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Liquid-Vapor Interfaces and Surface Tension in a Mesoscopic Model of Fluid with Nonlocal Interactions

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We analyze the problem of phase coexistence, surface tension and the interface patterns between liquid and vapour for the nonlocal free energy functional derived by Lebowitz, Mazel, and Presutti from a system of particles interacting through Kac potentials in the continuum. We study the sharp interface limit in *d* dimensions and characterize the shape of the interface profiles in the temperature region where a monotonicity property is valid. We further extend our analysis beyond this domain by performing numerical simulations.

KEY WORDS: Surface tension; constrained minima; Γ convergence.

1. INTRODUCTION

In this paper we study properties of interfaces and the sharp interface limit for a nonlocal functional in *d* dimensions. The statistical mechanics counterpart of the functional is a particle model analyzed by Lebowitz *et al.*,[21] and hereafter called the LMP model. This is a system of identical point particles in the continuum interacting via a two-body attractive Kac potential and a four-body, repulsive Kac potential. They prove that for a temperature range $T \in (T_0, T_c)$ the system exhibits a liquid-vapor phase transition, thus solving a long standing problem in rigorous Statistical Mechanics. In the limit when the range of the Kac potentials becomes infinite, the model is described by a van der Waals free energy functional of the form:

$$\mathscr{F}(\rho) = \int dr(E_\lambda(J \star \rho) - \beta^{-1} S(\rho)) \tag{1.1}$$

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where $\beta > 0$ is the inverse temperature and $\lambda \in \mathbb{R}$ is the chemical potential, $\rho(r)$, $r \in \mathbb{R}^d$, is the particle density profile, $J(r) \geqslant 0$, $r \in \mathbb{R}^d$ is an even positive kernel with support in the unit ball and with integral equal to 1, and "$\star$" denotes the convolution. E_λ is the mean field energy density

$$E_\lambda(s) = -\lambda s - \frac{s^2}{2} + \frac{s^4}{4!} \tag{1.2}$$

where the two last terms are remainding respectively of the two-body, attractive, and four-body repulsive Kac potentials in the underlying LMP model. $S(\rho)$ is the entropy density

$$S(\rho) = -\rho(\log \rho - 1) \tag{1.3}$$

The existence of a phase transition of liquid-vapor type is related to the fact that the global minimizers of the functional are constant functions, for any value of temperature and chemical potential. For $\beta > \beta_c = (kT_c)^{-1}$, there is a unique value of the chemical potential $\lambda = \lambda_\beta$, for which there are two distinct minimizers $\rho_{\beta,\pm}$, (with $\rho_{\beta,-} < \rho_{\beta,+}$). For other values, $\lambda \neq \lambda_\beta$ or $\beta \leqslant \beta_c$, the minimizer is unique.

In this paper, we study the sharp interface limit in $d \geqslant 2$ dimensions and prove the Γ-convergence of the excess free energy functional to a perimeter functional which assigns to an interface ∂E of a set $E \subset \mathbb{R}^d$ of bounded variation the free energy cost

$$H = \int_{\partial E} d\mu \, \mathrm{s}_\beta(\nu(r)) \tag{1.4}$$

where $d\mu$ is the $d-1$ surface area measure on ∂E, $\nu(r)$ is the outward normal to ∂E at r (defined almost everywhere); $\mathrm{s}_\beta(e)$, $|e| = 1$ is the surface tension of a flat surface whose normal is e.

Alberti and Bellettini,[1,2] have proved analogous results for general anisotropic interactions of ferromagnetic type including the free energy functionals arising from Ising spin system with ferromagnetic Kac potentials which generalize the first paper on this line of research due to Alberti *et al.*[3] These are the papers closer to ours in spirit and techniques, but there are by now many results on surface tension and Wulff theory for Ising type models. As the list of references is very long, we just mention that phase coexistence in two dimensions is fully described, see, for instance, refs. 15, 18–20, 23, 24 and that there are many results also in higher dimensions, refs. 6–10 and references therein.

Besides providing a further example of the generally accepted fact that H is the thermodynamic excess free energy of an interface, the interest in deriving (1.4) for the LMP model relies on an important mathematical (and physical) question about the validity of Γ-convergence when ferromagnetic-type inequalities do not hold, inequalities which were key ingredients in the proofs of Alberti and Bellettini. Our method is based on Peierls estimates on contours, and should extend to general functionals for which such estimates are valid; in particular they hold for the functionals associated to Ising models with ferromagnetic Kac potentials.

The other relevant issue in the definition of H is the identification of the surface tension. As explained by Alberti and Bellettini,[2] there is no need to give *a priori* the surface tension: $\mathrm{s}_\beta(e)$ depends on the model and it is selected by the limiting procedure. Thus it is the sharp interface limit that identifies the surface tension. In our model as well as in the model of Alberti and Bellettini it is given by the following expression. Given a unit vector $e \in \mathbb{R}^d$, let consider the rectangular domain $\mathscr{R}_e(L, h) = \mathscr{T}_e(L) \times [-h, h]$, where $h > 0$ and $\mathscr{T}_e(L)$ is a torus of side L in the orthogonal complement of e. Then we prove (see Theorems 2.4 and 2.5 in Section 2) that the excess free energy functional, (see (2.5) later for a definition of F) Γ-converges to H with

$$\mathrm{s}_\beta(e) = \liminf_{L \to \infty} \; \liminf_{h \to \infty} \frac{1}{L^{d-1}} \inf_{\rho \in L^\infty(\mathscr{R}_e(L, h))} F(\rho^{(\pm, h)}) \tag{1.5}$$

where $\rho^{(\pm, h)}$ is defined on the cylinder $\mathscr{C}_e = \mathscr{T}_e(L) \times \mathbb{R}$, equal to ρ in $\mathscr{R}_e(L, h)$ and constant and equal to the pure phases densities $\rho_{\beta, \pm}$ in the upper, respectively lower, part of the complement of $\mathscr{R}_e(L, h)$ in the direction e (see the next section for a precise definition).

Even if the fact that the infimum in (1.5) is a minimum does not play any role in the derivation of (1.4) it is of course relevant to actually show the existence of a minimizer (called *optimal profile* by Alberti and Bellettini) and to characterize its shape. A natural guess is that the optimal profile is a function ρ that depends only on the coordinate along e, $\rho(r) = \bar{\rho}(r \cdot e)$, $r \in \mathbb{R}^d$ and $\bar{\rho}$ is the optimal profile of a one dimensional functional.

Gayrard *et al.*,[17] have proven the existence of the one dimensional optimal profile $\bar{\rho}$ (that they call instanton) for all $\beta \in (\beta_c, \beta_0)$. In addition, they have shown that there is β^* such that for all $\beta \in (\beta_c, \beta^*)$ the minimizer is unique, strictly increasing and converges to $\rho_{\beta, \pm}$ exponentially fast. For $\beta \in (\beta^*, \beta_0)$ any minimizer approaches $\rho_{\beta, \pm}$ exponentially fast but presents oscillations when approaching the liquid phase in the sense that the set $\{x\colon \bar{\rho}(x) > \rho_{\beta, +}\} \subset \mathbb{R}$ is made of infinitely many disjoint intervals.

We prove that for $d \geqslant 2$ and $\beta \in (\beta_c, \beta^*)$, the minimizers of F depend only on the coordinate along the axis of the cylinder and that they reduce to the $d=1$ optimal profile found in ref. 17, in other words

$$s_\beta(e) = F^{(e)}(\bar{\rho}), \qquad \forall \beta \in (\beta_c, \beta^*)$$

where $F^{(e)}$ is a one dimensional functional defined in (2.10) later. For the other values of the temperature the validity of the above equality is not clear at all since nothing excludes the appearance of oscillations also in the directions orthogonal to e. In order to complete the analysis, we performed numerical simulations and computed the shape and the excess free energy of minimizers in two dimensions, for various interaction kernels. We thus got a strong belief that the same picture as before is valid for values of $\beta > \beta^*$, and that the minimizer is unique (up to translations) and described by the related one dimensional optimal profile.

2. DEFINITIONS AND RESULTS

We start this section with the precise definition of the excess free energy functional and recall its basic properties; we also state without proofs some of the results that Gayrard *et al.*,[17] gave in one dimension and for particular isotropic kernels but which are however valid in more generality. Our results are stated after this preliminary part.

Homogenous Solutions

Since $\int J = 1$ and $\int J \star S(\rho) = \int S(\rho)$ for any function ρ, we (formally) rewrite the free energy functional (1.1) as follow

$$\mathscr{F}(\rho) = \int (g_{\beta,\lambda}(J * \rho) + \beta^{-1}\{S(J * \rho) - J * S(\rho)\}) \quad g_{\beta,\lambda}(s) = E_\lambda(s) - \beta^{-1} S(s)$$

The term in the curly bracket is nonnegative and therefore the global minima of F are the constants that minimize $g_{\beta,\lambda}$. Let $\beta_c = (3/2)^{(3/2)}$ denote the inverse critical temperature. Then for all $\beta > \beta_c$, there is a unique $\lambda = \lambda_\beta$ such that the functional has two distinct minima, $\rho_{\beta,-}$ and $\rho_{\beta,+}$ with $g_{\beta,\lambda}(\rho_{\beta,+}) = g_{\beta,\lambda}(\rho_{\beta,-})$, (Fig. 1). In particular, they are solutions of the following *mean field equation*,

$$s = \varphi_\beta(s), \qquad \varphi_\beta(s) := \exp\{-\beta E'(s)\} \tag{2.1}$$

where $E'(s)$ is the derivative w.r.t. s of $E_{\lambda_\beta}(s)$ defined in (1.2). We denote by $\rho_{\beta,0}$ the third solution of (2.1), which is inbetween $\rho_{\beta,-}$ and $\rho_{\beta,+}$. The derivative of $\varphi_\beta(s)$ in a point s solution of (2.1) is

$$\varphi'_\beta(s) = \beta\varphi_\beta(s)[1-\tfrac{1}{2}s^2] = \beta s[1-\tfrac{1}{2}s^2]$$

It is not difficult to see that $\varphi'_\beta(\rho_{\beta,+})$ is a strictly decreasing function of β with value onto $(-\infty, 1)$. We define the two inverse temperatures β^* and β_0 through the equations:

$$\varphi'_{\beta^*}(\rho_{\beta^*,+}) = 0, \qquad \varphi'_{\beta_0}(\rho_{\beta_0,+}) = -1 \tag{2.2}$$

Those special values of β are related to properties of the evolution defined in (2.8) later, relevant for the study of the critical points of the free energy functional. For $\beta \in (\beta_c, \beta^*)$, it behaves just as in the ferromagnetic case, while for $\beta \in (\beta^*, \beta_0)$, the constant profile $\rho = \rho_{\beta,+}$ is only stable with respect to small perturbations. In particular the proof of Proposition 3.2 later strongly uses the positivity of $\varphi'_\beta(\rho_{\beta,+})$.

Noticing that the maximum of $\varphi_\beta(s)$ is reached at $s = \sqrt{2}$, independently of β, we set

$$R'' = \sup_{\beta \in (\beta_c, \beta_0)} \varphi_\beta(\sqrt{2}) \tag{2.3}$$

and we note that for $\beta > \beta^*$, $\rho_{\beta,+} \in (\sqrt{2}, R'')$. We also define

$$R' = \inf_{\beta \in (\beta_c, \beta_0)} \inf_{0 \leqslant s \leqslant R''} \varphi_\beta(s) \tag{2.4}$$

The Excess Free Energy Functional

From now on, we consider a situation of phase coexistence, and thus take $\beta > \beta_c$ and fix $\lambda = \lambda_\beta$. For notational convenience, we often drop β from the quantities we consider, for instance we write $\rho_\pm \equiv \rho_{\beta,\pm}$.

Following refs. 17 and 21, we define the excess free energy functional as follows.

$$F(\rho) = \int_{\mathbb{R}^d} (f(J \star \rho) + \beta^{-1}\{S(J \star \rho) - J \star S(\rho)\}) \tag{2.5}$$

where

$$f(s) = g_\beta(s) - g_\beta(\rho_+), \qquad g_\beta(s) = g_{\beta,\lambda_\beta}(s) = E_{\lambda_\beta}(s) - \beta^{-1}s[\log s - 1] \tag{2.6}$$

Observe that, as a functional with values in $[0, \infty]$, $F(\rho)$ is well defined on $L^1_{\text{loc}}(\mathbb{R}^d, \mathbb{R}_+)$. In fact by the Jensen's inequality the curly bracket on the right hand side of (2.5) is nonnegative, so that the whole functional is nonnegative.

Critical Points and Nonlocal Dynamics

The critical points of $F(\rho)$ are functions that satisfy the following equation:

$$\rho(r) = \Phi(\rho)(r), \qquad \Phi(\rho)(r) := \exp\{-\beta J \star E'_\beta(J \star \rho)(r)\} \tag{2.7}$$

The solutions of (2.7) are stationary solutions of the following nonlocal dynamic,

$$\frac{\partial \rho}{\partial t} = -\rho + \Phi(\rho) \tag{2.8}$$

We denote by $T_t(\rho)$ the flow solution of (2.8) with $\rho \in L^\infty(\mathbb{R}^d, \mathbb{R})$.

The proof of the following theorem is the same as the one of Theorem 4.6 of ref. 17.

Theorem 2.1. Recalling the definitions (2.3) and (2.4), $T_t(\rho)$ is well defined in $L^\infty(\mathbb{R}^d, [R', R''])$ and $T_t(\rho)$ belongs to $L^\infty(\mathbb{R}^d, [R', R''])$ for all t. Furthermore if $\rho \in L^\infty(\mathbb{R}^d, [R', R''])$ is such that $F(\rho) < \infty$, then $F(T_t(\rho)) \leqslant F(\rho)$ for all t.

From the above result it follows that we may restrict the domain of F to the functions with values in the interval $[R', R'']$.

One Dimensional Functionals and Interfaces

Given a unit vector $e \in \mathbb{R}^d$ and $x \in \mathbb{R}$ we set

$$j_e(x) = \int_{e^\perp} dr\, J(r + xe), \qquad e^\perp = \{r \in \mathbb{R}^d : r \cdot e = 0\} \tag{2.9}$$

and we call $F^{(e)}$ the one dimensional functional with interaction j_e, namely (recall (2.6))

$$F^{(e)}(\rho) = \int_{\mathbb{R}} dx \left(f(j_e \star \rho) + \frac{1}{\beta} \{S(j_e \star \rho) - j_e \star S(\rho)\} \right) \tag{2.10}$$

We define

$$\mathcal{N}_\beta := \{\rho \in L^\infty(\mathbb{R}, \mathbb{R}_+) : \limsup_{x\to-\infty} \rho(x) < \rho_{\beta,0}, \liminf_{x\to\infty} \rho(x) > \rho_{\beta,0}\} \tag{2.11}$$

Gayrard *et al.*[17] have completely characterized the value of $\tau_\beta(e)$ where

$$\tau_\beta(e) = \inf_{\rho\in\mathcal{N}_\beta} F^{(e)}(\rho) \tag{2.12}$$

Theorem 2.2 (ref. 17). For any $\beta \in (\beta_c, \beta_0)$ the infimum in (2.12) is a minimum, and any minimizer $\bar{\rho}_\beta \in L^\infty(\mathbb{R}, [R', R''])$ is a solution of (2.7) with J replaced by j_e. Moreover $\bar{\rho}_\beta(x) \to \rho_{\beta,\pm}$ as $x \to \pm\infty$ and the convergence is exponentially fast. For $\beta \in (\beta_c, \beta^*)$ there is a unique solution to (2.7) [up to translations], hence a unique minimizer, and this is a strictly increasing function. For $\beta \in (\beta^*, \beta_0)$ and for any minimizer $\bar{\rho}_\beta$, the set $\{x: \bar{\rho}_\beta(x) \geqslant \rho_{\beta,+}\}$ is made of infinitely many disjoint intervals.

Having set all the preliminaries, we now state our results starting with those concerning the surface tension.

Definition of Surface Tension

To impose periodic boundary conditions we modify the kernel J as follows. Given a unit vector e and $L > 0$ we consider a cube $\mathcal{Q}_e(L) \subset e^\perp$ of side L ($e^\perp$ is defined in (2.9)). We introduce the coordinate axes with the origin in the center of $\mathcal{Q}_e(L)$ and in this coordinate frame we consider the cylinder $\mathcal{C}_e(L) = [-L/2, L/2]^{d-1} \times \mathbb{R}$. Denoting by e_i the unit vectors in the ith direction, $i = 1,..., d-1$, we define

$$J_L(r) := \sum_{k\in\mathbb{Z}^{d-1}} J\left(r - L\sum_{i=1}^{d-1} k_i e_i\right), \qquad r \in \mathcal{C}_e(L) \tag{2.13}$$

We then denote by $T_t^{(L)}(\rho)$ the flow solution of (2.8) with J_L in place of J and $\rho \in L^\infty(\mathcal{C}_e(L), \mathbb{R})$. We also denote by

$$F^{\text{per}}(\rho) := \int_{\mathcal{C}_e(L)} (f(J_L \star \rho) + \beta^{-1}\{S(J_L \star \rho) - J_L \star S(\rho)\}) \tag{2.14}$$

Observe that the critical points of F^{per} are solutions of (2.7) with J_L in place of J.

Given $h > 0$ we denote by $\mathscr{R}_e(L, h)$ a rectangular slice of $\mathscr{C}_e(L)$ of height $2h$. As before we introduce coordinate axes so that this rectangle can be written as

$$\mathscr{R}_e(L, h) = \{r = (r_1,..., r_d) \in \mathbb{R}^d : |r_d| \leqslant h, |r_i| \leqslant L/2, i = 1,..., d-1\} \tag{2.15}$$

Given a function $\rho \in L^\infty(\mathscr{R}_e(L, h), [R', R''])$ we define $\rho^{(\pm, h)} \in L^\infty(\mathscr{C}_e(L), [R', R''])$ as

$$\rho^{(\pm, h)}(r) = \begin{cases} \rho(r), & \text{if} \quad r \in \mathscr{R}_e(L, h) \\ \rho_+ \mathbf{1}_{r_d \geqslant h} + \rho_- \mathbf{1}_{r_d < -h} & \text{otherwise} \end{cases} \tag{2.16}$$

We finally define the surface tension

$$\mathrm{s}_\beta(e) := \lim_{L \to \infty} \lim_{h \to \infty} \frac{1}{L^{d-1}} \inf_{\rho \in L^\infty(\mathscr{R}_e(L, h), [R', R''])} F^{\mathrm{per}}(\rho^{(\pm, h)}) \tag{2.17}$$

We then prove the following result.

Theorem 2.3. The limits on the right hand side of (2.17) exist. Let $\tau_\beta(e)$, $e \in \mathbb{R}^d$, $|e| = 1$ be the function defined in (2.12), then the following holds. For any $\beta \in (\beta_c, \beta_0)$

$$\mathrm{s}_\beta(e) \leqslant \tau_\beta(e) \tag{2.18}$$

For any $\beta \in (\beta_c, \beta^*)$

$$\mathrm{s}_\beta(e) = \tau_\beta(e) \tag{2.19}$$

We are not able to prove the upper bound for $\beta \in (\beta^*, \beta_0)$ but computer simulations strongly indicate its validity as we are going to explain in detail in Section 4.

Sharp Interface Limit

The energy H in (1.4) is the macroscopic value of the excess free energy, this means that the derivation of (1.4) is done in the limit of vanishing ratio between macro and micro variables. For simplicity we assume that the domain in macroscopic units is the unit torus $\mathscr{T} \subset \mathbb{R}^d$; For a scaling parameter $\varepsilon > 0$, the microscopic domain is thus $\varepsilon^{-1}\mathscr{T}$. At each macroscopic profile $u \in L^\infty(\mathscr{T}, [R', R''])$ we associate the microscopic profile $u^{(\varepsilon)} \in L^\infty(\varepsilon^{-1}\mathscr{T}, [R', R''])$

$$u^{(\varepsilon)}(r) = u(\varepsilon r), \qquad r \in \varepsilon^{-1}\mathscr{T} \tag{2.20}$$

We then define the scaled free energy $\mathscr{F}_\varepsilon$ with periodic interaction and with domain $L^\infty(\mathscr{T}, [R', R''])$ in the following way,

$$\mathscr{F}_\varepsilon(\rho) = \int_{\varepsilon^{-1}\mathscr{T}} (f(J \star \rho^{(\varepsilon)}) + \beta^{-1}\{S(J \star \rho^{(\varepsilon)}) - J \star S(\rho^{(\varepsilon)})\}) \tag{2.21}$$

canonically imbedded in $\mathbb{R}^d$ (recall the definition (2.13)).

A macroscopic state with the two coexisting phases is a function $u \in BV(\mathscr{T}, \{\rho_-, \rho_+\})$. $BV(\mathscr{T}, \{\rho_-, \rho_+\})$ denotes the set of functions defined in $\mathscr{T}$ with values in $\{\rho_-, \rho_+\}$ and with bounded variation.[16] Given u as above we denote by $E = \{r: u(r) = \rho_-\}$ and by μ the associated total variation measure. We recall that there is a set $\partial^* E \subset \partial E$, called essential boundary, such that the normal $\nu(r)$ at a point $r \in \partial^* E$ is defined μ-almost everywhere. If $\partial E \in C^1$ then $\partial^* E = \partial E$ and μ is the usual $d-1$ dimensional area measure.[1, 16]

Given $\delta > 0$ and u as above we define

$$\mathscr{F}^-(u) = \lim_{\delta \to 0} \liminf_{\varepsilon \to 0} \Big(\inf_{\|\rho - u\|_{L^1(\mathscr{T})} \leqslant \delta} \varepsilon^{d-1} \mathscr{F}_\varepsilon(\rho) \Big), \tag{2.22}$$

$$\mathscr{F}^+(u) = \lim_{\delta \to 0} \limsup_{\varepsilon \to 0} \Big(\inf_{\|\rho - u\|_{L^1(\mathscr{T})} \leqslant \delta} \varepsilon^{d-1} \mathscr{F}_\varepsilon(\rho) \Big) \tag{2.23}$$

The following result is the first step in the proof of the Γ convergence.

Theorem 2.4. For any $\beta \in (\beta_c, \beta_0)$ and for any $u \in BV(\mathscr{T}, \{\rho_-, \rho_+\})$ the following holds.

$$\mathscr{F}^-(u) = \mathscr{F}^+(u) = H(u) \tag{2.24}$$

where

$$H(u) = \int_{\partial^* E} d\mu(r)\, \mathrm{s}_\beta(\nu(r)) \tag{2.25}$$

where $d\mu$ is the measure on $\partial^* E$ associated to u.

To complete the analysis of the Γ-convergence a compactness property is needed, this is the content of the following theorem.

Theorem 2.5. If a family of functions $\{\rho_\varepsilon\} \subset L^\infty(\mathscr{T}, [R', R''])$ satisfies

$$\sup_{\varepsilon > 0} \varepsilon^{d-1} \mathscr{F}_\varepsilon(\rho_\varepsilon) \leqslant C \tag{2.26}$$

then it converges by subsequences in L^1 and any limit point is a BV function with values $\rho_\pm$. As a consequence, if $u \notin BV(\mathcal{T}, \{\rho_-, \rho_+\})$ then $\mathcal{F}^-(u) = \infty$.

As explained in ref. 1, see Corollary 1.8 there, from (2.24) and Theorem 2.5 it follows that the minimizers of $\mathcal{F}_\varepsilon$ under a mass constraint (that is with the integral over $\mathcal{T}$ equal to a fixed value c) converge in $L^1(\mathcal{T})$ to the minimizers of H under the same constraint.

The rest of the paper is organized as follows. In Section 3 we prove Theorem 2.3 and we give other properties of the surface tension. In Section 4 we present the computer simulation. In Section 5 we collect all the Peierls estimates and in Section 6 we prove Theorems 2.4 and 2.5.

3. SURFACE TENSION

In this section we first give the proof of the existence of the surface tension defined in (2.17) and prove Theorems 2.3. We define

$$S_e(L,h) := \frac{1}{L^{d-1}} \inf_{\rho \in L^\infty(\mathcal{R}_e(L,h),\,[R',R''])} F^{\mathrm{per}}(\rho^{(\pm,h)}) \tag{3.1}$$

The following holds.

Proposition 3.1. For any $L > 0$, $S_e(L,h)$ is a nonincreasing function of h. For any h fixed $S_e(L,h)$ has a limit as $L \to \infty$ and

$$\lim_{h\to\infty} \lim_{L\to\infty} S_e(L,h) = \mathrm{s}_\beta(e) \tag{3.2}$$

The proof of the proposition is omitted here since it can be drawn along the same lines as in Messager *et al.*[(22)3]

We consider $\bar\rho_\beta$ one of minimizers of $F^{(e)}$, see Theorem 2.2, and define

$$q_L(r) := \bar\rho_\beta(r_d)\, \chi_{\mathcal{Q}_e(L)}(z), \qquad r = (z, r_d) \in \mathcal{R}_e(L,h) \tag{3.3}$$

where χ_A is the characteristic function of the set A. We call $q_L^{(\pm,h)}(r)$, $r \in \mathcal{C}_e(L)$ the function equal to $q_L(r)$ for $r \in \mathcal{R}_e(L,h)$ and equal to ρ_+ (respectively ρ_-) for $r_d > h$ (respectively $r_d \leqslant h$). From Theorem 2.2, $|q_L^{(\pm,h)}(r) - q_L(r)| \leqslant ce^{-c'h}$ for all $|r_d| \geqslant h$, thus

$$|F^{\mathrm{per}}(q_L^{(\pm,h)}) - L^{d-1}F^{(e)}(\bar\rho_\beta)| \leqslant \bar c L^{d-1} e^{-\bar c' h} \tag{3.4}$$

[3] A detailed proof can be found in an extended version of this work, available at the authors' web page, see, for instance, http://univaq.it/~demasi/.

which implies that

$$s_\beta(e) \leqslant \tau_\beta(e) \tag{3.5}$$

The second part of Theorem 2.3 requires to show that, for any $\beta \in (\beta_c, \beta^*)$, q_L is the unique minimizer of F^{per}, i.e.,

$$\inf_{\rho \in L^\infty(\mathscr{R}_e(L, h), [R', R''])} F^{\text{per}}(\rho^{(\pm, h)}) \geqslant F^{\text{per}}(q_L) \tag{3.6}$$

that, by (3.4) and (3.5), proves (2.19).

The above inequality stems from the analysis of the evolution defined in (2.8) with J_L in place of J, and the fact that the functional decreases along its solutions. The key step is the following proposition whose proof strongly uses the Comparison Theorem that holds only for $\beta \in (\beta_c, \beta^*)$.

Proposition 3.2. For any $\beta \in (\beta_c, \beta^*)$ the following holds. For any $\rho \in L^\infty(\mathscr{R}_e(L, h), [R', R''])$ there is $\xi \in \mathbb{R}$ such that

$$\lim_{t \to \infty} \|T_t^{(L)}(\rho^{(\pm, h)}) - D_\xi(q_L)\|_\infty = 0, \qquad D_\xi(q_L)(r) = q_L(r + \xi e_d) \tag{3.7}$$

We postpone the proof of the above proposition and first complete the proof of Theorem 2.3.

Proof of (3.6). Let $\{\rho_n\}_{n \in \mathbb{N}} \subset L^\infty(\mathscr{R}_e(L, h), [R', R''])$ be any sequence such that

$$\lim_{n \to \infty} F^{\text{per}}(\rho_n^{(\pm, h)}) = \inf_{\rho \in L^\infty(\mathscr{R}_e(L, h), [R', R''])} F^{\text{per}}(\rho^{(\pm, h)}) \tag{3.8}$$

Since F^{per} is lower semicontinuous (see Proposition 4.5 of ref. 17) and decreases along the solutions of the evolution, from Proposition 3.2 it follows that there is sequence of real numbers ξ_n so that

$$F^{\text{per}}(\rho_n^{(\pm, h)}) \geqslant \liminf_{t \to \infty} F^{\text{per}}(T_t^{(L)}(\rho_n^{(\pm, h)})) \geqslant F^{\text{per}}(D_{\xi_n}(q_L)) = F^{\text{per}}(q_L)$$

From (3.8) we then get (3.6) and Theorem 2.3 is proved. ∎

Proof of Proposition 3.2. The proof is the same as the one given in the course of the proof of Theorem 7.3 of ref. 17. Indeed we face the same expository problem of Gayrard *et al.*: the full proof is an adaptation of the arguments given in the papers of refs. 12–14 that are too long and too similar to be repeated here.

The main point is to prove a stability result for the linear evolution

$$\partial_t u = \Omega u \tag{3.9}$$

obtained by linearizing the right hand side of (2.8) around q_L. Thus

$$\Omega u(r) = -u + \beta \bar{\rho}_\beta(r_d)\, J_L \star \left\{ \left[1 - \frac{(j_e \star \bar{\rho}_\beta)^2}{2} \right] J_L \star u \right\} \tag{3.10}$$

where, with our choice of the coordinate frame,

$$j_e(x-x') = \int_{\mathcal{Q}_e(L)} dz'\, J_L(r-r'), \quad r=(z,x),\, r'=(z',x'),\ z \in \mathcal{Q}_e(L),\ x, x' \in \mathbb{R}$$

We consider Ω as an operator in $L^\infty(\mathcal{C}_e(L), [R', R''])$ and we observe that

$$\Omega q'_L = 0, \qquad q'_L(r) = \bar{\rho}'_\beta(x)\, \chi_{\mathcal{Q}_e(L)}(z) \quad r=(z,x) \tag{3.11}$$

$\bar{\rho}'_\beta$ denoting the derivative. Thus 0 is an eigenvalue for Ω with eigenfunction q'_L and we now sketch the proof of the existence of a spectral gap, that is the proof of (3.12) later. Given $u \in L^\infty(\mathcal{C}_e(L), [R', R''])$ we denote by

$$N_u := \int_{\mathcal{C}_e(L)} dr\, \frac{q'_L(r)}{\beta \bar{\rho}_\beta(r_d)}\, u(r), \qquad \tilde{u} := u - N_u q'_L$$

Then there are $c>0$ and $\omega>0$ such that for all $u \in L^\infty(\mathcal{C}_e(L), [R', R''])$

$$\|e^{\Omega t}\tilde{u}\|_\infty \leqslant c e^{-\omega t}\, \|\tilde{u}\|_\infty \tag{3.12}$$

For $\beta \in (\beta_c, \beta^*)$ the square bracket on the right hand side of (3.10) is positive. Thus, to prove (3.12), we can exploit the fact that Ω is a Perron Frobenius operator by defining the transition probability kernel

$$K(r,r') := \frac{\beta \bar{\rho}_\beta(r_d)}{\bar{\rho}'_\beta(r_d)} \int dz\, J_L(r-z) \left[1 - \frac{(j_e \star \bar{\rho}(z_d))^2}{2} \right] J_L(z-r')\, \bar{\rho}'_\beta(r'_d) \tag{3.13}$$

and observing that

$$K = \frac{1}{q'_L} \circ [\Omega + 1] \circ q'_L, \qquad \int K(r,r')\, dr' = 1$$

By noticing that the measure

$$\mu(dr) := \frac{q'_L(r)^2}{\beta \bar{\rho}_\beta(r_d)}\, dr$$

is invariant under K, (3.12) is then obtained by showing a fast approach to equilibrium for the Markov evolution generated by K. Namely the following holds. There are c and α positive such that

$$\|q'_L[K^n(u-\mu(u))]\|_\infty \leqslant c e^{-\alpha n} \|u-\mu(u)\|_\infty, \qquad \mu(u) = \int \mu(dr)\, u(r) \quad (3.14)$$

By using the Dobrushin's theory of Gibbs measures at hight temperature it is possible to show (see refs. 13 and 14 for details) that (3.14) is implied by the following two properties of K.

There are I and for any $s>0$ an integer k_s and $b_s > 0$ so that

$$K^{k_s}(r, r') \geqslant b_s, \qquad \text{for all} \quad |r| \leqslant s, \quad \text{and for all} \quad r' \in I \qquad (3.15)$$

There are $\delta \in (0, 1)$ and $a > 0$ so that for all r

$$\int dr'\, K(r, r')\, w(r') \leqslant \delta w(r) + a, \qquad w = (q'_L)^{-1} > 0 \qquad (3.16)$$

(3.15) follows from the positivity of K and the fact that the first $d-1$ coordinates vary in a compact set. The value k_s diverges as $L \to \infty$, but this does not matter since the stability property is only needed for each fixed value of L.

To prove (3.16) we observe that since $\beta \in (\beta_c, \beta^*)$ there is s_0 so that

$$0 < p(x) := \beta \bar{\rho}_\beta(x)\, j_e \star \left[1 - \frac{(j_e \star \bar{\rho}_\beta)^2}{2}\right](x) < 1, \qquad \text{for all} \quad x \geqslant s_0 - 2$$

Then (3.16) follows with

$$\delta = p(s_0 - 2), \qquad a = \sup_{|x| \leqslant s_0 - 2} \frac{1}{\bar{\rho}'_\beta(x)}$$

As explained in ref. 17, after the spectral gap, the rest of the proof is the same as in ref. 13, so we omit the details. The proposition is proved. ∎

4. NUMERICAL ANALYSIS

In this section, we report various results obtained by computer simulations. The aim of this part is to get some insight about some aspects of the nonlocal functional (2.5), which are difficult to study. We first give the general frame in which this numerical work was done and report results obtained for various interaction kernels in one and two dimensions.

In order to cast the variational problem to a form easily amenable to computer simulation, we need both to have some control over the numerical parameters of the problem at hand, and to introduce a suitable discretized version of it. The first part can be conveniently provided by the following elementary mapping which gives an explicit parametrization of all the parameters, β, λ_β, ρ_+, and ρ_-, and in particular the phase diagram.

Phase Diagram

We first define two functions $g(s)$ and $v(s)$, $s \in (0, 1)$ as,

$$g(s) = \frac{1}{2s} \log\left(\frac{1+s}{1-s}\right) - 1, \qquad v(s) = \left(\frac{1+s^2}{2} + \frac{s^2}{3g(s)}\right)^{-1/2}$$

Since the function

$$s \to \beta(s) := \frac{3g(s)}{s^2 v(s)^3} \tag{4.1}$$

is strictly increasing from $(0, 1)$ onto $(\beta_c, +\infty)$, we can parametrize all quantities in term of $s \in (0, 1)$ instead of $\beta \in (\beta_c, +\infty)$. The other quantities, λ_β, ρ_+ and ρ_- are explicit elementary functions of s,

$$\lambda_\beta = \frac{-v(s)^3}{3}\left(1 + \frac{s^2}{g(s)}\,(1 - \log[v(s)\sqrt{1-s^2}])\right), \qquad \rho_\pm = v(s)(1 \pm s)$$

In addition, the expression given above shows that the chemical potential $\lambda_\beta < 0$.

A first use of the above parametrization consists in the drawing of the coexistence curve in the density-temperature plane (Fig. 1). The curve is asymmetric, mean-field like and independent on the interaction kernel.

Discretized Interaction Kernel

We now turn to the discretization scheme. As will be shown below, we need only to introduce a stepwise constant approximation of the interaction kernel.

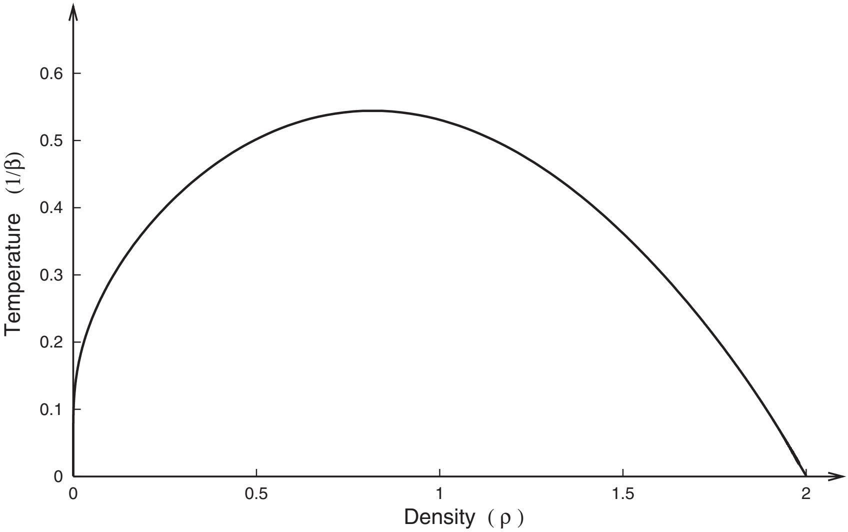

Fig. 1. Liquid-vapor phase diagram in the density-temperature plane for the local mean field limit of the LMP model.

Given $L > 0$, we consider a cylinder $\mathscr{C}(L) = [-L/2, L/2]^{d-1} \times \mathbb{R}$ in $\mathbb{R}^d$. We then take $h > 0$ such that L and h have commensurable values and choose $\epsilon > 0$ such that L and h are both integer multiples of ϵ. We finally consider finite rectangles of $\mathscr{C}(L)$, $\mathscr{R} = \mathscr{R}(L, h)$, as in (2.15), and introduce a partition of $\mathbb{R}^d$ in cubes of mesh ϵ, as follow.

Let $B_\epsilon(x)$ denote the cube in $\mathbb{R}^d$ with center in x and sidelength ϵ,

$$B_\epsilon(x) = \left\{ y \in \mathbb{R}^d : -\frac{\epsilon}{2} \leqslant x_i - y_i < \frac{\epsilon}{2}, i \in \{1,..., d\} \right\} \tag{4.2}$$

We consider the partition $\mathscr{B}^\epsilon = \{B_\epsilon(\epsilon k)\}_{k \in \mathbb{Z}^d}$ of $\mathbb{R}^d$, and its restriction on the rectangle, $\mathscr{B}^\epsilon_{\mathscr{R}} = \{B_\epsilon(\epsilon k)\}_{k \in \mathscr{R}_\epsilon}$ where $\mathscr{R}_\epsilon = \{k \in \mathbb{Z}^d : \epsilon k \in \mathscr{R}\}$.

Given an interaction kernel J defined on $\mathbb{R}^d$ as in Section 1, we introduce a step-wise constant approximation J^ϵ on $\mathbb{R}^d \times \mathbb{R}^d$ as follows:

$$J^\epsilon(z, z') = \epsilon^{-d} \int_{B_\epsilon(0)} J(q(z) - q(z') - \zeta)\, d\zeta \tag{4.3}$$

where $q(z)$ is the center of the unique cube in $\mathscr{B}^\epsilon$ which contains z. This definition breaks the continuous translational invariance of the interactions, so that the kernel J^ϵ now depends on two arguments (and not only on their difference as in the previous sections). J^ϵ is positive, has range not larger than $1+\epsilon$, and integral $\int J^\epsilon = 1$. As in the previous sections, we introduce a periodic extension of the interaction kernel on $\mathscr{C}(L)$ defined for all $r, r' \in \mathscr{C}(L)$ as

$$J^\epsilon_L(r, r') = \sum_{k \in \mathbb{Z}^{d-1}} J^\epsilon\left(r, r' - 2L \sum_{i=1}^{d-1} k_i e_{i+1}\right) \tag{4.4}$$

We now consider the functional defined as in Eq. (2.14), with the interaction kernel J^ϵ and denote it as $F^{(\varepsilon, L)}$. We have the following

Proposition 4.1. Recalling the definition (2.16), we consider F^{per} and $F^{(\varepsilon, L)}$ as functionals over $L^\infty(\mathscr{R}, [R', R''])$. The minima of $F^{(\varepsilon, L)}(\rho^{(\pm, h)})$, ρ defined in $\mathscr{R}$ are constant on each cube of the partition $\mathscr{B}^\epsilon_{\mathscr{R}}$ and we have

$$\lim_{\epsilon \to 0} \inf_{\rho \in L^\infty(\mathscr{R}, [R', R''])} F^{(\varepsilon, L)}(\rho^{(\pm, h)}) = \inf_{\rho \in L^\infty(\mathscr{R}, [R', R''])} F^{\text{per}}(\rho^{(\pm, h)}) \tag{4.5}$$

Proof. The fact that the functional takes its minima over profiles which are constant on each cube of the partition $\mathscr{B}^\epsilon_{\mathscr{R}}$ is due to the fact that $J^\epsilon \star \rho$ (and hence the energy part of the functional, $E_\lambda(J^\epsilon \star \rho)$) depends only on the mean of ρ in each cube,

$$\int dr'\, J^\epsilon(r, r')\, \rho(r') = \sum_{k \in \mathscr{R}^\varepsilon} J^\epsilon(r, \epsilon k) \int dr'\, \chi_{B_\epsilon(\epsilon k)}(r')\, \rho(r') \tag{4.6}$$

while the entropy term is concave,

$$\int dr'\, \chi_{B_\epsilon(\epsilon k)}(r')\, S(\rho(r')) \leqslant S\left(\int dr'\, \chi_{B_\epsilon(\epsilon k)}(r')\, \rho(r')\right) \tag{4.7}$$

The second part of the proposition follows from the uniform boundedness of the profiles. ∎

The above proposition thus allows us to reduce the functional space to a finite dimensional one, and all numerical simulations have been done in this setting.

Numerical Results

The questions to which we want to get some insight concern the existence and nature of the interfaces for large values of the inverse temperature β, the nature of the "transition" at β^* from monotonous to non-monotonous profiles, the possible existence of oscillatory pattern in the direction of the interface (for $d \geqslant 2$) , and the angular dependance of the interfacial energy for an anisotropic potential.

Numerical simulations were done on finite slices $\mathscr{R}(L, h)$ of $\mathscr{C}(L)$ as in (2.15) with fixed boundary conditions on the complement $\xi^{\pm}_{\mathscr{R}(L,h)^c}$. Minimization of free energy was done by a careful iteration of the map:

$$\rho \to \rho(1-\alpha) + \alpha\Phi(\rho) \tag{4.8}$$

where $\alpha > 0$ is taken sufficiently small so that free energy decreases under iteration. We skip here the technical details relative to the problems of convergence. In the one dimensional case, except for values of temperature close to T_c or 0, typical size of the grid $h \times \epsilon^{-1} \approx 10^5$ was found already sufficient for our purpose.

• Since the limiting value of β_0 for mathematical analysis is essentially of technical nature and related to the properties of the map $\rho = \Phi(\rho)$, no real change is expected for values $\beta > \beta_0$. On the other side, β^* has a more physical meaning since it separates monotonous from nonmonotonous density profiles. For $\beta > \beta^*$, the density profile has oscillations near the interface in the high density phase. In ref. 17, it was proven that either there is an infinite number of oscillations, or a finite number separating the interface from a constant density ρ_+ at finite distance. Numerical simulations were consistent with the first hypothesis (up to machine precision), but this might depend on the choice of the interaction kernel. We also give a proof for a particular kernel, $J(x) = \frac{1}{2} 1_{|x|<1}$ (see Proposition 4.2 later). Figure 2 illustrates typical one dimensional profiles for inverse temperatures both below and above β^*.

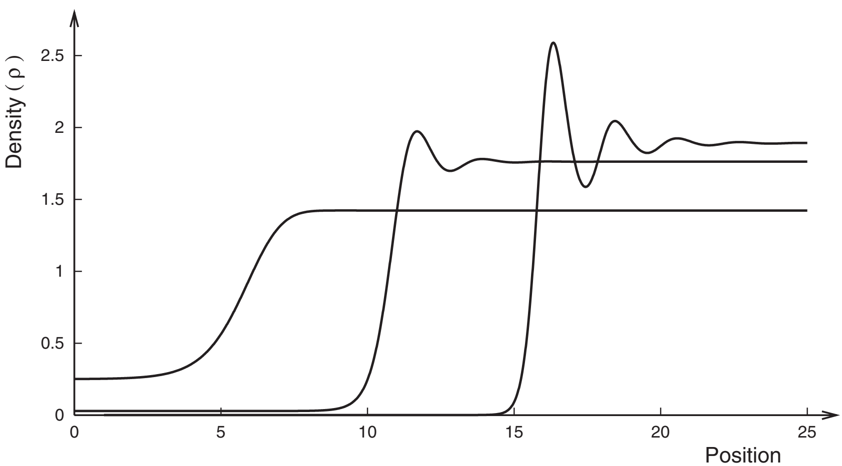

Fig. 2. Interface density profiles at various temperatures for the interaction kernel $J(x) = \frac{1}{2}\mathbf{1}_{\{|x|<1\}}$: From left to right: $\beta = 2.5$; $\beta = 5$; $\beta = 10$.

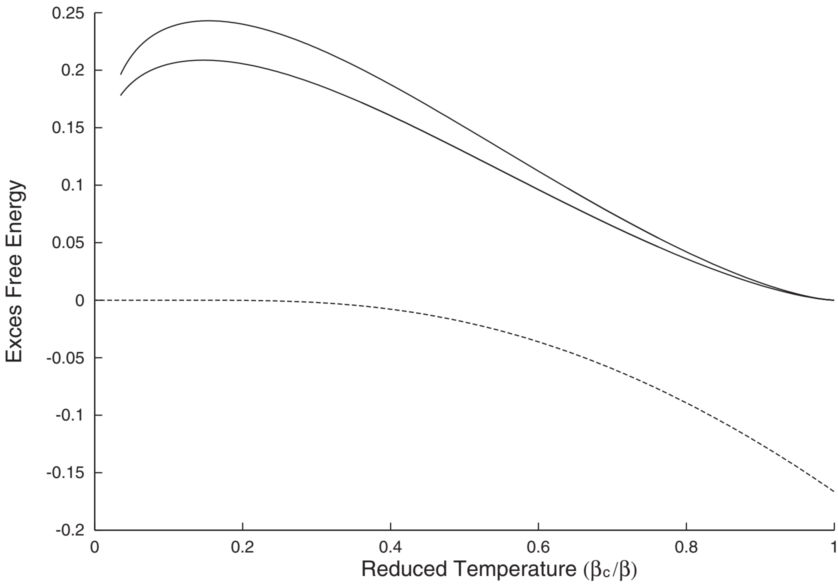

Fig. 3. Excess Free energy of the liquid-vapor interface in function of the reduced temperature $\frac{\beta_c}{\beta}$ for two interaction kernels. Upper plain curve: $J(x) = \frac{1}{2}\mathbf{1}_{\{|x|<1\}}$. Lower plain curve $J(x) = \frac{1}{\pi}\mathbf{1}_{\{|x|<1\}}\sqrt{1-x^2}$. No noticeable change occurs at $\beta = \beta^* \approx 1.35\beta_c$. Dotted line: free energy of the pure phases.

• Another question raised in ref. 17 is the nature of the "transition" at β^*. We thus computed the excess free energy for various interaction kernels in the whole range of temperature below T_c (Fig. 3) and it shows no evidence of any noticeable effect at β^*, thus probably ruling out the existence of a "secondary phase transition" at that point.

• We also investigated two dimensional systems with isotropic and nonisotropic interaction kernels and look for both the existence of oscillations in the direction of interface, and the dependance of surface tension on the interface orientation. In Proposition 3.1, it was proven that for $\beta < \beta^*$, the interface is uniform in all directions perpendicular to the cylinder axis. This stability result derives from the uniform positivity of the quantity $1-(J \star \bar{\rho})/2$ (see (3.13)). For $\beta > \beta^*$, this argument is no longer valid in the high density phase and one can ask whether spatial oscillation patterns form at the mesoscopic scale in direction perpendicular to the cylinder axis. Numerical results indicate that there is a subtle balance between the high and low density phase contributions to the excess free energy, and that the former, stabilizing contribution slightly dominates. Interface profiles where

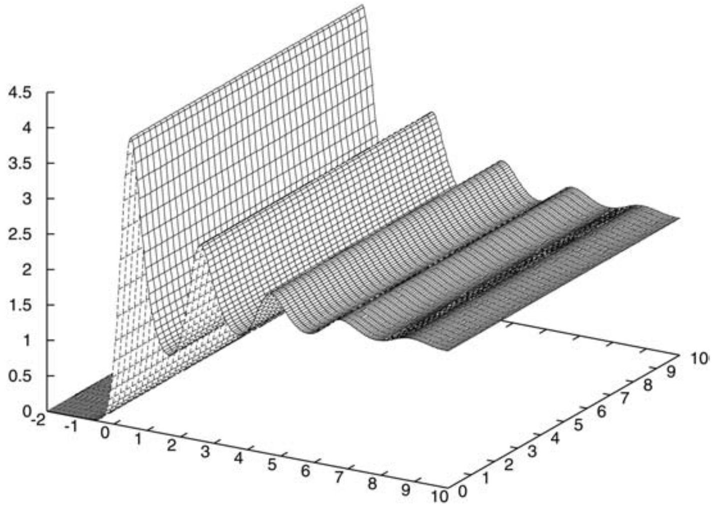

Fig. 4. Two dimensional interface profile at low temperature ($\beta = 25$) with uniform interaction in the unit square. Flat interface remains stable even for values of β much larger than β^*.

thus always found to be homogeneous in the $d-1$ dimensions perpendicular to the cylinder axis (Fig. 4).

We now consider the variation of the excess free energy with the orientation of the interface when nonisotropic interaction kernels are considered. The most typical case can be embodied by the two dimensional kernel describing uniform interactions inside a domain of elliptic shape. In such a case the one dimensional projection just amounts to a rescaling of the interaction range and the excess free energy changes accordingly. Let a (resp. b) be the major (minor) semiaxis length of the ellipse and θ be the angle between the major axis and the axis of the cylinder $\mathscr{C}(e)$. Then, by using only scaling arguments, it is not hard to show that the excess free energy $F^{(e)}$ depends on the orientation as

$$F^{(e)} = f_\beta \sqrt{a^2 \cos^2(\theta) + b^2 \sin^2(\theta)} \tag{4.9}$$

where f_β is a constant. The shape of the angular dependance is in this case completly independant on the model. The above shape is roughly still valid for kernels with compact support and interaction decreasing with the distance. Dropping the last condition changes the picture in some way. However, the stiffness matrix has been always found to be positive definite, so that no facetting phenomena has been found in the model.

We conclude this section by proving for a particular kernel, that there is no instanton constant and equal to ρ_+ on an half line. In ref. 17, it was proved that for $\beta > \beta^*$, the one dimensional instanton in the high density region converges at least exponentially fast to ρ_+ but has infinitely many oscillations. The following proposition thus prove in a particular case that these oscillations extend to the whole high density phase.

Proposition 4.2. Let ρ be the instanton solution of (2.5) in one space dimension associated to the interaction kernel

$$J(x) = \tfrac{1}{2}\, \mathbf{1}_{\{|x| < 1\}} \tag{4.10}$$

Then ρ cannot be constant and equal to ρ_+ on a half line.

Proof. The proof relies heavily on the particular choice for the kernel.

Suppose that such an instanton ρ exists, and let N be the leftmost point of the halfline on which ρ is constant and equal to ρ_+, $N = \inf\{x \in \mathbb{R} : \rho(y) = \rho_+ \ \forall y > x\}$.

We first take the derivative of (2.7), as

$$\begin{aligned} \rho'(x) &= -\beta\rho(x)(J' \star E'(J \star \rho))(x) \\ &= -\tfrac{1}{2}\, \beta\rho(x)(E'((J \star \rho)(x+1)) - E'((J \star \rho)(x-1))) \end{aligned} \tag{4.11}$$

In the second line, we made explicitely use of the special choice of the kernel, and in particular that its derivative is half the difference of two delta functions in 1 and -1.

Let us suppose $x \geqslant N$. By hypothesis, we have $\rho'(x) = 0$ and $(J \star \rho)(x+1) = \rho_+$. Hence (4.11) reduces to

$$E'((J \star \rho)(x-1)) = E'(\rho_+) \qquad \forall x \geqslant N \tag{4.12}$$

E' is not monotonous, but the reciprocal image of $E'(\rho_+)$ contains a finite number of elements. We thus rely on the continuity of $E'(J \star \rho)$ as a function of x to get,

$$(J \star \rho)(x-1) = \rho_+ \qquad \forall x \geqslant N \tag{4.13}$$

In order to conclude, we can take for instance the derivative of (4.13) and obtain, $\rho(x-2) = \rho(x)$ $\forall x \geqslant N$. Then ρ is also constant and equal to ρ_+ on the interval $[N-2, N]$, in contradiction with the definition of N. ∎

5. CONTOURS AND PEIERLS ESTIMATES

In this section we give the Peierls estimates on contours that are needed to prove Theorems 2.4 and 2.5. The proofs of our statements on contours are already known: some of them are given in ref. 17 for one dimension, others are similar to estimates given in ref. 21 for the more complicated particle models. We have learn them from E. Presutti who is writing the proofs in all details in ref. 25. For the reader convenience we state the definitions and the results on contours giving only some idea of the proofs.

We start with the following definitions that are the analogous of the ones given in ref. 17 in $d=1$ dimension.

• **Partitions and Boundaries.** We denote by $\mathscr{D}^{(\ell)}$ a decreasing sequence of partitions of $\mathbb{R}^d$ into cubes of side ℓ, $C_r^{(\ell)}$ denotes the cube of the partition which contains $r \in \mathbb{R}^d$. We say that a region $\Lambda \subset \mathbb{R}^d$ is $\mathscr{D}^{(\ell)}$-measurable if it is a union of cubes of the partition $\mathscr{D}^{(\ell)}$.

The $D^{(\ell)}$-outer boundary of a $\mathscr{D}^{(\ell)}$-measurable region Λ, denoted by $\delta_{\text{out}}^{\ell}[\Lambda]$ is the union of all the cubes C of $\mathscr{D}^{(\ell)}$ not in Λ which are connected to Λ (two sets are connected if their closures have nonempty intersection). The $\mathscr{D}^{(\ell)}$-inner boundary $\delta_{\text{in}}^{\ell}[\Lambda]$ is the $\mathscr{D}^{(\ell)}$-outer boundary of Λ^c.

• **Coarse-Graining.** Given the partition $\mathscr{D}^{(\ell)}$, we define the coarse-grained image of $\rho \in L^\infty(\mathbb{R}^d, [R', R''])$ with grain ℓ

$$M^{(\ell)}(\rho; r) = \frac{1}{\ell^d} \int_{C_r^{(\ell)}} dr'\, \rho(r') \tag{5.1}$$

• **Block Spins.** Given $\zeta > 0$, $\ell < 1$ and a profile $\rho \in L^\infty(\mathbb{R}^d, [R', R''])$ we define the function $\eta^{(\zeta, \ell)}(\rho; r) \in \{0, 1, -1\}$, $r \in \mathbb{R}^d$ as follows. $\eta^{(\zeta, \ell)}(\rho; r) = \pm 1$ if $|M^{(\ell)}(\rho; r) - \rho_\pm| \leqslant \zeta$, otherwise $\eta^{(\zeta, \ell)}(\rho; r) = 0$. We say that $\eta^{(\zeta, \ell)}(\rho; r)$ is the "block spin" representation of ρ with grain ℓ and accuracy ζ. In the applications ζ and ℓ are small.

• **Correct Points.** The correct points are defined in terms of parameters ζ and $\ell_- < 1 < \ell_+$. Given a function $\rho \in L^\infty(\mathbb{R}^d, [R', R''])$ a point $r \in \mathbb{R}^d$ is $+$ correct if $\eta^{(\zeta, \ell_-)}(\rho; r') = 1$ for all $r' \in C_r^{(\ell_+)} \cup \delta_{\text{out}}^{\ell_+}[C_r^{(\ell_+)}]$. The point is $-$ correct if $\eta^{(\zeta, \ell_-)}(\rho; r') = -1$ for all $r' \in C_r^{(\ell_+)} \cup \delta_{\text{out}}^{\ell_+}[C_r^{(\ell_+)}]$. We say that $r \in \mathbb{R}^d$ is uncorrect is it is neither $+$ nor $-$ correct.

Observe that the definition of correct points is such that the coarse grained image of the profile must be close to $\rho_\pm$ not only at the given point but also in a surrounding region, large enough to contain all points within interaction range.

In the applications ℓ_+ will be much larger than the range of the interaction. As in ref. 17, we will consider

$$\ell > 4; \qquad \ell_+ = \ell, \ \ell_- = \ell^{-1} \tag{5.2}$$

• **Contours.** The (ζ, ℓ)-contours of a function $\rho \in L^\infty(\mathbb{R}^d, [R', R''])$ are the pairs $\Gamma = (\mathrm{sp}(\Gamma), \eta_\Gamma)$, where $\mathrm{sp}(\Gamma)$, the spatial support of Γ, is one of the maximal connected component of $\{r \in \mathbb{R}^d : r \text{ is uncorrect}\}$ and η_Γ is the restriction to $\mathrm{sp}(\Gamma)$ of $\eta^{(\zeta, \ell_-)}(\rho; \cdot)$. When $\mathrm{sp}(\Gamma)$ is a bounded set, we call $c(\Gamma)$ the union of $\mathrm{sp}(\Gamma)$ and of its internal parts, namely $c(\Gamma)$ is the complement of the unbounded maximal connected component of $\mathrm{sp}(\Gamma)^c$. We then define $A_0 = \delta_{\mathrm{out}}^{\ell_+}[c(\Gamma)]$, $K_0 = \delta_{\mathrm{in}}^{\ell_+}[c(\Gamma)]$. By definition, $\eta_\Gamma \equiv 1$ or $\eta_\Gamma \equiv -1$ on K_0, in the former case we say that Γ is a $+$ contour, in the latter a $-$ contour.

Let Λ be a bounded, $\mathscr{D}^{(\ell_-)}$-measurable region; given $\rho^* \in L^\infty(\mathbb{R}^d, [R', R''])$ we define

$$\mathscr{X}_{\Lambda, \rho^*, +} = \{\rho \in \mathscr{M}^+_{\zeta, \ell_-; \Lambda} : \rho_{\Lambda^c} = \rho^*_{\Lambda^c}\} \tag{5.3}$$

where ρ_A denotes the function ρ restricted to the set A and where

$$\mathscr{M}^+_{\zeta, \ell_-; \Lambda} := \{\rho \in L^\infty(\mathbb{R}^d, [R', R'']) : \eta^{(\zeta, \ell_-)}(\rho; r) = 1, \text{ for all } r \in \Lambda\} \tag{5.4}$$

An analogous definition holds for the $-$ case and since the proofs are similar, for notational simplicity, we will restrict to the $+$ case.

In the next theorem we prove that if ℓ_- and ζ are small enough, then the minimizer of the excess free energy in $\mathscr{X}_{\Lambda, \rho^*, +}$, is point-wise close to ρ_+ in Λ, the closeness being exponential with the distance from the boundaries.

Theorem 5.1. There are ζ_0, ω, and c_ω all positive, so that for any $\zeta < \zeta_0$, $\ell_- < \ell_0(\zeta)$, the following holds.

For any bounded, $\mathscr{D}^{(\ell_-)}$-measurable region Λ and any ρ^* such that $\eta^{(\zeta, \ell_-)}(\rho^*; r) = 1$, for all $r \notin \Lambda$ at distance less than 4 from the boundary of Λ, the following holds.

- There is a unique minimizer ψ of $F(\cdot)$, recall (2.5), in $\mathscr{X}_{\Lambda, \rho^*, +}$;
- ψ is the unique solution of the equation

$$\begin{aligned} &\psi(r) = \exp\{-\beta J \star E'_\beta(J \star \psi)\}, \qquad r \in \Lambda \\ &\psi_{\Lambda^c} = \rho^*_{\Lambda^c} \end{aligned} \tag{5.5}$$

- ψ is continuous in Λ with values in $(\rho_+ - \zeta, \rho_+ + \zeta)$, and

$$|\psi_\Lambda(r) - \rho_+| \leqslant c_\omega e^{-\omega \operatorname{dist}(r, \Lambda^c_{\neq})} \tag{5.6}$$

where $\Lambda^c_{\neq} = \{r \in \Lambda^c : \operatorname{dist}(r, \Lambda) \leqslant 1, \rho^*_{\Lambda^c}(r) \neq \rho_+)\}$.

Proof. If $\rho \in \mathcal{M}^+_{\zeta, \ell_-; \Lambda}$ then, for ℓ_- small enough,

$$|J \star \rho - \rho_+| \leqslant \zeta + cR'' \ell_- \leqslant 2\zeta \tag{5.7}$$

Furthermore, given any ζ small enough there is ε so that

$$\rho_+ - \zeta \leqslant \inf_{|s - \rho_+| \leqslant \zeta + \varepsilon} \exp\{-\beta E'_\beta(s)\} \leqslant \sup_{|s - \rho_+| \leqslant \zeta + \varepsilon} \exp\{-\beta E'_\beta(s)\} \leqslant \rho_+ + \zeta \tag{5.8}$$

Therefore choosing ℓ_0 so that $cR''\ell_0 \leqslant \varepsilon$ we get

$$|\exp\{-\beta J \star E'_\beta(J \star \rho)\} - \rho_+| \leqslant \zeta \tag{5.9}$$

Let $T^\Lambda_t(\rho)$ be the solution of

$$\begin{aligned} &\partial_t \rho = -\rho + \exp\{-\beta J \star E'_\beta(J \star \rho)\}, \qquad \text{in } \Lambda \\ &\rho(r, 0) = \rho(r), \qquad \rho_{\Lambda^c}(r, t) = \rho^*_{\Lambda^c}(r), \qquad \forall t \geqslant 0 \end{aligned} \tag{5.10}$$

We further observe that for $\rho \in \mathcal{M}^+_{\zeta, \ell; \Lambda}$, the set $\mathcal{X}_{\Lambda, \rho^*, +}$ is T^Λ_t invariant, namely

$$\eta^{\zeta, \ell}(T^\Lambda_t(\rho), r) = 1, \qquad \forall r \in \Lambda \tag{5.11}$$

The proof of (5.11) is the same as the one of Lemma 6.2 of ref. 17.

Then, since $\mathcal{X}_{\Lambda, \rho^*, +}$ is closed in the topology of the uniform convergence on the compacts, if $u \in \mathcal{X}_{\Lambda, \rho^*, +}$ has finite free energy then $T^\Lambda_t(u)$ converges by subsequences uniformly on the compacts to a function ψ, see Proposition 4.7 of ref. 17. It is not difficult to prove that (i) and (ii) below hold.

(i) The function $\psi \in \mathcal{X}^0_{\Lambda, \rho^*, +}$ where

$$\mathcal{X}^0_{\Lambda, \rho^*, +} = \{\rho \in \mathcal{X}_{\Lambda, \rho^*, +} : \rho = \exp\{-\beta J \star E'_\beta(J \star \rho)\}, \text{ in } \Lambda\} \tag{5.12}$$

(ii) $F(\rho) \geqslant F(\psi)$ for all $\rho \in \mathcal{X}_{\Lambda, \rho^*, +}$ and the equality holds if and only if $\rho \in \mathcal{X}^0_{\Lambda, \rho^*, +}$.

To prove uniqueness, we assume that there are $\psi \neq \rho_+$ and $\phi \neq \rho_+$ both in $\mathscr{X}^0_{\Lambda, \rho^*, +}$. Then

$$|\psi - \phi| = |\exp\{-\beta J \star E'_\beta(J \star \phi)\} - \exp\{-\beta J \star E'_\beta(J \star \psi)\}| \tag{5.13}$$

and from (5.9) we know that $|\psi - \rho_+| \leqslant \zeta$ and $|\phi - \rho_+| \leqslant \zeta$, for all $r \in \Lambda$. Therefore, recalling the definition (2.1),

$$|\psi(r) - \phi(r)| \leqslant \Big(\sup_{|s-\rho_+| \leqslant 2\zeta} |\varphi'_\beta(s)|\Big) \, \|\psi - \phi\|_\infty \tag{5.14}$$

Since $|\varphi'_\beta(\rho_+)| < 1$, choosing ζ small enough, the sup in the bracket on the right hand side of (5.14) is strictly smaller than 1, which then implies that $\phi \equiv \psi$.

We are left with the proof of (5.6). We use (5.13) with $\phi \equiv \rho_+$ and setting

$$\varepsilon(\zeta) := \sup_{|s-\rho_+| \leqslant \zeta} |\varphi'_\beta(s)| < 1$$

we get, for any $r \in \Lambda$,

$$\begin{aligned} |\psi(r) - \rho_+| &= |\exp\{-\beta J \star E'_\beta(J \star \psi)\} - \exp\{-\beta E'_\beta(\rho_+)\}| \\ &\leqslant \varepsilon(\zeta) \left[\int_\Lambda J(r-r') \, |\psi(r') - \rho_+| + \int_{\Lambda^c} J(r-r') \, |\bar{\rho}_{\Lambda^c}(r') - \rho_+| \right] \end{aligned} \tag{5.15}$$

Using (5.15) iteratively, we get,

$$|\psi(r) - \rho_+| \leqslant \sum_{n=n_0(r)}^{\infty} \varepsilon(\zeta)^n \, 2R''$$

where $n_0(r)$ is the biggest integer less than $\mathrm{dist}(r, \Lambda^c_{\neq})$. This gives (5.6) and concludes the proof of the theorem. ∎

The next two theorems are the Peierls estimates needed to prove Theorem 2.4.

Theorem 5.2. For any $\zeta > 0$ small enough there is $\ell_0(\zeta) > 0$ and for any $\ell \geqslant \ell_0(\zeta)^{-1}$ there is $c > 0$ so that the following holds. Let $\rho \in L^\infty(\mathbb{R}^d; [R', R''])$ have a contour Γ. Then there is a function ψ equal to ρ on $c(\Gamma)^c$, equal to ρ_+ on $c(\Gamma) \setminus K_0$, with $\eta(\psi; r) = 1$ on K_0 and such that

$$F(\rho) \geqslant F(\psi) + c\zeta^2 \ell^{-2d} \, |\mathrm{sp}(\Gamma)| \tag{5.16}$$

Proof. Recalling (5.2), we consider Σ a $D^{(\ell_-)}$-measurable corridor in the middle of K_0 whose complement is made of two unconnected components at mutual distance $\geqslant 1$, calling Δ the bounded connected component of Σ^c. We also suppose that Σ has distance $\geqslant \ell/3$ from $\delta^1_{\text{in}}[K_0]$. By Theorem 5.1 applied to K_0 we can modify ρ into a new function ϕ, equal to ρ outside K_0, exponentially close to ρ_+ away from the boundaries, with $\eta(\phi; r) = 1$ on K_0 and such that

$$|\phi(r) - \rho_+| \leqslant c_\omega e^{-\omega\ell/4}, \qquad r \in \delta^\ell_{\text{out}}[\Delta] \cup \delta^\ell_{\text{in}}[\Delta] \tag{5.17}$$

We write

$$F(\phi) = F(\phi; \Delta) + F(\phi; \Delta^c) \tag{5.18}$$

where for any region Ω we have set

$$F(\phi; \Omega) := \int_\Omega (f(J \star \phi) + \beta^{-1}\{S(J \star \phi) - J \star S(\phi)\}) \geqslant 0 \tag{5.19}$$

Since ϕ is equal to ρ outside K_0, ϕ still has Γ as a contour and, as proved in ref. 21, see also Theorem 5.1 in ref. 17,

$$F(\phi; \Delta) \geqslant c'\zeta^2\ell^{-2d}\, |\text{sp}(\Gamma)| \tag{5.20}$$

Call ψ the function equal to ϕ on $(\Delta \cup \Sigma)^c$ and to ρ_+ elsewhere. Then by (5.17),

$$|F(\phi; \Delta^c) - F(\psi; \Delta^c)| \leqslant c''\, |\Sigma|\, e^{-\omega\ell/4}$$

and since $F(\psi; \Delta) = 0$,

$$F(\phi) \geqslant F(\psi; \Delta) + F(\psi; \Delta^c) - c''\, |\Sigma|\, e^{-\omega\ell/4} + c'\zeta^2\ell^{-2d}\, |\text{sp}(\Gamma)|$$

By choosing ℓ large enough we then get (5.16). ▮

As a corollary of Theorem 5.2, if ρ has n contours Γ_i, $i = 1,..., n$, then

$$F(\rho) \geqslant \sum_{i=1}^{n} c\zeta^2\ell^{-2d}\, |\text{sp}(\Gamma_i)| \tag{5.21}$$

(5.21) follows by successive applications of (5.16) and recalling that $F(\cdot) \geqslant 0$.

Theorem 5.2 is also used in the proof of the following theorem:

Theorem 5.3. There are ζ and ℓ such that the following holds. Let Λ and $\Delta \subset \Lambda$ be two bounded, $\mathscr{D}^{(\ell_+)}$-measurable regions; $\rho \in L^\infty(\mathbb{R}^d, [R', R''])$ with $\eta^{(\zeta, \ell_-)}(\rho; r) = 1$, $r \in \delta^{\ell_+}_{\text{out}}[\Lambda] \cup \delta^{\ell_+}_{\text{in}}[\Lambda]$. Then there is a positive constant C and a function ϕ in $L^\infty(\mathbb{R}^d, [R', R''])$, so that $\phi = \rho$ on Λ^c, $\phi = \rho_+$ on Δ, $\eta^{(\zeta, \ell_-)}(\phi; r) = 1$ on Λ and, finally, calling

$$\delta\Delta = \{r \in \Delta : \text{dist}(r, \Delta^c) \leqslant 2\}, \qquad \Lambda^c_{\neq} = \{r \in \Lambda^c, \rho(r) \neq \rho_+, \text{dist}(r, \Lambda^c) \leqslant 2\} \tag{5.22}$$

$$F(\rho) \geqslant F(\phi) - C\,|\Delta|\, e^{-\omega\, \text{dist}(\Delta, \Lambda^c_{\neq})} \tag{5.23}$$

ω and c_ω being the same as in Theorem 5.1.

Proof. By successive applications of Theorem 5.2 we can replace ρ by a new function ψ^* with lesser free energy and such that $\psi^* = \rho$ outside Λ and with $\eta^{(\zeta, \ell_-)}(\psi^* : r) = 1$ inside Λ. We next use Theorem 5.1 to replace ψ^* by a function ψ such that $\psi_{\Lambda^c} = \rho_{\Lambda^c}$ and (see (5.6))

$$|\psi_\Lambda(r) - \rho_+| \leqslant c_\omega e^{-\omega\, \text{dist}(r, \Lambda^c_{\neq})}, \qquad \text{for all} \quad r \in \Lambda \tag{5.24}$$

$$F(\rho) \geqslant F(\psi) \tag{5.25}$$

We then define a new function ϕ in the following way

$$\phi(r) = \rho_+, \quad \text{for all } r \in \Delta, \qquad \phi_{\Delta^c} = \psi_{\Delta^c}$$

Then there is a positive constant C so that

$$F(\phi) - F(\psi) \geqslant -C\,|\Delta|\, e^{-\omega\, \text{dist}(\Delta, \Lambda^c_{\neq})} \tag{5.26}$$

Theorem 5.3 is proved. ∎

6. Γ-CONVERGENCE

In this section we study the Γ convergence of the functional, that is we prove Theorems 2.4 and 2.5. We fix a function u in $BV(\mathscr{T}, \{\rho_-, \rho_+\})$ and we denote by E the set such that

$$u(r) = \rho_- \chi_E(r) + \rho_+ \chi_{E^c}(r) \tag{6.1}$$

χ_E is the characteristic function of the set E. We denote by $\partial^* E$ the essential boundary of E and by $d\mu$ the associated total variation measure. We decompose the proof of Theorem 2.4 into two propositions, proving successively a lower bound for $\mathscr{F}^-(u)$ and an upper bound for $\mathscr{F}^+(u)$.

Proposition 6.1 (Lower Bound). Let $\mathrm{s}_\beta(e)$, $|e|=1$, be as in (2.17) and u as above. Then, recalling the definition (2.22),

$$\mathscr{F}^-(u) \geqslant \int_{\partial^* E} d\mu\, \mathrm{s}_\beta(\nu(r)) \tag{6.2}$$

Proof. From the general theory of bounded variation functions,[16] the set E can be regarded (measure theoretically) as a C^1 set. That is for any $\alpha > 0$ there are C^1 hyper-surfaces $\mathscr{S}_1,..., \mathscr{S}_m$ whose closure are disjoint from each other, and compact sets $K_1,..., K_m$ with $K_i \subset \mathscr{S}_i \cap \partial^* E$ so that

$$d\mu|_{K_i} = dH^{d-1}, \qquad \int_{\partial^* E} d\mu - \sum_{i=1}^m \int_{K_i} dH^{d-1} \leqslant \alpha \tag{6.3}$$

where dH^{d-1} is the surface area. It is not difficult to see that the set E defined in (6.1) is made of essentially flat parts plus a small remainder. That is the following holds, see refs. 1 and 3. There are $n \geqslant 1$ disjoint measurable sets Σ_i, $i = 1,..., n$; and n cubes $R_i \subset \mathbb{R}^d$, $i = 1,..., n$ all of side h and unit vectors ν_i normal to a face of R_i with the following properties. Each Σ_i is contained in some K_{j_i} and denoting by $\nu(r)$ the unit normal to Σ_i at $r \in \Sigma_i$, we have

$$\sup_{r \in \Sigma_i} |\nu(r) - \nu_i| < \alpha, \qquad \left| h^{d-1} - \int_{\Sigma_i} d\mu \right| < \alpha h^{d-1} \tag{6.4}$$

Moreover,

$$\int_{R_i} dr\, |\chi^{\pm}_{R_i} - u| < \alpha h^d, \quad i = 1,..., n; \qquad \left| n h^{d-1} - \int_{\partial^* E} d\mu \right| < \alpha \tag{6.5}$$

where $\chi^{\pm}_{R_i} := \rho_+ \chi_{R_i^+} + \rho_- \chi_{R_i^-}$, $R_i^{\pm}$ being the upper and lower halves of R_i with respect to the direction ν_i.

We denote by $\chi_i^{(\varepsilon)}(r) = \chi^{\pm}_{R_i}(\varepsilon r)$, so that $\chi_i^{(\varepsilon)}$ is equal to $\rho_\pm$ resp. on an upper and lower half of $\varepsilon^{-1} R_i$.

Let ρ be such that $\|\rho - u^{(\varepsilon)}\|_{L^1(\varepsilon^{-1}\mathscr{T})} \leqslant \varepsilon^{-d}\delta$, then by the first inequality in (6.5),

$$\begin{aligned}\int_{\varepsilon^{-1}R_i} dr\, |\rho - \chi_i^{(\varepsilon)}| &\leqslant \int_{\varepsilon^{-1}R_i} dr\, |\rho - u^{(\varepsilon)}| + \int_{\varepsilon^{-1}R_i} dr\, |u^{(\varepsilon)} - \chi_i^{(\varepsilon)}| \\ &\leqslant \varepsilon^{-d} \left\{ \delta + \int_{R_i} dr\, |u - \chi^{\varepsilon}_{R_i}| \right\} =: \varepsilon^{-d} 2\alpha h^d \end{aligned} \tag{6.6}$$

having taken δ so small that

$$\delta < \alpha h^d \tag{6.7}$$

We fix $\alpha > 0$, take $\delta > 0$ so that (6.7) holds and then we let $\varepsilon \to 0$ and after $\alpha \to 0$.

The main step of the proof is the following *cut and paste lemma*: there is a function ρ^* such that

$$\mathscr{F}_\varepsilon(\rho) \geqslant \mathscr{F}_\varepsilon(\rho^*) - cn(\varepsilon^{-1}h)^{d-1}\sqrt{\alpha} \tag{6.8}$$

and with the following properties. For each i there is a rectangle Λ_i strictly contained in $\varepsilon^{-1}R_i$ with one side directed along v_i and length smaller than $2\varepsilon^{-1}h\sqrt{\alpha}$, the precise definition is given in (6.27) later. Calling $\partial_\pm \Lambda_i$ the top and bottom faces of Λ_i in the direction v_i, $\rho^*(r) = \rho_\pm$ for $\mathrm{dist}(r, \partial_\pm \Lambda_i) \leqslant 1$, $r \notin \Lambda_i$.

Let $\Lambda := \bigcup_{i=1}^n \Lambda_i$, then recalling the definition (5.19),

$$\mathscr{F}_\varepsilon(\rho^*) = \mathscr{F}_\varepsilon(\rho^*; \Lambda^c) + \sum_{i=1}^n \mathscr{F}_\varepsilon(\rho^*; \Lambda_i) \geqslant \sum_{i=1}^n \mathscr{F}_\varepsilon(\rho^*; \Lambda_i) \tag{6.9}$$

We have

$$|\mathscr{F}_\varepsilon(\rho^*; \Lambda_i) - \mathscr{F}_\varepsilon^{\mathrm{per}}(\rho^*; \Lambda_i)| \leqslant c\sqrt{\alpha}(\varepsilon^{-1}h)^{d-1} \tag{6.10}$$

where the superfix "per" refers to the free energy with interaction kernel J made periodic, see (2.13), on the sides of Λ_i (we have then used the bound on the height of Λ_i stated above). We denote by $\mathscr{C}_i$ the infinite cylinder containing Λ_i and by $\mathscr{F}_\varepsilon^{\mathrm{per}}$ the functional (2.14) with $\mathscr{C}_i$ in place of $\mathscr{C}_e(L)$.

Since ρ^* is equal to $\rho_\pm$ around top and bottom of Λ_i,

$$\mathscr{F}_\varepsilon^{\mathrm{per}}(\rho^*; \Lambda_i) = \mathscr{F}_\varepsilon^{\mathrm{per}}(\psi_i) \tag{6.11}$$

where ψ_i is a function on $\mathscr{C}_i$ which is equal to ρ^* on Λ_i and to $\rho_\pm$ above and below Λ_i. We then conclude from (6.8)–(6.9)–(6.11) that, for a suitable constant c'

$$\mathscr{F}_\varepsilon(\rho) \geqslant \sum_{i=1}^n \mathscr{F}_\varepsilon^{\mathrm{per}}(\psi_i) - c'n(\varepsilon^{-1}h)^{d-1}\sqrt{\alpha} \tag{6.12}$$

By (2.17),

$$\liminf_{\varepsilon \to 0} \varepsilon^{d-1} \mathscr{F}_\varepsilon^{\mathrm{per}}(\psi_i) \geqslant h^{d-1} s_\beta(v_i) \tag{6.13}$$

and from the second inequality in (6.4) we get

$$h^{d-1}\mathrm{s}_\beta(\nu_i) \geqslant \int_{\Sigma_i} d\mu\, \mathrm{s}_\beta(\nu_i) - h^{d-1}\alpha \tag{6.14}$$

while, by the second inequality in (6.5),

$$nh^{d-1} \leqslant \int_{\partial^* E} d\mu + \alpha \tag{6.15}$$

Therefore there is c' so that

$$\begin{aligned}
\mathscr{F}^-(u) &\geqslant \liminf_{\alpha \to 0} \sum_{i=1}^{n} [h^{d-1}\mathrm{s}_\beta(\nu_i) - ch^{d-1}\sqrt{\alpha}] \\
&\geqslant \lim_{\alpha \to 0} \left[\sum_{i=1}^{n} \int_{\Sigma_i} d\mu\, \mathrm{s}_\beta(\nu_i) - c'\sqrt{\alpha} \right] \\
&= \int_{\partial^* E} d\mu\, \mathrm{s}_\beta(\nu(r))
\end{aligned}$$

in the last equality we have used the first inequality in (6.4).

We are left with proof of the *cut and paste lemma* namely the existence of ρ^* and Λ_i which verify (6.8) and the other properties. This proof is similar to the "minimal section argument" of Benois *et al.*[5]

For notational simplicity we denote by $Q_i \equiv \varepsilon^{-1} R_i$ and by $L \equiv \varepsilon^{-1} h$ the side of Q_i. Moreover we assume that the coordinate axes are so that r_d is directed along ν_i and so that Q_i is the coordinate cube, that is

$$Q_i = \{ r = (r_1, ..., r_d) : |r_j| \leqslant L/2, \forall j = 1, ..., d \}$$

Recalling (6.6), we consider a function ρ such that $\|\rho - \chi_i^\varepsilon\|_{L^1(Q_i)} \leqslant \alpha L^d$ and we fix parameters ζ and ℓ in such a way that Theorem 5.3 holds. We need to look for a layer in $r_d > 0$ where ρ is close to ρ_+ and want also that in the reflected layer in the bottom, ρ is close to ρ_-. We choose the layer thickness equal to ℓ_+, see (5.2). The kth layer, $k \in \mathbb{Z}$, is then (to have lighter notation we omit the dependence on i in the definition below)

$$S_k = \{ r \in Q_i : |r_d - \ell_+ k| \leqslant \ell_+/2 \} \tag{6.16}$$

Observe that for all k, $|S_k| = |S_0| = \ell_+ L^{d-1}$, and $Q_i = \bigcup_{k=0}^{K} (S_k \cup S_{-k})$ where K is the integer part of $L/2\ell_+$. Let

$$N = \min \left\{ m \in \mathbb{N} : m \geqslant \sqrt{\alpha} \frac{L}{2\ell_+} \right\} \tag{6.17}$$

We define for any $1 \leqslant m \leqslant N$

$$\Sigma_m := S_{2m-1} \cup S_{2m} \cup S_{2m+2N-1} \cup S_{2m+2N},$$
$$\Sigma_{-m} := S_{-2m+1} \cup S_{-2m} \cup S_{-2m-2N+1} \cup S_{-2m-2N} \tag{6.18}$$

Observe that they are mutually disjoint and that $|\Sigma_m \cup \Sigma_{-m}| = 8\,|S_0|$. Let

$$a_m = \frac{1}{8\,|S_0|} \int_{\Sigma_m \cup \Sigma_{-m}} dr\, |\rho(r) - \chi_i^\varepsilon(r)| \tag{6.19}$$

We now prove that, for L large enough, i.e., ε small enough,

$$a := \min_{m \leqslant N} a_m \leqslant \sqrt{\alpha} \tag{6.20}$$

In fact, by assumption,

$$\alpha L^d \geqslant \int_{Q_i} dr\, |\rho(r) - \chi_i^\varepsilon(r)| \geqslant \sum_{m=1}^{N} 8\,|S_0|\, a_m \geqslant 8\,|S_0|\, Na$$

then by (6.17), $\alpha L^d > 8a\ell_+ L^{d-1} \sqrt{\alpha}\, L/2\ell_+$, which proves (6.20).

Call m the integer where the minimum in (6.20) is achieved, so that

$$\int_{\Sigma_m \cup \Sigma_{-m}} dr\, |\rho - \chi_i^\varepsilon| \leqslant \sqrt{\alpha}\, 8\ell_+ L^{d-1}$$

Recalling that $C_r^{(\ell_-)}$ is the cube of the partition $\mathscr{D}^{(\ell_-)}$ with contains r, we define

$$\mathscr{C}_{m,+} := \{C_r^{(\ell_-)} \subset \Sigma_m : \eta^{(\zeta,\ell_-)}(\rho; r) < 1\}$$
$$\mathscr{C}_{m,-} := \{C_r^{(\ell_-)} \subset \Sigma_{-m} : \eta^{(\zeta,\ell_-)}(\rho; r) > -1\}$$

We then have that

$$\sqrt{\alpha}\, 8\ell_+ L^{d-1} \geqslant \int_{\Sigma_m \cup \Sigma_{-m}} dr\, |\rho - \chi_i^\varepsilon| \geqslant \sum_{C \in \mathscr{C}_{m,+} \cup \mathscr{C}_{m,-}} \int_C |\rho - \chi_i^\varepsilon| \geqslant \zeta\, |\mathscr{C}_{m,+} \cup \mathscr{C}_{m,-}|$$

which implies that

$$|\mathscr{C}_{m,+} \cup \mathscr{C}_{m,-}| \leqslant \frac{8\ell_+}{\zeta} L^{d-1} \sqrt{\alpha} \tag{6.21}$$

We further define $\mathscr{C}_0^{(i)}(L)$ as the union of all cubes $C^{(\ell_+)}$ such that both $C^{(\ell_+)}$ and $\delta_{\text{out}}^{\ell_+}[C^{(\ell_+)}]$ are contained in Q_i. Notice that, for suitable constants c and c',

$$\left|\delta_{\text{out}}^{\ell_+}[\mathscr{C}_0^{(i)}(L)] \cap \left\{ \bigcup_{k=-4N}^{4N} S_k \right\}\right| \leqslant cNL^{d-2} \leqslant c'L^{d-1}\sqrt{\alpha}$$

We then have

$$\mathscr{M}_{m,i} := \delta_{\text{out}}^{\ell_+}[\mathscr{C}_0^{(i)}(L)] \cup \mathscr{C}_{m,+} \cup \mathscr{C}_{m,-}, \qquad |\mathscr{M}_{m,i}| \leqslant \bar{c}L^{d-1}\sqrt{\alpha} \tag{6.22}$$

We perform the same construction for all i and we define the function

$$\psi = \rho \quad \text{in} \left[\bigcup_{i=1}^{n} \mathscr{M}_{m,i}\right]^c, \qquad \psi = \chi_i^\varepsilon \quad \text{in } \mathscr{M}_{m,i},\ i = 1,..., n$$

so that from (6.22) we get that there is a constant $c_0 > 0$ so that

$$\mathscr{F}_\varepsilon(\rho) \geqslant \mathscr{F}_\varepsilon(\psi) - c_0 n L^{d-1}\sqrt{\alpha} \tag{6.23}$$

We next consider the following subsets of Q_i,

$$\Lambda_+ = \bigcup_{j=2m}^{2m+2N-1} S_j \cap \mathscr{C}_0^{(i)}(L), \qquad \Lambda_- = \bigcup_{j=-2m}^{-2m-2N+1} S_j \cap \mathscr{C}_0^{(i)}(L)$$

We are going to apply Theorem 5.3 to Λ_+, $\Delta_+ = S_{2m+N} \cap \mathscr{C}_0^{(i)}(L)$ and to Λ_-, $\Delta_- = S_{-2m-N} \cap \mathscr{C}_0^{(i)}(L)$. For simplicity we only consider the former.

Since

$$\eta^{(\zeta,\ell_-)}(\psi; r) = 1, \qquad r \in \delta_{\text{out}}^{\ell_+}[\Lambda_+] \tag{6.24}$$

the conditions on the internal and external boundaries of the domain, which appear among the hypotheses of Theorem 5.3 are verified. Moreover, recalling (5.22) and the fact that $\Delta_+ = S_{2m+N} \cap \mathscr{C}_0^{(i)}(L)$

$$\Lambda_{+,\neq}^c \subset S_{2m-1} \cup S_{2m+2N}, \qquad \text{dist}(\Delta_+, \Lambda_{+,\neq}^c) \geqslant \ell_+ N/2 \tag{6.25}$$

Then from Theorem 5.3 it follows that there is ϕ_i equal to ψ outside $\Lambda_\pm$ and equal to χ_i^ε on $S_{2m+N} \cap \mathscr{C}_0^{(i)}(L)$ and $S_{-2m-N} \cap \mathscr{C}_0^{(i)}(L)$, such that

$$\mathscr{F}_\varepsilon(\psi; Q_i) \geqslant \mathscr{F}_\varepsilon(\phi_i; Q_i) - (2c_\omega e^\omega |S_0|)\, e^{-\omega \ell_+ N/2} \tag{6.26}$$

The *cut and paste lemma* is then proven with

$$\Lambda_i = \bigcup_{j=-2m-N}^{2m+N} S_j \cap \mathscr{C}_0^{(i)}(L) \tag{6.27}$$

and $\rho^* = \phi_i$ in Λ_i for all i and $\rho^* = \rho$ elsewhere.

The proposition is proved. ▮

For the upper bound we need another property of BV functions that says that BV sets can be approximated by polyhedral sets. As explained in Definition 5.1 of ref. 1 a polyhedral set A is an open set whose boundary ∂A is contained in the union of finitely many hyperplanes. The faces of A are the intersection of ∂A with each one of these hyperplanes and the normal to ∂A is defined for all points different from the edge points (i.e., points that belong to al least two different faces). Given $u \in BV$ let E be as in (6.1). Then there exists a sequence of BV functions u_k equal to $\rho_\pm$ inside and outside of polyhedral sets E_k that converges in variation norm as $k \to \infty$ to u. Furthermore for any continuous function $g(e)$ defined in the unit ball, the following holds

$$\lim_{k \to \infty} \int_{\partial^* E_k} d\mu_k \, g(\nu(r)) = \int_{\partial^* E} d\mu \, g(\nu(r)) \tag{6.28}$$

With this we easily get the upper bound.

Proposition 6.2 (Upper Bound). Let $\mathrm{s}_\beta(e)$, $|e| = 1$ be as in (2.17) and u as above. Then, recalling the definition (2.23),

$$\mathscr{F}^+(u) \leqslant \int_{\partial^* E} d\mu \, \mathrm{s}_\beta(\nu(r)) \tag{6.29}$$

Proof. We will show that there exists $\rho^{(\varepsilon)} \in L^1(\varepsilon^{-1}\mathscr{T}, [R', R''])$, $\varepsilon > 0$, so that

$$\lim_{\varepsilon \to 0} \varepsilon^d \, \|\rho^{(\varepsilon)} - u^{(\varepsilon)}\|_{L^1(\varepsilon^{-1}\mathscr{T})} = 0, \qquad \limsup_{\varepsilon \to 0} \, \varepsilon^{d-1} \mathscr{F}_\varepsilon(\rho^{(\varepsilon)}) \leqslant \int_{\partial^\star E} d\mu(r) \, \mathrm{s}_\beta(\nu(r)) \tag{6.30}$$

which clearly implies (6.29). The choice of $\rho^{(\varepsilon)}$ involves a diagonalization procedure. Let u_k be the functions that approximate u and that are equal to $\rho_\pm$ inside and outside polyhedral sets E_k with boundary ∂E_k. For each k, we will construct functions $\rho^{(\varepsilon, L, h, k)}$ so that

$$\limsup_{h \to 0} \limsup_{L \to \infty} \limsup_{\varepsilon \to 0} \varepsilon^d \|\rho^{(\varepsilon, L, h, k)} - u_k^{(\varepsilon)}\|_{L^1(\varepsilon^{-1}\mathscr{T})} = 0 \tag{6.31}$$

$$\limsup_{h \to 0} \limsup_{L \to \infty} \limsup_{\varepsilon \to 0} \varepsilon^{d-1} \mathscr{F}_\varepsilon(\rho^{(\varepsilon, L, h, k)}) \leqslant \int_{\partial E_k} d\mu_k(r)\, \mathrm{s}_\beta(\nu(r)) \tag{6.32}$$

Since

$$\varepsilon^d \|u_k^{(\varepsilon)} - u^{(\varepsilon)}\|_{L^1(\varepsilon^{-1}\mathscr{T})} = \|u_k - u\|_{L^1(\mathscr{T})} \to 0, \qquad \text{as} \quad k \to \infty$$

we then get from (6.31) and (6.32)

$$\limsup_{k \to \infty} \limsup_{h \to 0} \limsup_{L \to \infty} \limsup_{\varepsilon \to 0} \varepsilon^d \|\rho^{(\varepsilon, L, h, k)} - u^{(\varepsilon)}\|_{L^1(\varepsilon^{-1}\mathscr{T})} = 0 \tag{6.33}$$

$$\limsup_{k \to \infty} \limsup_{h \to 0} \limsup_{L \to \infty} \limsup_{\varepsilon \to 0} \varepsilon^{d-1} \mathscr{F}_\varepsilon(\rho^{(\varepsilon, L, h, k)})$$

$$\leqslant \limsup_{k \to \infty} \int_{\partial E_k} d\mu_k(r)\, \mathrm{s}_\beta(\nu(r)) \tag{6.34}$$

By (6.28),

$$\lim_{k \to \infty} \int_{\partial E_k} d\mu_k(r)\, \mathrm{s}_\beta(\nu(r)) = \int_{\partial^* E} d\mu(r)\, \mathrm{s}_\beta(\nu(r)) \tag{6.35}$$

because s_β is a bounded continuous function of the unit normal ν. By (6.33)–(6.35), there are $L = L(\varepsilon)$, $h = h(\varepsilon)$, and $k = k(\varepsilon)$ so that the family $\rho^{(\varepsilon, L(\varepsilon), h(\varepsilon), k(\varepsilon))}$ satisfies (6.30). Thus the proof of (6.29), follows from the existence of a family $\rho^{(\varepsilon, L, h, k)}$ satisfying (6.31) and (6.32), which we prove next.

Here k is fixed and we will drop it from the notation, thus writing, in the sequel, E for a polyhedral set and denoting, as usual, $u = \rho_- \chi_E + \rho_+ \chi_{E^c}$. The faces of E are called Σ_i, and their normal ν_i, directed toward the plus phase. On each hyperplane which contains $\varepsilon^{-1}\Sigma_i$, we introduce a partition into $d-1$ dimensional cubes of side L, the orientation of the cubes of the partition being the same for all ε. As already said, we will take $L \to \infty$ after $\varepsilon \to 0$, with a third parameter, $h \to \infty$ after $\varepsilon \to 0$ and $L \to \infty$. We first define $\rho^{(\varepsilon, L, h)}$ around $\varepsilon^{-1}\Sigma_1$. On each rectangle $\mathscr{R}_{\nu_1}(L, h)$ of height $2h$ and mid cross section a cube entirely contained in $\varepsilon^{-1}\Sigma_1$. Recalling the definition (3.1) and letting $\rho^{(\varepsilon, L, h, \pm)}$ the function equal to $\rho^{(\varepsilon, L, h)}$ inside $\mathscr{R}_{\nu_1}(L, h)$ and equal to $\chi^\pm$ in $\mathscr{R}_{\nu_1}(L, h)^c$, we choose $\rho^{(\varepsilon, L, h)}$ so that

$$\frac{1}{L^{d-1}} F^{\mathrm{per}}(\rho^{(\varepsilon, L, h, \pm)}) \leqslant S_{\nu_1}(L, h) + \varepsilon \tag{6.36}$$

When the mid cross section of $\mathscr{R}_{v_1}(L, h)$ is not entirely contained in $\varepsilon^{-1}\Sigma_1$, we set $\rho^{(\varepsilon, L, h)} = \rho_\pm$ in the part of $\mathscr{R}_{v_1}(L, h)$ which is (vertically, w.r.t. v_1) above and below $\varepsilon^{-1}\Sigma_1 \cap \mathscr{R}_{v_1}(L, h)$. We follow the same rule in the other faces, except for points (if any) where $\rho^{(\varepsilon, L, h)}$ has already been defined. On the remaining of the space we set $\rho^{(\varepsilon, L, h)} = u^{(\varepsilon)}$.

Once h is fixed, if L is large enough, any rectangle $\mathscr{R}_{v_i}(L, h)$ at distance $> L$ from the boundary of $\varepsilon^{-1}\Sigma_i$ has no intersection with any of the other rectangles, then, for a suitable constant c,

$$\varepsilon^{d-1}\mathscr{F}_\varepsilon(\rho^{(\varepsilon, L, h)}) \leqslant \sum_i \left([S_{v_i}(L, h) + \varepsilon]\, |\Sigma_i| + cLh\varepsilon\right) \tag{6.37}$$

From Proposition 3.1 and (6.37), (6.32)–(6.33) follow, thus completing the proof of the upper bound of Γ-convergence. ∎

We now prove Theorem 2.5, the arguments we use are similar to the ones given in ref. 4 and rely on the Peierls estimates given in Section 5.

Proof of Theorem 2.5. Recalling the definition (2.21) of $\mathscr{F}_\varepsilon$, we consider a family of functions $\rho_\varepsilon \in L^\infty(\mathscr{T}, [R', R''])$ that satisfies

$$\sup_{\varepsilon > 0} \varepsilon^{d-1}\mathscr{F}_\varepsilon(\rho_\varepsilon) \leqslant C \tag{6.38}$$

Given any ζ and ℓ that satisfy the hypothesis of Theorem 5.2 at each element of the family ρ_ε it corresponds a set of contours $\Gamma_1,..., \Gamma_n$, (to avoid heavy notation we do not explicit the dependence on ρ_ε of n and of the contours). We define the BV sets

$$A_\varepsilon^\pm = \{r \in \varepsilon^{-1}\mathscr{T} : r \text{ is} \pm \text{correct}\} \tag{6.39}$$

and we let

$$\chi_{(\pm, \varepsilon)}(r) = \chi_{A_\varepsilon^\pm}(\varepsilon^{-1} r), \qquad \chi^{(\pm, \varepsilon)} \in BV(\mathscr{T}; \{0, 1\}) \tag{6.40}$$

From (5.21) and from (6.38) we get there is a positive constant c so that

$$c\zeta^2\ell^{-2d} \sum_{i=1}^n |\mathrm{sp}(\Gamma_i)| \leqslant \mathscr{F}_\varepsilon(\rho_\varepsilon) \leqslant C\varepsilon^{-d+1} \tag{6.41}$$

Denoting by $\mathscr{P}$ the perimeter functional on $BV(\mathscr{T}; \{0, 1\})$ (the Hausdorff area of "the reduced boundary") from (6.41) we get

$$\mathscr{P}(\chi_{(\pm, \varepsilon)}) \leqslant c' = (2d\ell_+)^{d-1}\, c \tag{6.42}$$

By compacteness of $\mathscr{P}$, there is a subsequence ε_n and $\chi_\pm \in BV(\mathscr{T}; \{0, 1\})$, $\mathscr{P}(\chi_\pm) \leqslant c'$, so that

$$\lim_{n\to\infty} \|\chi_{(\pm,\varepsilon_n)} - \chi_\pm\|_{L^1} = 0 \tag{6.43}$$

Since $A_\varepsilon^+ \cup A_\varepsilon^- \cup (\bigcup_{i=1}^n \mathrm{sp}(\Gamma_i)) = \varepsilon^{-1}\mathscr{T}$, from (6.41) we get

$$1 \geqslant \int_{\mathscr{T}} [\chi_{(+,\varepsilon)}(r) + \chi_{(-,\varepsilon)}(r)]\, dr \geqslant 1 - \ell_+^d c\varepsilon \tag{6.44}$$

and thus,

$$\int_{\mathscr{T}} [\chi_+(r) + \chi_-(r)]\, dr = 1 \tag{6.45}$$

To conclude the proof of the theorem it is sufficient to show that

$$\lim_{n\to\infty} \|\chi_{(\pm,\varepsilon_n)} \rho_{\varepsilon_n} - u^{(\pm)}\|_{L^1} = 0, \qquad u^{(\pm)} = \rho_\pm \chi_{(\pm)} \tag{6.46}$$

For notational simplicity, we restrict to the plus case. We now show that there is a sequence $\delta_n \to 0$ slowly enough, such that

$$\lim_{n\to\infty} \varepsilon_n^d \int_{A_{\varepsilon_n}^+ \cap \{|\rho^{(\varepsilon_n)} - \rho_+| \geqslant \delta_n\}} |\rho^{(\varepsilon_n)} - \rho_+| = 0, \qquad \rho^{(\varepsilon_n)}(r) = \rho_{\varepsilon_n}(\varepsilon r) \tag{6.47}$$

Since $|\rho^{(\varepsilon_n)} - \rho_+| \leqslant 2R''$, it suffices to prove that

$$\lim_{n\to\infty} \varepsilon_n^d\, |A_{\varepsilon_n}^+ \cap \{|\rho^{(\varepsilon_n)} - \rho_+| \geqslant \delta_n\}| = 0 \tag{6.48}$$

Recalling the definitions (2.5) since $g'_\beta(\rho_+) = 0$ and $g''_\beta(\rho_+) > 0$, there are $\gamma > 0$ small enough and $b > 0$ so that

$$f(s) = g_\beta(s) - g_\beta(\rho_+) \geqslant b(s - \rho_+)^2, \qquad \text{for all} \quad s \in (\rho_+ - \gamma, \rho_+ + \gamma)$$

On the other hand from (5.7) we get that

$$|J \star \rho^{(\varepsilon_n)}(r) - \rho_+| \leqslant 2\zeta, \qquad \text{for all} \quad r \in A_{\varepsilon_n}^+$$

Thus choosing $\zeta < \gamma$ we get

$$f(J \star \rho)(r) \geqslant b\delta_n^2, \qquad \forall r \in A_\varepsilon^+ \cap \{\big||\rho^{(\varepsilon_n)} - \rho_+| \geqslant \delta_n\big|\} \tag{6.49}$$

hence

$$\varepsilon_n^d \left|A_\varepsilon^+ \cap \{|\rho^{(\varepsilon_n)} - \rho_+| \geqslant \delta_n|\}\right| \leqslant \frac{\varepsilon_n^d}{b\delta_n^2} \int_{A_\varepsilon^+ \cap \{|\rho^{(\varepsilon_n)} - \rho_+| \geqslant \delta_n|\}} f(J \star \rho^{(\varepsilon_n)})\, dr$$
$$\leqslant \frac{\varepsilon_n^d}{b\delta_n^2} \mathscr{F}_\varepsilon(\rho^{(\varepsilon_n)})$$

that proves (6.48) if $\varepsilon_n/\delta_n^2 \to 0$.

To conclude the proof of the theorem we take $u \notin BV(\mathscr{T}, \{\rho_-, \rho_+\})$, then we suppose by contradiction that $\mathscr{F}_-(u) < \infty$, then there is a family $u_\varepsilon \in L^\infty(\mathscr{T}, [R', R''])$, so that $u_\varepsilon \to u$ in $L^1(\mathscr{T})$ and $\mathscr{F}_\varepsilon(u^{(\varepsilon)}) \to \mathscr{F}_-(u)$. Then there is C so that $\varepsilon^{d-1}\mathscr{F}_\varepsilon(u_\varepsilon) < C$ and a subsequence converging in $L^1(\mathscr{T})$ to a function in $BV(\mathscr{T}, \{\rho_-, \rho_+\})$, against the assumption that u is not in BV. The theorem is proved. ▮

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