\varepsilon = -1$ towards $\bar{u}_\varepsilon = 0$ (in view of the symmetry exhibited by the energy when changing $u \to -u$, it is sufficient to consider only the case $\bar{u}_\varepsilon \leq 0$). In fact, for $d \geq 2$ non-trivial minimizers emerge at some $\bar{u}_\varepsilon = -1 + \delta$ with $\varepsilon \lesssim \delta \lesssim \varepsilon^{2/3} |\ln \varepsilon|^{1/3}$ [6, 24], while for $d = 1$ they emerge for some $\varepsilon \lesssim \delta \lesssim \varepsilon^{1/2}$ [6, 23]. The nature of the transition towards non-trivial minimizers is quite delicate and at present not well understood.

In the absence of general results for non-trivial minimizers of $\mathcal{E}_\varepsilon$ for $\varepsilon \lesssim 1$, $\bar{u}_\varepsilon \in (-1,1)$ and $\ell \gg 1$ in $d \geq 2$, one can consider different asymptotic regimes that admit further analytical characterization. One such regime was analyzed in [12], where the behavior of the minimizers of $\mathcal{E}_\varepsilon$ was studied in the limit $\varepsilon \to 0$ for $\bar{u}_\varepsilon = -1 + \lambda \varepsilon^{2/3} |\ln \varepsilon|^{1/3}$, with $\lambda > 0$ and $\ell > 0$ fixed, in the case $d = 2$. In this regime, non-trivial minimizers are expected to consist of well separated "droplets" of the minority phase, i.e., regions where $u \simeq +1$ surrounded by the sea of the majority phase where $u \simeq -1$, separated by narrow domain walls of thickness $\sim \varepsilon$. It was found that there exists an explicit critical value of $\lambda = \lambda_c > 0$ such that the minimizers of $\mathcal{E}_\varepsilon$ are non-trivial for all $\lambda > \lambda_c$, while for $\lambda \leq \lambda_c$ the minimizers are "asymptotically trivial", namely, that the energy of the minimizers converges to that of $u = \bar{u}_\varepsilon$, and the minimizer converges to $u = \bar{u}_\varepsilon$ in a certain sense as $\varepsilon \to 0$. Moreover, the threshold value λ_c corresponding to the onset of non-trivial minimizers was found to be independent of ℓ, suggesting that the transition should persist to the macroscopic limit $\ell \to \infty$ with $\varepsilon \ll 1$ and $\bar{u}_\varepsilon$ fixed (i.e., when commuting the order of the $\varepsilon \to 0$ and $\ell \to \infty$ limits). The obtained non-trivial minimizers exhibit a kind of a homogenization limit, with mass distributing uniformly on average throughout the domain. Furthermore, by performing a two-scale expansion of the energy, one can make more precise conclusions about the detailed properties of the minimizers and, in particular, formulate a variational problem in the whole space that determines the placement of the connected components of the minimizers in terms of the so-called renormalized energy, whose minimizers are conjectured to concentrate on the vertices of a hexagonal lattice [13].

Here, we would like to understand how the transition to non-trivial minimizers happens when $\varepsilon \to 0$ and $\ell \gtrsim 1$ in the physical three-dimensional case. Therefore, from now on we fix $d = 3$ throughout the rest of the paper. Once again, in this regime the minimizers are expected to exhibit a two-phase character, with the minority phase occupying a small fraction of space. To this end, we define

$$\bar{u}_\varepsilon := -1 + \lambda \varepsilon^{2/3}, \tag{1.3}$$

where $\lambda > 0$ is fixed. Our main result is the following theorem.

Theorem 1.1. *Let $\ell > 0$ and $\lambda > 0$, and let $\mathcal{E}_\varepsilon$ be defined in* (1.1) *with $\bar{u}_\varepsilon$ given by* (1.3)*. Then, there exists a universal constant $\lambda_c > 0$ such that if u_ε is a minimizer of $\mathcal{E}_\varepsilon(u)$ among all $u \in H^1(\mathbb{T}_\ell)$ satisfying* (1.2)*, and $\mu_\varepsilon \in \mathcal{M}^+(\mathbb{T}_\ell)$ is such that $d\mu_\varepsilon(x) = \frac{1}{2}\varepsilon^{-2/3}(1 + \operatorname{sgn} u_\varepsilon(x))\, dx$, we have as $\varepsilon \to 0$:*

(i) $\mu_\varepsilon \rightharpoonup 0$ *in* $\mathcal{M}(\mathbb{T}_\ell)$ *if* $\lambda \le \lambda_c$.

(ii) $\mu_\varepsilon \rightharpoonup \bar{\mu}$ *in* $\mathcal{M}(\mathbb{T}_\ell)$, *where* $d\bar{\mu} = \frac{1}{2}(\lambda - \lambda_c)dx$, *if* $\lambda > \lambda_c$.

(iii) $\varepsilon^{-4/3}\mathcal{E}_\varepsilon(u_\varepsilon) \to \min\{\lambda^2\ell^3, \lambda_c(2\lambda - \lambda_c)\ell^3\}$.

Thus, the onset of non-trivial minimizers in three space dimensions occurs sooner in terms of $0 < 1+\bar{u}_\varepsilon \ll 1$ than the corresponding transition in two dimensions. In particular, cylindrical morphologies obtained by trivially extending the two-dimensional minimizers into the third dimension are no longer global energy minimizers. One would, therefore, expect that the emergent non-trivial minimizers consist of a collection of well separated small droplets of the minority phase surrounded by the sea of the majority phase. Furthermore, the size and the distance between the droplets would scale differently (cf. [15]) from those in two dimensions, and in contrast to the latter [12, 13] we can no longer conclude that the droplets are nearly spherical. Still, we are able to express the shape and size of the individual droplets in terms of the non-local isoperimetric problem in the whole space that goes back to Gamow [4,11] (for details, see the following sections). In particular, this allows us to obtain a quantitative estimate for the threshold λ_c, using balls as competitors in the whole space problem and a recent quantitative non-existence result for the Gamow's liquid drop model [9].

Theorem 1.2. *With the notation of Theorem 1.1, we have*

$$\frac{3}{4\sqrt[3]{2}} \le \lambda_c \le \frac{3}{2\sqrt[3]{5}}. \tag{1.4}$$

Note that numerically the bound in Theorem 1.4 appears to be fairly tight: $0.5952 < \lambda_c < 0.8773$, with the lower bound to within 33% of the value of the upper bound. Note that if the conjecture that the minimizers of Gamow's liquid drop model are balls is true, then the upper bound in Theorem 1.4 should in fact yield equality.

Our proof relies on our previous results obtained for the three-dimensional sharp interface version of the Ohta-Kawasaki energy [15]. Together with the approach from [24, Section 4], the result in Theorem 1.1 is obtained along the lines of the arguments in [12], suitably adapted from the two-dimensional to the three-dimensional case. Note, however, that the results in [15] cannot be directly combined with those of [24], since the sharp interface energy studied in [15] does not include the effect of *charge screening*. In fact, there is no transition from trivial to non-trivial minimizers in the unscreened sharp interface energy. Therefore, as a first step towards the proof one needs to adapt the results of [15] to the case of screened sharp interface energy and obtain an asymptotic characterization of its minimizers as $\varepsilon \to 0$.

As in [15], we separate the non-local energy into the near-field and far-field contributions, with screening appearing explicitly in the latter. At the same time, the self-interaction energy of the droplets turns out to be still well approximated by that of Gamow's liquid drop model. Combining the far-field with the near-field contributions to the energy then allows to establish a Γ-convergence result for the screened sharp interface energy to an energy functional which is quadratic in the limit charge density, with the notion of convergence being the weak convergence of measures. Along the way, we establish uniform estimates for the connected components of the minimizers similar to those in [15], which, in turn, allows to characterize non-existence of nontrivial minimizers of the screened sharp interface energy below the threshold for all ε sufficiently small.

Once the Γ-convergence result is established for the screened sharp interface energy, we proceed as in [12] by introducing a piecewise-constant charge density associated with the admissible configurations for the diffuse interface energy that eliminates the small deviations of the charge density from their equilibrium values ± 1 for the double-well potential (for a more detailed explanation of the need of such a step, see the beginning of Sec. 2.2 in [12]). We then adapt the arguments of [12, Section 6] to obtain the corresponding Γ-convergence result for the diffuse interface energy to the same quadratic functional in the limit charge density as for the screened sharp interface energy. Finally, explicitly minimizing the limit energy we obtain the main result of our paper contained in Theorem 1.1. Furthermore, we relate the value of the threshold λ_c with the optimal energy per unit mass for Gamow's liquid drop model. In addition, we use recent results in [9, 10] characterizing the minimizers of the latter problem to obtain sharp quantitative bounds on the value of the threshold.

To summarize, our paper provides an extension of various recent results for the diffuse interface Ohta-Kawasaki energy to the case of a macroscopic three-dimensional domain, establishing a sharp transition from trivial to nontrivial minimizers in the asymptotic limit of vanishingly thin interfaces. Most of the techniques used in our proofs are adaptations of those that appeared in the earlier studies of this problem in different settings. The main novelty of our results, however, is the way these arguments are combined to yield a nontrivial scaling for the transition to nontrivial minimizers and the limit energy functional for the three-dimensional Ohta-Kawasaki energy. To our knowledge, this is the first sharp asymptotic result for this energy in the regime of strong compositional asymmetry and large number of droplets (for the case of finitely many droplets, see [5]). We note that the present lack of knowledge about the minimizers of Gamow's liquid drop model prevents us to go to the next order in a two-scale Γ-expansion to describe local interactions of droplets via a "renormalized energy" [27]. In particular, it is not known at present whether the minimizer per unit mass exists only for a unique value of the mass (this would be true if minimizers were balls). Thus, further insights into the solution of Gamow's model would be needed to carry out the programme realized for the two-dimensional Ohta-Kawasaki energy in [13].

Our paper is organized as follows. In Sec. 2, we introduce the different energies appearing in our study and state a number of results related to each of the associated variational problems. Also in this section, we prove Theorem 2.2 that gives a quantitative lower bound for the self-interaction energy per unit mass for Gamow's liquid drop model. Then, in Sec. 3 we state the Γ-convergence result for the sharp interface energy in Theorem 3.2, followed by a proof. Also in Sec. 3, we provide some further results about the connected components of minimizers of the screened sharp interface energy, see Theorem 3.4 and Corollary 3.5. Finally, in Sec. 4 we state and prove the corresponding Γ-convergence result for the diffuse interface energy, see Theorem 4.1. The results in Theorems 1.1 and 1.2 are then obtained as simple corollaries of the above theorems.

2 Setting

In this section, we introduce the basic notation used throughout the rest of the paper, together with the assumptions and some technical results.

2.1 The diffuse interface energy

We begin by generalizing the diffuse energy functional in (1.1) to one involving an arbitrary symmetric double-well potential $W(u)$:

$$\mathcal{E}_\varepsilon(u) := \int_{\mathbb{T}_\ell} \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + W(u) + \frac{1}{2}(u - \bar{u}_\varepsilon)(-\Delta)^{-1}(u - \bar{u}_\varepsilon) \right) dx, \tag{2.1}$$

with $W(u)$ satisfying [24]:

(i) $W \in C^2(\mathbb{R})$, $W(u) = W(-u)$, and $W \geq 0$,

(ii) $W(+1) = W(-1) = 0$ and $W''(+1) = W''(-1) > 0$,

(iii) $W''(|u|)$ is monotonically increasing for $|u| \geq 1$, $\lim_{|u|\to\infty} W''(u) = +\infty$, and $|W'(u)| \leq C(1 + |u|^q)$, for some $C > 0$ and $1 < q < 5$.

This energy is clearly well-defined and bounded on the admissible class

$$\mathcal{A}_\varepsilon := \left\{ u \in H^1(\mathbb{T}_\ell) \ : \ \frac{1}{\ell^3} \int_{\mathbb{T}_\ell} u \, dx = \bar{u}_\varepsilon \right\}, \tag{2.2}$$

with the non-local term interpreted, as usual, with the help of the Green's function $G_0(x)$ solving

$$-\Delta G_0(x) = \delta(x) - \ell^{-3}, \qquad \int_{\mathbb{T}_\ell} G_0(x) \, dx = 0 \tag{2.3}$$

in $\mathcal{D}'(\mathbb{T}_\ell)$. Explicitly, the energy takes the form

$$\mathcal{E}_\varepsilon(u) = \int_{\mathbb{T}_\ell} \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + W(u) \right) dx + \frac{1}{2} \int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} (u(x) - \bar{u}_\varepsilon) G_0(x-y)(u(y) - \bar{u}_\varepsilon) \, dx \, dy, \tag{2.4}$$

noting that the last term in the right-hand side is well-defined by Young's inequality.

Under the assumptions above, every critical point $u \in \mathcal{A}_\varepsilon$ of $\mathcal{E}_\varepsilon$ solves weakly the Euler-Lagrange equation, which can be written as (see [24, Section 4])

$$-\varepsilon^2 \Delta u + W'(u) + v = \Lambda, \qquad -\Delta v = u - \bar{u}_\varepsilon, \tag{2.5}$$

where $v \in H^3(\mathbb{T}_\ell)$ is a zero-average solution of the second equation in (2.5) and $\Lambda \in \mathbb{R}$ is the Lagrange multiplier satisfying

$$\Lambda = \frac{1}{\ell^3} \int_{\mathbb{T}_\ell} W'(u) \, dx, \tag{2.6}$$

as can be seen by integrating the first equation in (2.5) over $\mathbb{T}_\ell$. In particular, we have

$$v(x) = \int_{\mathbb{T}_\ell} G_0(x-y)(u(y) - \bar{u}_\varepsilon) dy, \tag{2.7}$$

and $u, v \in C^\infty(\mathbb{T}_\ell)$, solving (2.5) classically [24, Section 4]. Also, by the direct method of calculus of variations, minimizers of $\mathcal{E}_\varepsilon$ are easily seen to exist for all choices of the parameters.

2.2 The sharp interface energy with screening

For $\varepsilon \ll 1$, minimizers of $\mathcal{E}_\varepsilon$ are expected to consist of functions which take values close to ± 1, except for narrow transition regions of width of order ε [24]. As usual, we define the energy of an optimal one-dimensional transition layer connecting $u = \pm 1$ [21]:

$$\sigma := \int_{-1}^{1} \sqrt{2W(s)} \, ds > 0. \tag{2.8}$$

We also define

$$\kappa := \frac{1}{\sqrt{W''(1)}} > 0, \tag{2.9}$$

characterizing the effect of charge screening appearing in the sharp interface version of the energy $\mathcal{E}_\varepsilon$, which we introduce in the sequel. With some obvious modifications, the results of [24, Section 4] apply to $\mathcal{E}_\varepsilon$ defined in (2.1), with the corresponding sharp interface energy E_ε defined as

$$E_\varepsilon(u) := \frac{\varepsilon\sigma}{2} \int_{\mathbb{T}_\ell} |\nabla u| \, dx + \frac{1}{2} \int_{\mathbb{T}_\ell} (u - \bar{u}_\varepsilon)(-\Delta + \kappa^2)^{-1}(u - \bar{u}_\varepsilon) \, dx, \tag{2.10}$$

where u belongs to the admissible class

$$\mathcal{A} := BV(\mathbb{T}_\ell; \{-1, 1\}). \tag{2.11}$$

Specifically, in the considered scaling regime we have the following relation between the two energies (see the following sections):

$$\frac{\min\limits_{u \in \mathcal{A}_\varepsilon} \mathcal{E}_\varepsilon(u)}{\min\limits_{u \in \mathcal{A}} E_\varepsilon(u)} \to 1 \qquad \text{as} \quad \varepsilon \to 0. \tag{2.12}$$

Notice that the neutrality constraint in (1.2) is no longer present in the case of the sharp interface energy.

The energy in (2.10) may be rewritten with the help of the Green's function as

$$E_\varepsilon(u) := \frac{\varepsilon\sigma}{2} \int_{\mathbb{T}_\ell} |\nabla u| \, dx + \frac{1}{2} \int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} (u(x) - \bar{u}_\varepsilon) G(x - y)(u(y) - \bar{u}_\varepsilon) \, dx \, dy, \tag{2.13}$$

where G solves

$$-\Delta G(x) + \kappa^2 G(x) = \delta(x) \qquad \text{in} \quad \mathcal{D}'(\mathbb{T}_\ell). \tag{2.14}$$

Notice that G has an explicit representation

$$G(x) = \frac{1}{4\pi} \sum_{\mathbf{n} \in \mathbb{Z}^3} \frac{e^{-\kappa|x - \mathbf{n}\ell|}}{|x - \mathbf{n}\ell|}. \tag{2.15}$$

In particular, we have

$$G(x) \simeq \frac{1}{4\pi|x|} \qquad |x| \ll 1, \qquad\qquad G(x) \geq c \qquad \forall x \in \mathbb{T}_\ell, \tag{2.16}$$

for some $c > 0$ depending on κ and ℓ. Also, integrating (2.14) we get

$$\int_{\mathbb{T}_\ell} G(x) dx = \kappa^{-2}. \tag{2.17}$$

The latter allows us to rewrite the energy E_ε in an equivalent form in terms of $\chi \in BV(\mathbb{T}_\ell; \{0, 1\})$, where

$$\chi(x) := \frac{1 + u(x)}{2} \qquad\qquad x \in \mathbb{T}_\ell, \tag{2.18}$$

as

$$E_\varepsilon(u) = \frac{\varepsilon^{4/3}\lambda^2\ell^3}{2\kappa^2} + \varepsilon\sigma \int_{\mathbb{T}_\ell} |\nabla\chi|\, dx - \frac{2\varepsilon^{2/3}\lambda}{\kappa^2} \int_{\mathbb{T}_\ell} \chi\, dx + 2 \int_{\mathbb{T}_\ell}\int_{\mathbb{T}_\ell} G(x-y)\chi(x)\chi(y)\, dx\, dy, \tag{2.19}$$

where we also used (1.2).

We now introduce a version of the energy E_ε written in terms of the rescaling

$$\tilde{\chi}(x) := \chi(\ell x/\ell_\varepsilon) \quad x \in \mathbb{T}_{\ell_\varepsilon}, \qquad \ell_\varepsilon := \left(\frac{4}{\sigma\varepsilon}\right)^{1/3} \ell. \tag{2.20}$$

With this definition we have $\tilde{\chi} \in \widetilde{\mathcal{A}}_{\ell_\varepsilon}$, where

$$\widetilde{\mathcal{A}}_{\ell_\varepsilon} := BV(\mathbb{T}_{\ell_\varepsilon}; \{0,1\}), \tag{2.21}$$

for every $\chi \in \mathcal{A}$, and $E_\varepsilon(\chi) = \widetilde{E}_{\ell_\varepsilon}(\tilde{\chi})$, with

$$\begin{aligned}\widetilde{E}_{\ell_\varepsilon}(\tilde{\chi}) := &\frac{\varepsilon^{4/3}\lambda^2\ell^3}{2\kappa^2} - \frac{\varepsilon^{5/3}\sigma\lambda}{2\kappa^2} \int_{\mathbb{T}_{\ell_\varepsilon}} \tilde{\chi}\, dx \\ &+ \left(\frac{\varepsilon^{5/3}\sigma^{5/3}}{4^{2/3}}\right) \left[\int_{\mathbb{T}_{\ell_\varepsilon}} |\nabla\tilde{\chi}|\, dx + \frac{1}{2}\int_{\mathbb{T}_{\ell_\varepsilon}} \tilde{\chi}\left(-\Delta + 4^{-2/3}\varepsilon^{2/3}\sigma^{2/3}\kappa^2\right)^{-1} \tilde{\chi}\, dx\right].\end{aligned} \tag{2.22}$$

Introducing G_ε, which solves

$$-\Delta G_\varepsilon(x) + 4^{-2/3}\kappa^2\varepsilon^{2/3}\sigma^{2/3} G_\varepsilon(x) = \delta(x) \qquad \text{in } \mathbb{T}_{\ell_\varepsilon}, \tag{2.23}$$

we can then express the energy $\widetilde{E}_{\ell_\varepsilon}$ as

$$\begin{aligned}\widetilde{E}_{\ell_\varepsilon}(\tilde{\chi}) := &\frac{\varepsilon^{4/3}\lambda^2\ell^3}{2\kappa^2} - \frac{\varepsilon^{5/3}\sigma\lambda}{2\kappa^2} \int_{\mathbb{T}_{\ell_\varepsilon}} \tilde{\chi}\, dx \\ &+ \left(\frac{\varepsilon^{5/3}\sigma^{5/3}}{4^{2/3}}\right) \left[\int_{\mathbb{T}_{\ell_\varepsilon}} |\nabla\tilde{\chi}|\, dx + \frac{1}{2}\int_{\mathbb{T}_{\ell_\varepsilon}} G_\varepsilon(x-y)\tilde{\chi}(x)\tilde{\chi}(y)\, dx\, dy\right].\end{aligned} \tag{2.24}$$

Note that, as in (2.15), we have the following representation for G_ε:

$$G_\varepsilon(x) = \frac{1}{4\pi} \sum_{\mathbf{n}\in\mathbb{Z}^3} \frac{e^{-4^{-1/3}\varepsilon^{1/3}\sigma^{1/3}\kappa|x-\mathbf{n}\ell_\varepsilon|}}{|x-\mathbf{n}\ell_\varepsilon|}. \tag{2.25}$$

2.3 The whole space energy

As was shown by us in [15], in the absence of screening, i.e., with $\kappa = 0$ and $u \in \mathcal{A}$ also satisfying (1.2), the asymptotic behavior of the minimizers of E_ε in (2.10) with $\bar{u}_\varepsilon$ satisfying (1.3) can be expressed in terms of those for the energy defined on the whole of $\mathbb{R}^3$:

$$\widetilde{E}_\infty(\tilde{\chi}) := \int_{\mathbb{R}^3} |\nabla \tilde{\chi}| \, dx + \frac{1}{8\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\tilde{\chi}(x)\tilde{\chi}(y)}{|x-y|} \, dx \, dy, \tag{2.26}$$

which is well defined in the admissible class

$$\widetilde{\mathcal{A}}_\infty := BV(\mathbb{R}^3; \{0,1\}). \tag{2.27}$$

In particular, the optimal self-energy per unit volume of the minority phase is

$$f^* := \inf_{\tilde{\chi} \in \widetilde{\mathcal{A}}_\infty} \frac{\widetilde{E}_\infty(\tilde{\chi})}{\int_{\mathbb{R}^3} \tilde{\chi} \, dx}. \tag{2.28}$$

Note that within the nuclear physics context, this is precisely the dimensionless form of the celebrated Gamow's liquid drop model of the atomic nucleus [11] (for a recent mathematical overview, see [4]). In particular, the value of f^* corresponds to the energy per nucleon in the tightest bound nucleus.

The relationship between E_ε and $\widetilde{E}_\infty$ can be seen formally by passing to the limit $\varepsilon \to 0$ in (2.24) with $\tilde{\chi}$ taken to be the characteristic function of a fixed bounded set restricted to $\mathbb{T}_{\ell_\varepsilon}$. Then we have

$$\left(\frac{4^{2/3}}{\varepsilon^{5/3} \sigma^{5/3}} \right) \left(\widetilde{E}_{\ell_\varepsilon}(\tilde{\chi}) - \frac{\varepsilon^{4/3} \lambda^2 \ell^3}{2\kappa^2} \right) \to -\frac{\lambda f^*}{\lambda_c} \int_{\mathbb{R}^3} \tilde{\chi} \, dx + \widetilde{E}_\infty(\tilde{\chi}), \tag{2.29}$$

where $\tilde{\chi}$ was extended by zero to the whole of $\mathbb{R}^3$, and we defined

$$\lambda_c := 2^{-1/3} \sigma^{2/3} \kappa^2 f^*. \tag{2.30}$$

The following result was recently established about minimizers of the problem in the whole space [9, 15].

Theorem 2.1. *There exists a bounded, connected open set $F^* \subset \mathbb{R}^3$ with smooth boundary such that*

$$f^* = \frac{\widetilde{E}_\infty(\tilde{\chi}_{F^*})}{\int_{\mathbb{R}^3} \tilde{\chi}_{F^*} \, dx}, \tag{2.31}$$

where χ_{F^*} is the characteristic function of the set F^*.

It has been conjectured that the minimizer of $\widetilde{E}_\infty$ with fixed mass is given by a ball whenever such a minimizer exists [5]. Therefore, taking a ball of radius R as a test function in (2.28) and optimizing in R, one obtains an estimate

$$f^* \leq 3^{5/3} \cdot 2^{-2/3} \cdot 5^{-1/3}. \tag{2.32}$$

The above conjecture would imply that the inequality in (2.32) is in fact an equality. Proving such a result is a difficult hard analysis problem that currently appears to be out of reach. Nevertheless, we can establish a first quantitative lower bound for the value of f^*, using equipartition of energy of F^* established in [10] and a quantitative upper bound on $|F^*|$ obtained in [9]. Note that the resulting lower bound equals about 67% of the upper bound in (2.32). This is one of the main results of the present paper.

Theorem 2.2. *We have*

$$f^* \geq \frac{3^{5/3}}{4}. \tag{2.33}$$

Proof. Let F^* be a minimizer from Theorem 2.1, and write

$$f^* = \frac{P(F^*) + V(F^*)}{|F^*|}, \tag{2.34}$$

where $P(F^*)$ is the perimeter of F^* and $V(F^*)$ is the Coulombic self-energy of F^*. By the result from [10], the energy exhibits a kind of equipartition

$$V(F^*) = \frac{1}{2} P(F^*), \tag{2.35}$$

which can be easily seen by considering the sets λF^* as competitors for f^* and taking advantage of the homogeneity of P and V with respect to dilations. Thus, we have

$$f^* = \frac{3P(F^*)}{2|F^*|}. \tag{2.36}$$

Therefore, applying the isoperimetric inequality yields

$$f^* \geq \left(\frac{243\pi}{2|F^*|} \right)^{1/3}. \tag{2.37}$$

The proof is then concluded by recalling the quantitative upper bound $|F^*| \leq 32\pi$ from [9]. □

2.4 The limit energy

For $\mu \in \mathcal{M}^+(\mathbb{T}_\ell) \cap H^{-1}(\mathbb{T}_\ell)$, define

$$E_0(\mu) := \frac{\lambda^2 \ell^3}{2\kappa^2} - \frac{2}{\kappa^2}(\lambda - \lambda_c) \int_{\mathbb{T}_\ell} d\mu + 2 \int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} G(x-y) d\mu(x) d\mu(y). \tag{2.38}$$

Note that $\mu \in \mathcal{M}^+(\mathbb{T}_\ell) \cap H^{-1}(\mathbb{T}_\ell)$ implies that μ is a non-negative Radon measure that has bounded Coulombic energy:

$$\int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} G(x-y)\, d\mu(x)\, d\mu(y) < \infty. \tag{2.39}$$

where G is the screened Coulombic kernel from (2.15). The converse is also true, i.e., a positive Radon measure with bounded Coulombic energy defines a bounded linear functional on $H^1(\mathbb{T}_\ell)$. This fact follows from the following lemma, whose proof is a straightforward adaptation of the proof of [12, Lemma 3.2] in two dimensions. In particular, it allows to extend the definition of E_0 to arbitrary positive Radon measures on $\mathbb{T}_\ell$, with $E_0(\mu) < +\infty$ if and only if $\mu \in H^{-1}(\mathbb{T}_\ell)$.

Lemma 2.3. *Let $\mu \in \mathcal{M}^+(\mathbb{T}_\ell)$ and let (2.39) hold. Then*

(i) $\mu \in H^{-1}(\mathbb{T}_\ell)$, in the sense that it can be extended to a bounded linear functional over $H^1(\mathbb{T}_\ell)$.

(ii) If

$$v(x) := \int_{\mathbb{T}_\ell} G(x-y)\, d\mu(y), \tag{2.40}$$

then $v \in H^1(\mathbb{T}_\ell)$. Furthermore, v solves

$$-\Delta v + \kappa^2 v = \mu, \tag{2.41}$$

weakly in $H^1(\mathbb{T}_\ell)$, and

$$\nabla v(x) = \int_{\mathbb{T}_\ell} \nabla G(x-y)\, d\mu(y), \tag{2.42}$$

in the sense of distributions.

(iii) If v is as in (ii), we have $\kappa^2 \int_{\mathbb{T}_\ell} v\, dx = \int_{\mathbb{T}_\ell} d\mu$ and

$$\int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} G(x-y)\, d\mu(x)\, d\mu(y) = \int_{\mathbb{T}_\ell} \left(|\nabla v|^2 + \kappa^2 v^2\right) dx. \tag{2.43}$$

According to Lemma 2.3, the energy E_0 may be equivalently rewritten in terms of the associated potential v in (2.40) as

$$E_0(\mu) = \frac{\lambda^2 \ell^3}{2\kappa^2} - 2(\lambda - \lambda_c) \int_{\mathbb{T}_\ell} v \, dx + 2 \int_{\mathbb{T}_\ell} \left(|\nabla v|^2 + \kappa^2 v^2 \right) dx, \tag{2.44}$$

and minimizing $E_0(\mu)$ over $\mu \in \mathcal{M}^+(\mathbb{T}_\ell) \cap H^{-1}(\mathbb{T}_\ell)$ is the same as minimizing the right-hand side of (2.44) with respect to all $v \in H^1(\mathbb{T}_\ell)$ such that $v \geq 0$ in $\mathbb{T}_\ell$ and $-\Delta v + \kappa^2 v \in \mathcal{M}^+(\mathbb{T}_\ell)$. By inspection, the latter is minimized by $v = \bar{v}$, where

$$\bar{v} = \begin{cases} 0, & \lambda \leq \lambda_c, \\ \frac{1}{2\kappa^2}(\lambda - \lambda_c), & \lambda > \lambda_c. \end{cases} \tag{2.45}$$

In terms of the measures, we can state this result as follows:

Proposition 2.4. *The energy $E_0(\mu)$ is minimized by a unique measure $\bar{\mu}$ among all $\mu \in \mathcal{M}^+(\mathbb{T}_\ell) \cap H^{-1}(\mathbb{T}_\ell)$, with $\bar{\mu} = 0$ for all $\lambda \leq \lambda_c$, and $d\bar{\mu} = \frac{1}{2}(\lambda - \lambda_c)dx$ for $\lambda > \lambda_c$, respectively. Moreover, we have*

$$E_0(\bar{\mu}) = \begin{cases} \frac{\lambda^2 \ell^3}{2\kappa^2}, & \lambda \leq \lambda_c, \\ \frac{\lambda_c(2\lambda - \lambda_c)\ell^3}{2\kappa^2}, & \lambda > \lambda_c, \end{cases} \tag{2.46}$$

and (2.41) *is solved by $v(x) = \bar{v}$.*

3 Sharp interface energy E_ε

In this section, we consider the sharp-interface functional E_ε defined in (2.10) in the limit $\varepsilon \to 0$ with $\bar{u}_\varepsilon$ given by (1.3) and positive $\sigma, \lambda, \kappa, \ell$ fixed. For a given $u_\varepsilon \in \mathcal{A}$, we introduce a measure μ_ε that is continuous with respect to the Lebesgue measure on $\mathbb{T}_\ell$ and whose density is an appropriately rescaled characteristic function of the minority phase:

$$d\mu_\varepsilon(x) := \frac{1}{2} \varepsilon^{-2/3}(1 + u_\varepsilon(x))dx. \tag{3.1}$$

Note that by definition the measure μ_ε is non-negative. We also introduce the potential v_ε via

$$-\Delta v_\varepsilon + \kappa^2 v_\varepsilon = \mu_\varepsilon \qquad \text{in} \quad \mathbb{T}_\ell. \tag{3.2}$$

Our first result establishes compactness of sequences with bounded energy after a suitable rescaling.

Theorem 3.1 (Equicoercivity)**.** *Let* $(u_\varepsilon) \in \mathcal{A}$ *be such that*

$$\limsup_{\varepsilon\to 0} \varepsilon^{-4/3} E_\varepsilon(u_\varepsilon) < +\infty, \tag{3.3}$$

and let μ_ε *and* v_ε *be defined in* (3.1) *and* (3.2)*, respectively. Then, up to extraction of a subsequence, we have*

$$\mu_\varepsilon \rightharpoonup \mu \ \textit{in}\ \mathcal{M}(\mathbb{T}_\ell), \qquad v_\varepsilon \rightharpoonup v \ \textit{in}\ H^1(\mathbb{T}_\ell), \tag{3.4}$$

as $\varepsilon \to 0$*, for some* $\mu \in \mathcal{M}^+(\mathbb{T}_\ell) \cap H^{-1}(\mathbb{T}_\ell)$ *and* $v \in H^1(\mathbb{T}_\ell)$ *satisfying*

$$-\Delta v + \kappa^2 v = \mu \qquad \textit{in} \quad \mathbb{T}_\ell. \tag{3.5}$$

Proof. Inserting (3.1) into (2.10) and dropping the perimeter term, following the argument of [24] we arrive at (see also (2.19))

$$E_\varepsilon(u_\varepsilon) \geq \frac{\lambda^2 \ell^3}{2\kappa^2} - \frac{2\lambda}{\kappa^2} \int_{\mathbb{T}_\ell} d\mu_\varepsilon(x) + 2 \int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} G(x-y) d\mu_\varepsilon(x) d\mu_\varepsilon(y), \tag{3.6}$$

where we used (2.17) and (1.3) and took into account the translational invariance of the problem in $\mathbb{T}_\ell$. By (2.16) we get

$$E_\varepsilon(u_\varepsilon) \geq -\frac{2\lambda}{\kappa^2} \mu_\varepsilon(\mathbb{T}_\ell) + 2c\mu_\varepsilon^2(\mathbb{T}_\ell), \tag{3.7}$$

where we again recall that μ_ε is nonnegative by definition. It then follows that

$$\mu_\varepsilon(\mathbb{T}_\ell) < C, \tag{3.8}$$

for some constant $C > 0$ independent of ε, which implies that $\mu_\varepsilon \rightharpoonup \mu$ for a subsequence. The above considerations together with Lemma 2.3(iii) and (3.3) show that

$$\int_{\mathbb{T}_\ell} \left(|\nabla v_\varepsilon|^2 + \kappa^2 v_\varepsilon^2 \right) dx = \int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} G(x-y) d\mu_\varepsilon(x) d\mu_\varepsilon(y) < C, \tag{3.9}$$

and upon extraction of a further subsequence we get $v_\varepsilon \rightharpoonup v$ in $H^1(\mathbb{T}_\ell)$. Finally, (3.5) follows by passing to the limit in (3.2). □

We now proceed to the main result of this section which establishes the Γ-limit of the screened sharp interface energy, similar to its two-dimensional analog in [12, Theorem 1].

Theorem 3.2 (Γ-convergence of E_ε)**.** *As* $\varepsilon \to 0$ *we have*

$$\varepsilon^{-4/3} E_\varepsilon \overset{\Gamma}{\rightharpoonup} E_0, \tag{3.10}$$

with respect to the weak convergence of measures. More precisely, we have *i) Lower bound: Suppose that* $(u_\varepsilon) \in \mathcal{A}$ *and let* μ_ε *be defined as in* (3.1)*, and suppose that*

$$\mu_\varepsilon \rightharpoonup \mu \text{ in } \mathcal{M}(\mathbb{T}_\ell), \tag{3.11}$$

as $\varepsilon \to 0$*, for some* $\mu \in {\mathcal{M}_\ell}^+(\mathbb{T}_\ell)$*. Then*

$$\liminf_{\varepsilon\to 0} \varepsilon^{-4/3} E_\varepsilon(u_\varepsilon) \geq E_0(\mu). \tag{3.12}$$

ii) Upper bound: Given $\mu \in \mathcal{M}^+(\mathbb{T}_\ell)$*, there exists* $(u_\varepsilon) \in \mathcal{A}$ *such that for the corresponding* μ_ε *as in* (3.1) *we have*

$$\mu_\varepsilon \rightharpoonup \mu \text{ in } \mathcal{M}(\mathbb{T}_\ell), \tag{3.13}$$

as $\varepsilon \to 0$*, and*

$$\limsup_{\varepsilon\to 0} \varepsilon^{-4/3} E_\varepsilon(u_\varepsilon) \leq E_0(\mu). \tag{3.14}$$

Proof. Assume first that $\mu \in \mathcal{M}^+(\mathbb{T}_\ell) \cap H^{-1}(\mathbb{T}_\ell)$, so that $E_0(\mu) < +\infty$. As in the proof of Propositions 5.1 and 5.2 in [15], we separate the contributions of the near-field and far-field interaction, i.e. for $0 < \rho \leq \frac{1}{4}$ we write

$$G_\rho(x) = \eta_\rho(x) G(x), \qquad H_\rho(x) := G(x) - G_\rho(x), \tag{3.15}$$

where $\eta_\rho(x)$ is a smooth cutoff function depending on $|x|$ which is monotonically increasing from 0 to 1 as $|x|$ goes from 0 to ρ, with $\eta_\rho(x) = 0$ for all $|x| < \frac{1}{2}\rho$ and $\eta_\rho(x) = 1$ for all $|x| > \rho$. With the help of (2.19), for any $u_\varepsilon \in \mathcal{A}$ we decompose the energy as $E_\varepsilon = E_\varepsilon^{(1)} + E_\varepsilon^{(2)}$, where

$$\begin{aligned} \varepsilon^{-4/3} E_\varepsilon^{(1)}(u_\varepsilon) &= \frac{\lambda^2 \ell^3}{2\kappa^2} - \frac{2\lambda}{\kappa^2} \int_{\mathbb{T}_\ell} d\mu_\varepsilon(x) + 2 \int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} G_\rho(x-y)\, d\mu_\varepsilon(x)\, d\mu_\varepsilon(y), \\ \varepsilon^{-4/3} E_\varepsilon^{(2)}(u_\varepsilon) &= \varepsilon^{-1/3} \sigma \int_{\mathbb{T}_\ell} |\nabla \chi_\varepsilon|\, dx + 2\varepsilon^{-4/3} \int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} H_\rho(x-y) \chi_\varepsilon(x) \chi_\varepsilon(y)\, dx\, dy, \end{aligned} \tag{3.16}$$

where χ_ε is as in (2.18) with u replaced with u_ε. The term $E_\varepsilon^{(1)}$ is continuous with respect to the weak convergence of measures, hence

$$\int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} G_\rho(x-y)\, d\mu_\varepsilon(x)\, d\mu_\varepsilon(y) \to \int_{\mathbb{T}_\ell} \int_{\mathbb{T}_\ell} G_\rho(x-y)\, d\mu(x)\, d\mu(y) \qquad \text{as } \varepsilon \to 0. \tag{3.17}$$

The proof of the lower bound for $E_\varepsilon^{(2)}$ follows with similar arguments as in [15]. After the rescaling in (2.20), one can write

$$\varepsilon^{-4/3} E_\varepsilon^{(2)}(u_\varepsilon) = \left(\frac{\varepsilon^{1/3} \sigma^{5/3}}{4^{2/3}} \right) \left[\int_{\mathbb{T}_{\ell_\varepsilon}} |\nabla \tilde{\chi}_\varepsilon| dx + \frac{1}{2} \int_{\mathbb{T}_{\ell_\varepsilon}} \int_{\mathbb{T}_{\ell_\varepsilon}} \widetilde{H}_\rho^\varepsilon(x-y) \tilde{\chi}_\varepsilon(x) \tilde{\chi}_\varepsilon(y)\, dx\, dy \right], \tag{3.18}$$

where $\tilde{\chi}_\varepsilon(x) := \chi_\varepsilon(x\ell/\ell_\varepsilon)$ and

$$\widetilde{H}^\varepsilon_\rho(x) := (1 - \eta_\rho(x\ell/\ell_\varepsilon))G_\varepsilon(x). \tag{3.19}$$

Observe that by (2.25) and monotonicity of $\eta_\rho(x)$ in $|x|$ we have

$$\widetilde{H}^\varepsilon_\rho(x) \geq (1-\rho)\Gamma^\#_{\rho_0}(x),$$

where $\Gamma^\#_{\rho_0}(x) := (1 - \eta_{\rho_0}(x))\Gamma^\#(x)$ and $\Gamma^\#(x) := \frac{1}{4\pi|x|}$ is the restriction of the Newton potential on the torus, for any $\rho_0 > 0$ and all ε small enough depending only on κ, σ and ρ_0. The rest of the proof follows exactly as in [15].

Finally, if $\mu \notin H^{-1}(\mathbb{T}_\ell)$, then $E_0(\mu) = +\infty$ and the upper bound is trivial, while the lower bound follows via a contradiction argument from the compactness established in Theorem 3.1. □

As a direct consequence of Theorems 3.1 and 3.2, we have the following characterization of the minimizers of the sharp interface energy in the limit $\varepsilon \to 0$.

Corollary 3.3. *Let $(u_\varepsilon) \in \mathcal{A}$ be minimizers of E_ε. Let μ_ε be defined in* (3.1) *and let v_ε be the solution of* (3.2) *respectively. Then as $\varepsilon \to 0$, we have*

$$\mu_\varepsilon \rightharpoonup \bar{\mu} \text{ in } \mathcal{M}(\mathbb{T}_\ell), \qquad v_\varepsilon \rightharpoonup \bar{v} \text{ in } H^1(\mathbb{T}_\ell), \tag{3.20}$$

where $\bar{\mu}$ and $\bar{v}$ are as in Proposition 2.4.

We note that for $\lambda \gg \lambda_c$ the minimum energy per unit volume for minimizers in Proposition 3.3 approaches asymptotically to that of the unscreened sharp interface energy studied in [15], indicating that the presence of an additional screening does not affect the limit behavior of the energy at higher densities than those appearing in (1.3). We would thus expect that the same result would still hold for the sharp interface energy even for $1 + \bar{u}_\varepsilon = o(1)$ as $\varepsilon \to 0$, consistently with a recent result for the sharp interface energy without screening [8].

We conclude by proving an analog of [15, Theorem 3.6] that provides uniform bounds on the diameter of the connected components of minimizers of E_ε as $\varepsilon \to 0$, and convergence of most of the connected components to minimizers of Gamow's model per unit mass.

Theorem 3.4 (Minimizers: droplet structure)**.** *For $\lambda > 0$, let $(u_\varepsilon) \in \mathcal{A}$ be regular representatives of minimizers of E_ε, and assume that the sets $\{u_\varepsilon = +1\}$ are non-empty for ε sufficiently small. Let N_ε be the number of connected components of the set $\{u_\varepsilon = +1\}$, let $\chi_{\varepsilon,k} \in BV(\mathbb{R}^3; \{0,1\})$ be the characteristic function of the k-th connected component of the support of the periodic extension of $\{u_\varepsilon = +1\}$ to the whole of $\mathbb{R}^3$ modulo translations in $\mathbb{Z}^3$, and let $x_{\varepsilon,k} \in \operatorname{supp}(\chi_{\varepsilon,k})$. Then there exists $\varepsilon_0 > 0$ such that the following properties hold:*

i) There exist constants $C, c > 0$ depending only on σ, κ, λ and ℓ such that, for all $\varepsilon \le \varepsilon_0$ we have

$$0 < v_\varepsilon \le C \qquad \text{and} \qquad \int_{\mathbb{R}^3} \chi_{\varepsilon,k}\, dx \ge c\,\varepsilon, \tag{3.21}$$

where v_ε solves (3.2). Moreover we have

$$\operatorname{supp}(\chi_{\varepsilon,k}) \subseteq B_{C\varepsilon^{1/3}}(x_{\varepsilon,k}). \tag{3.22}$$

ii) If $\lambda > \lambda_c$, where where λ_c is given by (2.30), there exist constants $C, c > 0$ as above such that, for all $\varepsilon \le \varepsilon_0$ we have

$$c(\lambda - \lambda_c)\varepsilon^{-1/3} \le N_\varepsilon \le C(\lambda - \lambda_c)\varepsilon^{-1/3}. \tag{3.23}$$

Moreover, there exists $\widetilde{N}_\varepsilon \le N_\varepsilon$ with $\widetilde{N}_\varepsilon / N_\varepsilon \to 1$ as $\varepsilon \to 0$ and a subsequence $\varepsilon_n \to 0$ such that for every $k_n \le \widetilde{N}_{\varepsilon_n}$ the following holds: After possibly relabeling the connected components, we have

$$\tilde{\chi}_n \to \tilde{\chi} \qquad\qquad \text{in } L^1(\mathbb{R}^3), \tag{3.24}$$

where $\tilde{\chi}_n(x) := \chi_{\varepsilon_n,k_n}(\varepsilon_n^{1/3}(x + x_{\varepsilon_n,k_n}))$, and $\tilde{\chi} \in \widetilde{\mathcal{A}}_\infty$ is a minimizer of the right-hand side of (2.28).

Proof. The proof can be obtained as in [15, Theorem 3.6], with some simplifications due to the absence of a volume constraint. We outline the necessary modifications below. As stated above, the constants in the estimates below depend on σ, κ, λ and ℓ, and may change from line to line.

For $\tilde{u}_\varepsilon(x) := u_\varepsilon(\ell x/\ell_\varepsilon)$, we define $F \subset \mathbb{T}_{\ell_\varepsilon}$ to be the set $\{\tilde{u}_\varepsilon = +1\}$, which by our assumption is non-empty for ε sufficiently small. Then we can write $v_\varepsilon(x) = (\sigma/4)^{2/3} v_F(\ell x/\ell_\varepsilon)$, where $v_F(x) := \int_{\mathbb{T}_{\ell_\varepsilon}} G_\varepsilon(x-y)\chi_F(y)dy$, and G_ε is defined in (2.25). The first step in the proof is to obtain an L^∞-bound on the potential v_F analogous to the one in [15, Lemma 6.3]:

$$0 < v_F \le C\varepsilon^{-2/9}. \tag{3.25}$$

Observe that by strict positivity of G_ε we clearly have $v_F > 0$. On the other hand, the upper bound follows exactly as in [15, Lemma 6.3], due to the fact that $G_\varepsilon(x) \le C/|x|$ for some $C > 0$, since

$$G_\varepsilon(x) = \frac{\ell}{\ell_\varepsilon} G\left(\frac{\ell x}{\ell_\varepsilon}\right) = \frac{1}{4\pi} \sum_{\mathbf{n} \in \mathbb{Z}^3} \frac{e^{-\kappa \ell |(x/\ell_\varepsilon) - \mathbf{n}\ell|}}{|x - \mathbf{n}\ell|}, \tag{3.26}$$

in view of (2.15).

Next, we need to estimate the gradient of v_F pointwise in terms v_F itself, as in [15, Lemma 6.5], which relies on [15, Eq. (6.15)]. It is easy to see that the latter estimate still holds in the present setting, with the constants depending on κ and ℓ. The proof then follows as in [15], with a few simplifications due to positivity of G. Also, since v_F satisfies

$$-\Delta v_F + \left(\frac{\varepsilon\sigma}{4}\right)^{2/3} \kappa^2 v_F = \left(\frac{\sigma}{4}\right)^{2/3} \chi_F \qquad \text{in } \mathbb{T}_{\ell_\varepsilon}, \tag{3.27}$$

by positivity of v_F we have that v_F is subharmonic outside $\overline{F}$. Thus, v_F attains its global maximum in $\mathbb{T}_{\ell_\varepsilon}$ for some $\bar{x} \in \overline{F}$, and the analog of [15, Eq. (6.19)] holds true:

$$v_F(x) \geq \frac{3}{4} v_F(\bar{x}) - C \qquad \text{for all } x \in B_r(\bar{x}), \tag{3.28}$$

for some $C > 0$ and $r > 0$.

Proceeding as in [15, Lemma 6.7 and Proposition 6.2], we establish a lower density estimate for F: Given $x_0 \in \overline{F}$ and letting F_0 be the connected component of F containing x_0, we have

$$|F_0 \cap B_r(x_0)| \geq cr^3 \qquad \text{for all } r \leq C \min\left(1, \|v_F\|_\infty^{-1}\right) \leq C\varepsilon^{2/9}, \tag{3.29}$$

for some c, $C > 0$, where the last inequality follows from (3.25). The assertion in (3.21) then follows as in [15, Theorem 6.9] from (3.25), (3.28) and (3.29). The idea of the proof in [15] is to find a suitable competitor F' which is obtained by cutting from F a ball of radius independent of ε, centered at the point where the potential v_F attains its maximum. Compared to [15], the proof here is simpler since we don't have a volume constraint, so that we can allow competitors with smaller volume than F. Arguing by contradiction, if the maximum of v_F is large, then necessarily the density of F in the ball has to be small, otherwise the energy of F' would be less that the energy of F. However, this contradicts the density estimate in (3.29). Finally, exactly as in [15, Lemma 6.11], the bound on the potential and the density estimate (3.29) also imply the diameter bound

$$\operatorname{diam}(F_0) \leq C, \tag{3.30}$$

for some constant $C > 0$, which gives (3.22). This concludes the proof of part *i*).

The proof of part *ii*) follows as in the proof of [15, Theorem 3.6], with the exception that the estimate on N_ε in (3.23) now follows from (3.21) and the fact that, recalling Corollary 3.3,

$$\lim_{\varepsilon \to 0} \int_{\mathbb{T}_\ell} d\mu_\varepsilon = \bar{\mu}(\mathbb{T}_\ell) = \frac{1}{2}(\lambda - \lambda_c), \tag{3.31}$$

where $\bar{\mu}$ is as in Proposition 2.4. □

The results obtained in Theorem 3.4 allow us to establish a sharp transition from trivial to non-trivial minimizers at the level of the sharp interface energy near $\lambda = \lambda_c$ for all $\varepsilon \ll 1$.

Corollary 3.5. *There exists $\varepsilon_0 = \varepsilon_0(\sigma, \kappa, \lambda, \ell) > 0$ such that if λ_c is given by (2.30), then:*

i) For any $\lambda < \lambda_c$ and $\varepsilon < \varepsilon_0$ we have that $u = -1$ is the unique minimizer of E_ε in $\mathcal{A}$.

ii) For $\lambda > \lambda_c$ and $\varepsilon < \varepsilon_0$ we have that $u = -1$ is not a minimizer of E_ε in $\mathcal{A}$.

Proof. Since the statement in *ii)* follows immediately from Corollary 3.3, we only need to demonstrate *i)*. The strategy is analogous to the one used in the proof of [24, Proposition 3.2]. For $\lambda < \lambda_c$, let u_ε be a minimizer of E_ε over $\mathcal{A}$, and assume, by contradiction, that $u_\varepsilon \neq -1$ for a sequence of $\varepsilon \to 0$. Let $\chi_{\varepsilon,k}$ be as in Theorem 3.4. By (2.15) we have

$$E_\varepsilon(u_\varepsilon) \geq \frac{\varepsilon^{4/3}\lambda^2\ell^3}{2\kappa^2} + \sum_{k=1}^{N_\varepsilon} \Bigg(\varepsilon\sigma \int_{\mathbb{R}^3} |\nabla \chi_{\varepsilon,k}| dx - \frac{2\varepsilon^{2/3}\lambda}{\kappa^2} \int_{\mathbb{R}^3} \chi_{\varepsilon,k} dx \\ + \frac{1}{2\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{e^{-\kappa|x-y|}}{|x-y|} \chi_{\varepsilon,k}(x) \chi_{\varepsilon,k}(y)\, dx\, dy \Bigg). \tag{3.32}$$

At the same time, since by Theorem 3.4 the diameter of the support of $\chi_{\varepsilon,k}$ is bounded above by $C\varepsilon^{1/3}$, for every $\delta > 0$ we have $e^{-\kappa|x-y|} \geq 1 - \delta$ for all ε sufficiently small and all $x, y \in \operatorname{supp}(\chi_{\varepsilon,k})$. Introducing $\tilde{\chi}_{\varepsilon,k}(x) := \chi_{\varepsilon,k}(\ell_\varepsilon x/\ell)$ as in (2.20), we can then write

$$E_\varepsilon(u_\varepsilon) \geq \frac{\varepsilon^{4/3}\lambda^2\ell^3}{2\kappa^2} - \frac{\varepsilon^{5/3}\sigma\lambda}{2\kappa^2} \sum_{k=1}^{N_\varepsilon} \int_{\mathbb{R}^3} \tilde{\chi}_{\varepsilon,k} dx \\ + \frac{\varepsilon^{5/3}\sigma^{5/3}}{4^{2/3}} \sum_{k=1}^{N_\varepsilon} \left(\int_{\mathbb{R}^3} |\nabla \tilde{\chi}_{\varepsilon,k}| dx + \frac{1-\delta}{8\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\tilde{\chi}_{\varepsilon,k}(x)\tilde{\chi}_{\varepsilon,k}(y)}{|x-y|} dx\, dy \right) \\ \geq \frac{\varepsilon^{4/3}\lambda^2\ell^3}{2\kappa^2} - \frac{\varepsilon^{5/3}\sigma\lambda}{2\kappa^2} \sum_{k=1}^{N_\varepsilon} \int_{\mathbb{R}^3} \tilde{\chi}_{\varepsilon,k} dx + \frac{\varepsilon^{5/3}\sigma^{5/3}(1-\delta)}{4^{2/3}} \sum_{k=1}^{N_\varepsilon} \widetilde{E}_\infty(\tilde{\chi}_{\varepsilon,k}). \tag{3.33}$$

Now we substitute the definitions of f^* and λ_c in (2.28) and (2.30), respectively, into (3.33). This yields

$$E_\varepsilon(u_\varepsilon) \geq \frac{\varepsilon^{4/3}\lambda^2\ell^3}{2\kappa^2} + \frac{\varepsilon^{5/3}\sigma\left((1-\delta)\lambda_c - \lambda\right)}{2\kappa^2} \sum_{k=1}^{N_\varepsilon} \int_{\mathbb{R}^3} \tilde{\chi}_{\varepsilon,k} dx. \tag{3.34}$$

In particular, for $\lambda < \lambda_c$ one can choose δ small enough, so that $E_\varepsilon(u_\varepsilon) > \varepsilon^{4/3}\lambda^2\ell^3/(2\kappa^2) = E_\varepsilon(-1)$ for all ε sufficiently small, contradicting minimality of u_ε. ☐

4 Diffuse interface energy $\mathcal{E}_\varepsilon$

We now consider the diffuse-interface functional $\mathcal{E}_\varepsilon$ defined in (1.1) in the limit $\varepsilon \to 0$ with, as before, $\bar{u}_\varepsilon$ given by (1.3) and positive $\sigma, \lambda, \kappa, \ell$ fixed.

Let

$$d\mu_\varepsilon^0(x) := \frac{1}{2}\varepsilon^{-2/3}\left(1 + u_\varepsilon^0(x)\right) dx, \tag{4.1}$$

where

$$u_\varepsilon^0(x) := \begin{cases} +1 & \text{if } u_\varepsilon(x) > 0, \\ -1 & \text{if } u_\varepsilon(x) \le 0, \end{cases} \tag{4.2}$$

and let v_ε^0 satisfy

$$-\Delta v_\varepsilon^0 + \kappa^2 v_\varepsilon^0 = \mu_\varepsilon^0 \qquad \text{in} \quad \mathbb{T}_\ell. \tag{4.3}$$

With this notation, we are now in the position to state the main technical result of this paper.

Theorem 4.1 (Equicoercivity and Γ-convergence of $\mathcal{E}_\varepsilon$)**.** *For $\lambda > 0$ and $\ell > 0$, let $\mathcal{E}_\varepsilon$ be defined by (2.1) with W satisfying the assumptions of Sec. 2.1, let $\bar{u}_\varepsilon$ given by* (1.3)*, and let σ and κ be given by* (2.8) *and* (2.9)*, respectively. Then, as $\varepsilon \to 0$ we have*

$$\varepsilon^{-4/3}\mathcal{E}_\varepsilon \overset{\Gamma}{\rightharpoonup} E_0(\mu), \tag{4.4}$$

where $\mu \in \mathcal{M}^+(\mathbb{T}_\ell) \cap H^{-1}(\mathbb{T}_\ell)$. More precisely, we have

i) Compactness and lower bound: Let $(u_\varepsilon) \in \mathcal{A}_\varepsilon$ be such that $\limsup_{\varepsilon\to 0} \|u_\varepsilon\|_{L^\infty(\mathbb{T}_\ell)} \le 1$ *and*

$$\limsup_{\varepsilon \to 0} \varepsilon^{-4/3}\mathcal{E}_\varepsilon(u_\varepsilon) < +\infty. \tag{4.5}$$

Then, up to extraction of a subsequence, we have

$$\mu_\varepsilon^0 \rightharpoonup \mu \textit{ in } \mathcal{M}(\mathbb{T}_\ell), \qquad v_\varepsilon^0 \rightharpoonup v \textit{ in } H^1(\mathbb{T}_\ell), \tag{4.6}$$

as $\varepsilon \to 0$, where $\mu \in \mathcal{M}^+(\mathbb{T}_\ell) \cap H^{-1}(\mathbb{T}_\ell)$ and $v \in H^1(\mathbb{T}_\ell)$ satisfy

$$-\Delta v + \kappa^2 v = \mu \qquad \textit{in} \quad \mathbb{T}_\ell. \tag{4.7}$$

Moreover, we have

$$\liminf_{\varepsilon \to 0} \varepsilon^{-4/3}\mathcal{E}_\varepsilon(u_\varepsilon) \ge E_0(\mu). \tag{4.8}$$

ii) Upper bound: Given $\mu \in \mathcal{M}^+(\mathbb{T}_\ell) \cap H^{-1}(\mathbb{T}_\ell)$ and $v \in H^1(\mathbb{T}_\ell)$ solving (4.7), there exist $(u_\varepsilon) \in \mathcal{A}_\varepsilon$ such that for the corresponding μ_ε^0, v_ε^0 as in (4.1) and (4.3) we have

$$\mu_\varepsilon^0 \rightharpoonup \mu \text{ in } \mathcal{M}(\mathbb{T}_\ell), \qquad v_\varepsilon^0 \rightharpoonup v \text{ in } H^1(\mathbb{T}_\ell), \tag{4.9}$$

as $\varepsilon \to 0$, and

$$\limsup_{\varepsilon\to 0} \varepsilon^{-4/3}\mathcal{E}_\varepsilon(u_\varepsilon) \le E_0(\mu). \tag{4.10}$$

Proof. As in [24], the basic strategy is to relate the minimization problem for $\mathcal{E}_\varepsilon$ to that for E_ε and apply the results in Theorems 3.1 and 3.2. The proof relies on the fact, first observed in [24], that the energy $\mathcal{E}_\varepsilon$ is asymptotically equivalent to E_ε in the following sense: For any $\delta > 0$ and $u_\varepsilon \in \mathcal{A}_\varepsilon$ satisfying some mild technical conditions (see below) there is $\tilde{u}_\varepsilon \in \mathcal{A}$ such that

$$E_\varepsilon[\tilde{u}_\varepsilon] \le (1+\delta)\mathcal{E}_\varepsilon(u_\varepsilon), \tag{4.11}$$

for all $\varepsilon \ll 1$, and, conversely, for any $\tilde{u}_\varepsilon \in \mathcal{A}$, again, satisfying some mild technical conditions, there is $u_\varepsilon \in \mathcal{A}_\varepsilon$ such that

$$\mathcal{E}_\varepsilon[u_\varepsilon] \le (1+\delta)E_\varepsilon(\tilde{u}_\varepsilon), \tag{4.12}$$

for all $\varepsilon \ll 1$. The proof then proceeds exactly as in the two-dimensional case [12, Theorem 1], with modifications appropriate to three space dimensions. We outline the key differences below.

For (4.11) to hold, we need to verify the assumptions of [24, Proposition 4.2], which are equivalent to checking that $\|u_\varepsilon\|_\infty \to 1$, $\mathcal{E}_\varepsilon(u_\varepsilon) \to 0$ and $\|v_\varepsilon\|_\infty \to 0$ as $\varepsilon \to 0$, where $v_\varepsilon(x) := \int_{\mathbb{T}_\ell} G_0(x-y)(u_\varepsilon(y) - \bar{u}_\varepsilon)dy$. The first and second conditions are clearly satisfied by the assumptions of the theorem. To check the third condition, we note that the non-local part of the energy may be written in terms of v_ε as

$$\frac{1}{2}\int_{\mathbb{T}_\ell}\int_{\mathbb{T}_\ell} (u_\varepsilon(x) - \bar{u}_\varepsilon)G_0(x-y)(u_\varepsilon(y) - \bar{u}_\varepsilon)\,dx\,dy = \frac{1}{2}\int_{\mathbb{T}_\ell} |\nabla v_\varepsilon|^2 dx. \tag{4.13}$$

Since $\int_{\mathbb{T}_\ell} v_\varepsilon(x)\,dx = 0$ we have by Poincaré's inequality that the right-hand side of (4.13) is bounded below by a multiple of $\|v_\varepsilon\|_2^2$. In turn, the latter is bounded below by a multiple of $\|v_\varepsilon\|_\infty^5$, in view of the fact that by elliptic regularity we have $\|\nabla v_\varepsilon\|_\infty \le C$ for some $C > 0$ depending only on ℓ, for all $\varepsilon \ll 1$. Therefore, from $\mathcal{E}_\varepsilon(u_\varepsilon) \to 0$ we also obtain that $\|v_\varepsilon\|_\infty \to 0$ as $\varepsilon \to 0$. Thus, by (4.11) $\tilde{u}_\varepsilon$ satisfies the assumptions of Theorem 3.1, and so there exists $\mu \in \mathcal{M}(\mathbb{T}_\ell)$ such that, upon extraction of subsequences, $\mu_\varepsilon \rightharpoonup \mu$ in $\mathcal{M}(\mathbb{T}_\ell)$, where the measure μ_ε defined by (3.1) with u_ε replaced by $\tilde{u}_\varepsilon$. For those subsequences, Theorem 3.2 holds true for μ_ε as well.

Now, from the construction of $\tilde{u}_\varepsilon$ in the proof of [24, Lemma 4.1] we know that $\tilde{u}_\varepsilon(x) = u^0_\varepsilon(x)$ for all $x \in \mathbb{T}_\ell$ such that $|u_\varepsilon(x)| > 1 - \delta^2$. Hence from the bound on $\mathcal{E}_\varepsilon(u_\varepsilon)$ and the assumptions on W we get that $\|\tilde{u}_\varepsilon - u^0_\varepsilon\|_1 \leq C\varepsilon^{4/3}\delta^{-4}$ for some $C > 0$ and all $\varepsilon \ll 1$. This implies that $\mu^0_\varepsilon \rightharpoonup \mu$ in $\mathcal{M}(\mathbb{T}_\ell)$ as well $\varepsilon \to 0$. Together with the conclusions of Theorems 3.1 and 3.2, this gives the compactness and the lower bound statement of Theorem 4.1, in view of arbitrariness of δ.

For (4.12) to hold, we need to verify the assumptions of [24, Proposition 4.3] on $\tilde{u}_\varepsilon \in \mathcal{A}$, namely, that the connected components of the support of $\{\tilde{u}_\varepsilon = +1\}$ are smooth and at least ε^α apart for some $\alpha \in [0, 1)$, have boundaries whose curvature is bounded by $\varepsilon^{-\alpha}$, and that $\|\tilde{v}_\varepsilon\|_\infty \to 0$ as $\varepsilon \to 0$, where $\tilde{v}_\varepsilon(x) := \int_{\mathbb{T}_\ell} G(x-y)(\tilde{u}_\varepsilon(y) - \bar{u}_\varepsilon)dy$. Clearly the first two assumptions hold true for the recovery sequence in the proof of Theorem 3.2 with any $\alpha \in (\frac{1}{3}, 1)$, provided that $\varepsilon \ll 1$. The third assumption is satisfied for all $\varepsilon \ll 1$, in view of the fact that the non-local part of the sharp interface energy can be written as

$$\frac{1}{2}\int_{\mathbb{T}_\ell}\int_{\mathbb{T}_\ell} (\tilde{u}_\varepsilon(x) - \bar{u}_\varepsilon)G_0(x-y)(\tilde{u}_\varepsilon(y) - \bar{u}_\varepsilon)\,dx\,dy = \frac{1}{2}\int_{\mathbb{T}_\ell} \left(|\nabla \tilde{v}_\varepsilon|^2 + \kappa^2 \tilde{v}_\varepsilon^2\right) dx, \qquad (4.14)$$

and the desired estimate follows from $E_\varepsilon(\tilde{u}_\varepsilon) \to 0$ just like in the case of the diffuse interface energy. Thus, the proof of the upper bound is concluded by taking the functions u_ε appearing in (4.12), associated with the recovery sequence $(\tilde{u}_\varepsilon)$ from Theorem 3.2, once again, in view of arbitrariness of δ. □

Similarly to the sharp interface energy, as a direct consequence of Theorem 4.1 we have the following characterization of the minimizers of the diffuse interface energy in the limit $\varepsilon \to 0$.

Corollary 4.2. *Under the assumptions of Theorem 4.1, let $(u_\varepsilon) \in \mathcal{A}_\varepsilon$ be minimizers of $\mathcal{E}_\varepsilon$. Let μ^0_ε be defined in* (4.1) *and v^0_ε be the solution of* (4.3)*, respectively. Then as $\varepsilon \to 0$, we have*

$$\mu^0_\varepsilon \rightharpoonup \bar{\mu} \text{ in } \mathcal{M}(\mathbb{T}_\ell), \qquad v^0_\varepsilon \rightharpoonup \bar{v} \text{ in } H^1(\mathbb{T}_\ell), \qquad (4.15)$$

where $\bar{\mu}$ and $\bar{v}$ are as in Proposition 2.4.

We emphasize that the limit behavior of the minimal energy obtained in (4.2) *differs* from that of the unscreened sharp interface energy one would naively associate with $\mathcal{E}_\varepsilon$. In particular, the minimal energy exhibits a threshold behavior, contrary to that of the minimizers of the unscreened sharp interface energy studied in [8, 15].

Proof of Theorems 1.1 and 1.2. The statement of Theorem 1.1 is simply the restatement of Corollary 4.2 that does not specify the precise values of the constants appearing there. In turn, the statement of Theorem 1.2 uses the explicit values of $\sigma = \frac{2\sqrt{2}}{2}$ and $\kappa = \frac{1}{\sqrt{2}}$ for (1.1), together with the bounds on f^* obtained in (2.32) and (2.33). □

Acknowledgements. HK was supported by DFG via grant #392124319. CBM was supported, in part, by NSF via grants DMS-1313687 and DMS-1614948. MN was partially supported by INDAM-GNAMPA, and by the University of Pisa Project PRA 2017 "Problemi di ottimizzazione e di evoluzione in ambito variazionale".

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