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Density Oscillations at the Interface Between Vapor and Liquid

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We study the interface between liquid and vapor in the context of the van der Waals theory, considering the non-local free energy functional recently derived by Lebowitz, Mazel, and Presutti from a system of particles in the continuum with Kac potentials. We prove that the density profile between vapor and liquid is monotone when the inverse temperature is between the critical value β_c and a second critical value $\beta^* > \beta_c$, becoming oscillatory after β^* and overshooting the equilibrium density of the liquid phase infinitely often.

KEY WORDS: Non-local equations; fronts between phases.

1. INTRODUCTION

In a recent paper,[1] Lebowitz, Mazel, and Presutti, LMP, have proved that systems of identical point particles in the continuum have liquid-vapor phase transitions. The interaction among particles is given by a very specific class of two-body attractive plus four-body repulsive Kac potentials. By taking full advantage of the choice, LMP have proved that, after coarse graining, the effective temperature of the system becomes lower and the Pirogov–Sinai method applies.

The robustness of the analysis makes it conceivable that phase coexistence, surface tension and Wulff shape might be approached as well. Indeed such a program has been successfully carried through for Ising

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models with Kac potentials. Phase transitions are proved in refs. 2, 3, and 4, validity of Wulff construction is more recent,[5] while older results,[6–8] show that the surface tension converges to the v.d.W. [van der Waals] surface tension as γ (the inverse range of the Kac potential) goes to 0. The main obstacle in extending the results from Ising to LMP is the extensive use in the former of ferromagnetic inequalities which are missing in the latter due to the four-body repulsive interaction (whose presence is, on the other hand, essential to ensure stability of matter). Also at the level of the v.d.W. theory, ferromagnetic inequalities are important. The results about interface profiles (instantons) and their free energy (surface tension) for the non-local free energy functionals derived from the Ising system with Kac potentials extensively use comparison inequalities inherited from the underlying ferromagnetic spin system. Again, in the non-local functional derived from LMP comparison inequalities are not valid and our purpose here is to start an investigation of the issue at the level of the v.d.W. theory.

Our results show the appearance of very interesting physical structures which, even though derived from a particular model, may hopefully have more general nature. We have found that there exist two temperature regimes (below the critical temperature). In the first one, despite the absence of ferromagnetic inequalities, the interface behaves just as in the ferromagnetic Ising case. In fact the density profile which connects the vapor and the liquid phases is monotononically increasing and the convergence to the asymptotic values exponentially fast.

As the temperature decreases past a "second critical value," the picture changes abruptly and the instanton profile presents oscillations when approaching (still in an exponential fashion) the liquid phase, with infinitely many oscillations above and below the limit value (overshooting effects). The appearence of oscillatory patterns of the density-density correlations in a liquid are known, both experimentally and theoretically, see ref. 9 and references therein. There are indications of their occurrence also at the vapor-liquid interface, but the issue is more controversial and we address the reader to the survey by Croxton.[10]

2. THE LMP NON-LOCAL, FREE ENERGY FUNCTIONALS

The scaling limit of the LMP particle model, see ref. 1, is described by the non-local, free energy functionals

$$\mathscr{F}_{\beta,\lambda;\Lambda}(\rho) = \int_\Lambda dr \left(E_\lambda(J * \rho) - \frac{S(\rho)}{\beta} \right) \tag{2.1}$$

where Λ is a d-dimensional torus, β the inverse temperature, λ the chemical potential, $\rho \in L^1(\Lambda, \mathbb{R}_+)$ a density profile,

$$E_\lambda(s) = -\lambda s - \frac{s^2}{2} + \frac{s^4}{4!} \tag{2.2}$$

the mean field energy density; $J = J(r, r') = \mathbf{1}_{|r-r'| \leqslant R_d}$ is a probability kernel, $J * \rho$ being the convolution in the torus Λ. Finally $S(\rho) = -\rho(\log \rho - 1)$ is the entropy density.

The terms s^2 and s^4 are reminiscent of the two and four-body interactions in the particle model, their different signs in (2.2) being related to the attractive and repulsive nature of the 2 and 4 body interactions. The particular combination of the convolution terms in (2.1) is very specific and characteristic of the LMP model, it reflects its atypical feature (for systems with repulsive interactions) that the minimizers of the free energy are spatially homogeneous, i.e., constant functions, for any value of temperature and chemical potential. This is readily seen by rewriting $\mathscr{F}_{\beta, \lambda; \Lambda}$ as

$$\mathscr{F}_{\beta, \lambda; \Lambda}(\rho) = \int_\Lambda dr \left(F_{\beta, \lambda}(J * \rho) + \frac{1}{\beta} \{S(J * \rho) - J * S(\rho)\} \right) \tag{2.3}$$

$$F_{\beta, \lambda}(s) = E_\lambda(s) + \frac{s}{\beta} (\log s - 1) \tag{2.4}$$

By concavity the integral of the curly bracket is minimized by taking $\rho(r)$ equal to a constant independent of r; by choosing the constant equal to a minimizer of (2.4) we then get a minimizer for the full functional $\mathscr{F}_{\beta, \lambda; \Lambda}$.

Thus the minimization of $\mathscr{F}_{\beta, \lambda; \Lambda}$ reduces to that of $F_{\beta, \lambda}(s)$ which is elementary. For $\beta \leqslant \beta_c = (3/2)^{3/2}$, $F_{\beta, \lambda}$ has for any λ a unique minimizer. For $\beta > \beta_c$, there is a unique value of λ, $\lambda = \lambda_\beta$, where $F_{\beta, \lambda}$ has two distinct minimizers, $0 < \rho_{\beta, -} < \rho_{\beta, +}$ (for $\lambda \neq \lambda_\beta$ the minimizer is unique). Denoting, by an abuse of notation, $E_\beta \equiv E_{\lambda_\beta}$ and writing $E'_\beta(s)$ for the derivative of $E_\beta(s)$ w.r.t. s, the equilibrium densities satisfy the mean field equation m.f.e.

$$s = \exp\{-\beta E'_\beta(s)\} =: \varphi_\beta(s) \tag{2.5}$$

Such equation has three roots, $\rho_{\beta, -} < \rho_{\beta, 0} < \rho_{\beta, +}$; the two extremal are stable the central one unstable. As a consequence $\varphi'_\beta(\rho_{\beta, +}) < 1$. We then define $\beta^* > \beta_c$ and $\beta_0 > \beta^*$ so that

$$1 > \varphi'_\beta(\rho_{\beta, +}) > 0, \qquad \text{for} \quad \beta_c < \beta < \beta^* \tag{2.6}$$

At β^* the derivative becomes 0, $\varphi'_{\beta^*}(\rho_{\beta^*,+})=0$, and

$$0>\varphi'_\beta(\rho_{\beta,+})>-1, \qquad \text{for} \quad \beta^*<\beta<\beta_0 \tag{2.7}$$

Since for any β, $s=\sqrt{2}$ is the only root of $\varphi'_\beta(s)=0$, $\rho_{\beta^*,+}=\sqrt{2}$. The interval (β_c,β_0) is the one considered in LMP and we will also restrict our analysis to β in (β_c,β_0).

3. VAN DER WAALS SURFACE TENSION

Coexistence of phases is studied by imposing conditions which favor different phases in different parts of the domain. By assuming planar symmetry and denoting by x the coordinate along the normal to the symmetry plane, we can integrate out the remaining coordinates thus reducing to a $d=1$ problem. The functional obtained in this way (and after taking the thermodynamic limit) is

$$\mathscr{F}_\beta(\rho)=\int_{\mathbb{R}} dx\left(\left[F_{\beta,\lambda_\beta}(j*\rho)-F_{\beta,\lambda_\beta}(\rho_{\beta,+})\right]+\frac{1}{\beta}\{S(j*\rho)-j*S(\rho)\}\right) \tag{3.1}$$

where $\rho\in L^1_{\mathrm{loc}}(\mathbb{R},\mathbb{R}_+)$, $j(x,y)=j(0,y-x)$ and

$$j(0,x)=\int dx_2\cdots dx_d\, J(0,(x,x_2,\ldots,x_d)) \tag{3.2}$$

$j(x,y)$ is a C^1 probability kernel supported by $|x-y|\leqslant 1$.

As we have subtracted the equilibrium value $F_{\beta,\lambda_\beta}(\rho_{\beta,+})$, $\mathscr{F}_\beta(\rho)$ is the excess free energy [rather than the free energy] of the profile ρ; as a functional with values in $[0,\infty]$ (the latter included), $\mathscr{F}_\beta(\rho)$ is well defined on $L^1_{\mathrm{loc}}(\mathbb{R},\mathbb{R}_+)$, as $j*\rho$ is well defined and both integrands in (3.1) are non negative. Denoting by

$$\mathscr{N}_\beta:=\{\rho\in L^\infty(\mathbb{R},\mathbb{R}_+): \liminf_{x\to\infty}\rho(x)>\rho_{\beta,0},\ \limsup_{x\to-\infty}\rho(x)<\rho_{\beta,0}\} \tag{3.3}$$

the v.d.W. surface tension is

$$\tau_\beta:=\inf_{\rho\in\mathscr{N}_\beta}\mathscr{F}_\beta(\rho) \tag{3.4}$$

We call instanton any element in $\mathscr{N}_\beta$ which satisfies the space dependent m.f.e.

$$\rho(\cdot)=\Phi_\beta(\rho;\cdot), \qquad \Phi_\beta(\rho;\cdot)=\exp\{-\beta j*E'_\beta(j*\rho)\} \tag{3.5}$$

The instantons are the critical points of (3.1). Our main result is:

Theorem 3.1. For any $\beta \in (\beta_c, \beta_0)$ the inf in (3.4) is a minimum, and any minimizer $\bar{\rho}_\beta$ is an instanton. 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 instanton [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 $\{x\colon \bar{\rho}_\beta(x) \geqslant \rho_{\beta,+}\}$ is made of infinitely many disjoint intervals.

The theorem will be proved in the sequel. In Section 4 we will introduce a dynamics under which the free energy functional decreases (more precisely it does not increase). We will use extensively such dynamics to modify density profiles into others with smaller free energy. In particular we will prove, see Theorem 4.6, that we can restrict the analysis to the space $L^\infty(\mathbb{R}; [R', R''])$, with R' and R'' suitable, positive constants. In Section 5 we will prove extensive bounds on the free energy of profiles which deviate from equilibrium, namely that the free energy of a profile ρ is bounded from below by the volume of the region where it either differs from $\rho_{\beta,\pm}$ or "oscillates between the two." Such Peierls-type estimates will be used to prove in Section 6 the existence of instantons which minimize the free energy in $\mathscr{N}_\beta$, while in Section 7 we will establish properties on the asymptotic behavior of the instantons, as a simple consequence of the analysis of the solutions of the mean field equation (3.5). In Section 8 we will draw some concluding remarks.

4. NON-LOCAL DYNAMICS

Stochastic dynamics for the LMP model may be defined as a birth-death process (a "contact process" in the continuum) whose generator is self-adjoint in L^2 of any Gibbs measure. Its scaling limit as $\gamma \to 0$ should give rise to a deterministic non-local dynamics described by an equation of the form

$$\frac{\partial \rho}{\partial t} = -\rho + \Phi_\beta(\rho; \cdot) \tag{4.1}$$

Notice that the stationary solutions of (4.1) are also solutions of the m.f.e. (3.5). While interesting on its own right, (4.1) is for us here merely a tool for investigating $\mathscr{F}_\beta$, so our analysis of (4.1) will be very partial and only aimed at establishing properties needed for the proof of Theorem 3.1.

We are going to regard (4.1) as evolution equation on the space $L^\infty(\mathbb{R}; [a, b])$, with $0 < a < b < \infty$ to be suitably chosen. Namely, $\rho(x, t)$,

$x \in \mathbb{R}$, $t \geqslant 0$, is a solution of (4.1) if it is a measurable function with values in $[a, b]$, it is differentiable in t for any x and it satisfies (4.1). We will also consider partial dynamics, where, given a measurable region Λ, $\rho^{\Lambda}(x, t)$ is required to solve (4.1) only in Λ, while $\rho^{\Lambda}(x, t) = \rho^{\Lambda}(x, 0)$ for all $x \in \Lambda^c$ and $t \geqslant 0$. We will denote by $T_t(\rho)$ and $T_t^{\Lambda}(\rho)$ the corresponding solutions starting at $t = 0$ from ρ. If $\Lambda = \mathbb{R}$, $T_t^{\Lambda} \equiv T_t$.

Since $\Phi_\beta(\rho; \cdot)$ is Lipschitz if $\rho \in L^\infty$, existence and uniqueness, i.e., well-posedness of T_t and T_t^{Λ}, are easily settled in the following proposition, whose proof is omitted.

Proposition 4.1. Suppose there are $0 < a < b < \infty$ so that

$$a \leqslant \Phi_\beta(\rho; \cdot) \leqslant b, \qquad \text{for all} \quad \rho \in L^\infty(\mathbb{R}; [a, b]) \tag{4.2}$$

then $T_t(\rho)$ and $T_t^{\Lambda}(\rho)$ are well defined.

In the next corollary we will define pairs which satisfy (4.2). Let

$$R'' = \sup_{\beta \in (\beta_c, \beta_0)} \varphi_\beta(\sqrt{2}) \tag{4.3}$$

Recall that $\varphi_\beta(s)$ is defined in (2.5) and that its maximum is reached at $s = \sqrt{2}$, independently of β. Moreover for $\beta > \beta^*$, $\rho_{\beta,+} \in (\sqrt{2}, R'')$.

Corollary 4.2. Let $b \geqslant R''$ and

$$a \leqslant \inf_{\beta \in (\beta_c, \beta_0)} \inf_{0 \leqslant s \leqslant b} \varphi_\beta(s) \tag{4.4}$$

Then the pair a, b satisfies (4.2) for any $\beta \in (\beta_c, \beta_0)$ and consequently, $T_t(\rho)$ and $T_t^{\Lambda}(\rho)$ are well defined on $L^\infty(\mathbb{R}, [a, b])$.

Proof. Recalling (3.5) and (2.5), if $\rho \in L^\infty(\mathbb{R}, [a, b])$

$$\Phi_\beta(\rho; \cdot) \in \Big[\inf_{s \in [a, b]} \varphi_\beta(s), \sup_{s \in [a, b]} \varphi_\beta(s)\Big] \tag{4.5}$$

hence (4.2) follows from (4.3)–(4.4). The corollary is proved. ∎

The essential property of the flows T_t and T_t^{Λ} is that they dissipate free energy:

Theorem 4.3. Let a and b satisfy (4.2), $\rho \in L^\infty(\mathbb{R}; [a, b])$ and such that $\mathscr{F}_\beta(\rho) < \infty$. Then for any $t \geqslant 0$ and any measurable region Λ (possibly $\Lambda = \mathbb{R}$, in which case $T_t^{\Lambda} \equiv T_t$)

$$\mathscr{F}_\beta(T_t^\Lambda(\rho)) - \mathscr{F}_\beta(\rho) \leqslant -\int_0^t ds\, I_\beta(T_s^\Lambda(\rho); \Lambda) \tag{4.6}$$

$$I_\beta(\rho; \Lambda) = \int_\Lambda dx\, (-\rho + \Phi_\beta(\rho; x)) \frac{1}{\beta} (-\log \rho + \log \Phi_\beta(\rho; x)) \tag{4.7}$$

$I_\beta(\rho; \Lambda) \geqslant 0$ with equality iff ρ solves (3.5) in Λ.

Proof. If Λ is bounded, (4.6) is simply derived as an equality by differentiating $\mathscr{F}_\beta(T_t^\Lambda(\rho))$ w.r.t. the time t. Otherwise we call $\Lambda_n = \Lambda \cap [-n, n]$ and use the previous result for Λ bounded, to write

$$\mathscr{F}_\beta(T_t^{\Lambda_n}(\rho)) - \mathscr{F}_\beta(\rho) = -\int_0^t ds\, I_\beta(T_s^{\Lambda_n}(\rho); \Lambda_n) \tag{4.8}$$

By the validity of a barrier lemma, see Proposition 4.4 below, $T_t^{\Lambda_n}(\rho) \to T_t^\Lambda(\rho)$ uniformly on the compacts. By the lower semicontinuity of $\mathscr{F}_\beta$, see Proposition 4.5 below, we have

$$\lim_{n \to \infty} \mathscr{F}_\beta(T_t^{\Lambda_n}(\rho)) \geqslant \mathscr{F}_\beta(T_t^\Lambda(\rho))$$

while, by Fatou's lemma,

$$\lim_{n \to \infty} \int_0^t ds\, I_\beta(T_s^{\Lambda_n}(\rho); \Lambda_n) \geqslant \int_0^t ds\, I_\beta(T_s^\Lambda(\rho); \Lambda)$$

Then the limit of (4.8) yields (4.6). The Theorem is proved. ∎

Proposition 4.4 [Barrier Lemma]. Let a and b satisfy (4.2), then there are constants $B > 0$ and C so that the following holds. Let $\rho_i \in L^\infty(\mathbb{R}; [a, b])$, $i = 1, 2$, call $\rho_i(\cdot, t) = T_t(\rho_i)$, let $V \geqslant e^2 B$ and $t > 0$, then

$$|\rho_1(0, t) - \rho_2(0, t)| \leqslant e^{(B-1)t} \sup_{|x| \leqslant Vt} |\rho_1(x) - \rho_2(x)| + C \exp\left\{ -tV \log \frac{V}{eB} \right\} \tag{4.9}$$

Moreover, for any measurable region Λ, let $\rho^\Lambda(\cdot, t) = T_t^\Lambda(\rho)$, $\rho(\cdot, t) = T_t(\rho)$, $\rho \in L^\infty(\mathbb{R}; [a, b])$, and $d_\Lambda(x) = \mathrm{dist}(x, \Lambda^c)$,

$$|\rho(x, t) - \rho^\Lambda(x, t)| \leqslant C \exp\left\{ -d_\Lambda(x) \log\left(\frac{d_\Lambda(x)}{eBt} \right) \right\} \tag{4.10}$$

Proof. By writing (4.1) in integral form we get

$$T_t(\rho_1)-T_t(\rho_2)=e^{-t}[\rho_1-\rho_2]+\int_0^t ds\, e^{-(t-s)}\{\Phi_\beta(T_s(\rho_1);\cdot)-\Phi_\beta(T_s(\rho_2);\cdot)\}$$

Let $z \in [0, 1]$ be an interpolating parameter, and write

$$K_s(z, x) := \Phi_\beta(zT_s(\rho_1)+(1-z)\, T_s(\rho_2); x)$$

Then

$$T_t(\rho_1)-T_t(\rho_2)=e^{-t}[\rho_1-\rho_2]+\int_0^t ds\, e^{-(t-s)}\int_0^1 dz\, \frac{d}{dz}\, K_s(z,\cdot)$$

Let

$$B := \sup_{r\in[a,b]} \varphi'_\beta(r) \tag{4.11}$$

(φ_β is defined in (2.5)), then,

$$\left|\frac{d}{dz} K_s(z, x)\right| \leqslant B(j * j * |\rho_1(\cdot, s)-\rho_2(\cdot, s)|)(x)$$

hence

$$|\rho_1(x, t)-\rho_2(x, t)|$$
$$\leqslant e^{-t}\, |\rho_1(x, 0)-\rho_2(x, 0)|+B\int_0^t ds\, e^{-(t-s)} \sup_{|x-y|\leqslant 2} |\rho_1(y, s)-\rho_2(y, s)|$$

because $j(x, y)$ is supported by $|x-y| \leqslant 1$ ($R_d = 1$ for $d = 1$).

Iterating the inequality and calling N the smallest integer larger or equal to $Vt/2$, we get:

$$|\rho_1(0, t)-\rho_2(0, t)| \leqslant \sum_{n<N} e^{-t}\, \frac{(Bt)^n}{n!} \sup_{|x|\leqslant Vt} |\rho_1(x, 0)-\rho_2(x, 0)|+C\, \frac{(Bt)^N}{N!}$$

where $C=\varphi_\beta(\sqrt{2})$, as $\Phi_\beta(\cdot;\cdot)$ is bounded by the maximum of $\varphi_\beta(s)$, which is reached at $s=\sqrt{2}$. Use of the Stirling formula, then yields (4.9).

To prove (4.10), we proceed in the same way, iterating N times, with N the smallest integer larger or equal to $d_\Lambda(x)/2$. The proposition is proved. ▮

Proposition 4.5 (Lower Semicontinuity). Let $\rho_n \in L^\infty(\mathbb{R})$ be a sequence converging to ρ uniformly on the compacts. Then

$$\liminf_{n \to \infty} \mathscr{F}_\beta(\rho_n) \geqslant \mathscr{F}_\beta(\rho) \tag{4.12}$$

Proof. By (3.1), $\mathscr{F}_\beta$ is an integral of a positive function, then (4.12) follows by using Fatou's lemma. The proposition is proved. ▮

Theorem 4.6. Let R'' as in (4.3) and

$$R' = \inf_{\beta \in (\beta_c, \beta_0)} \inf_{0 \leqslant s \leqslant R''} \varphi_\beta(s) \tag{4.13}$$

Then $T_t(\rho)$ and $T_t^A(\rho)$ are well defined on $L^\infty(\mathbb{R}, [R', R''])$ and the inf of $\mathscr{F}_\beta$ in $\mathscr{N}_\beta$ is the same as the inf in $\mathscr{N}_\beta \cap L^\infty(\mathbb{R}, [R', R''])$. Finally, any instanton is in $L^\infty(\mathbb{R}, [R', R''])$.

Proof. The statement about well-posedness for $T_t(\rho)$ and $T_t^A(\rho)$ is already proved in Corollary 4.2, setting $b = R''$.

The statement in the theorem is a consequence of the following inequality valid for any ρ such that $\mathscr{F}_\beta(\rho) < \infty$

$$\mathscr{F}_\beta(\rho^{**}) \leqslant \mathscr{F}_\beta(\rho) \qquad \text{where} \quad \rho^{**} := \max\{R', \min\{\rho, R''\}\} \tag{4.14}$$

As the proofs are similar we will only prove "the upper half" of the above inequality, namely that

$$\mathscr{F}_\beta(\rho^{*}) \leqslant \mathscr{F}_\beta(\rho) \qquad \text{where} \quad \rho^{*} := \min\{\rho, R''\} \tag{4.15}$$

We will first show that for any $A > R''$ there is $\delta_A > 0$ so that the following holds. Let $\mathscr{F}_\beta(\rho) < \infty$, $n > 0$, call

$$X_{A,n}(\rho) := \{x \in [-n, n] : \rho(x) > A\} \tag{4.16}$$

If $|X_{A,n}(\rho)| > 0$, there is $\rho^{(1)}$ such that $\mathscr{F}_\beta(\rho^{(1)}) \leqslant \mathscr{F}_\beta(\rho)$, $\rho^{(1)} = \rho$ outside $X_{A,n}(\rho)$ and

$$R'' \leqslant \rho^{(1)} \leqslant \rho - \delta_A \qquad \text{on} \quad X_{A,n}(\rho) \tag{4.17}$$

To prove (4.17), we shorthand $\Lambda = X_{A,n}(\rho)$ and set $\rho^{(1)} = T_t^\Lambda(\rho)$ with $t = (A - R'')/(2A)$, then, by Theorem 4.3, $\mathscr{F}_\beta(\rho^{(1)}) \leqslant \mathscr{F}_\beta(\rho)$. Since $\Phi_\beta \geqslant 0$,

$$\frac{\partial \rho}{\partial t} \geqslant -\rho$$

hence, on $\Lambda = X_{A,n}(\rho)$ and for $s \leqslant t$

$$T_s^A(\rho) \geqslant A - As \geqslant A - \frac{A - R''}{2} \tag{4.18}$$

which proves the first inequality in (4.17). On the other hand, since $\Phi_\beta \leqslant R''$,

$$\frac{\partial T_s^A(\rho)}{\partial s} \leqslant -T_s^A(\rho) + R''$$

hence, by (4.18), on $\Lambda = X_{A,n}(\rho)$

$$T_t^A(\rho) \leqslant \rho - t\left(A - \frac{A - R''}{2} - R''\right) = \rho - \frac{(A - R'')^2}{4A} \tag{4.19}$$

thus proving (4.17), with δ_A given by the last term in (4.19).

If $|X_{A,n}(\rho^{(1)})| > 0$, we apply the previous procedure starting from $\rho^{(1)}$ (instead of ρ) and get a new function $\rho^{(2)}$; by induction we either obtain an infinite sequence $\rho^{(k)}$, or a finite one, if, for some k, $|X_{A,n}(\rho^{(k)})| = 0$. In the former case, $\rho^{(k)} \to \rho^{(\infty)}$ (by monotonicity), $\mathscr{F}_\beta(\rho^{(\infty)}) \leqslant \mathscr{F}_\beta(\rho)$ (by lower semicontinuity, Proposition 4.5) and $|X_{A,n}(\rho^{(\infty)})| = 0$ because

$$\{x \in X_{A,n}(\rho^{(\infty)}) : \rho^{(\infty)} \geqslant A\} \subseteq \bigcap_{k \geqslant 1} \{x \in X_{A,n}(\rho) : \rho \geqslant A + k\delta_A\}$$

The Lebesgue measure of the set on the r.h.s. vanishes because, by assumption (see below (3.1)) ρ is locally integrable, hence a.e. finite in $[-n, n]$.

We call $\rho_{A,n}$ the function $\rho^{(\infty)}$ if the sequence $\rho^{(k)}$ is infinite, otherwise $\rho_{A,n}$ is the last term of the sequence. In any case we have $\mathscr{F}_\beta(\rho_{A,n}) \leqslant \mathscr{F}_\beta(\rho)$, $\rho_{A,n} \leqslant A$ a.e. in $[-n, n]$ (because $|X_{A,n}(\rho_{A,n})| = 0$) and $\rho_{A,n} = \rho$ outside $X_{A,n}(\rho)$.

By monotonicity we can set

$$\rho_n := \lim_{A \to R''} \rho_{A,n}$$

and again, by lower semicontinuity, $\mathscr{F}_\beta(\rho_n) \leqslant \mathscr{F}_\beta(\rho)$; by construction $\rho_n \leqslant R''$ a.e. on $[-n, n]$, while $\rho_n = \rho$ whenever $\rho \leqslant R''$, i.e., $\rho_n(x) = \min\{\rho(x), R''\}$ a.e. in $[-n, n]$. Finally, $\rho_n = \rho$ outside $[-n, n]$. Then again by monotonicity

$$\rho^* = \lim_{n \to \infty} \rho_n$$

and by lower semicontinuity, $\mathscr{F}_\beta(\rho^*) \leqslant \mathscr{F}_\beta(\rho)$ thus proving (4.15).

Finally if ρ solves (3.5), $\rho \in [R', R'']$ by (4.5). The theorem is proved. ▮

Since

$$T_t(\rho) = e^{-t}\rho + \int_0^t ds\, e^{-(t-s)} \Phi_\beta(T_s(\rho); \cdot)$$

$T_t(\rho)(x) - e^{-t}\rho(x)$ is differentiable in x with derivative uniformly bounded in $L^\infty(\mathbb{R}, [R', R''])$. Analogous property holds for $T_t^\Lambda(\rho)$, so that, by the Ascoli–Arzelà theorem we have proved:

Proposition 4.7. Let $\rho \in L^\infty(\mathbb{R}, [R', R''])$ and $\{t_j\}$ a divergent sequence. Then there is a divergent subsequence $\{t'_j\}$ so that $T_{t'_j}(\rho)$ converges uniformly on the compacts of $\mathbb{R}$. Analogous property holds for T_t^Λ.

The last property of dynamics we need is:

Theorem 4.8. Let $\rho \in L^\infty(\mathbb{R}, [R', R''])$ and $\mathscr{F}(\rho) < \infty$. Then any limit point u of $T_t(\rho)$ [in the sense of uniform convergence on the compacts] satisfies (3.5) and $\mathscr{F}(u) \leqslant \mathscr{F}(\rho)$. Analogously, if Λ is a measurable region, any limit point u of $T_t^\Lambda(\rho)$ satisfies (3.5) in Λ and $\mathscr{F}(u) \leqslant \mathscr{F}(\rho)$.

The proof of Theorem 4.8 is based on the fact that if u does not satisfy (3.5), then $T_t(u)$ (or $T_t^\Lambda(u)$) has positive free energy dissipation. By using regularity of dynamics, we then find that the orbit $T_t(\rho)$ (or $T_t^\Lambda(\rho)$) dissipates an infinite amount of free energy, against the assumption that $\mathscr{F}_\beta(\rho) < \infty$. We omit the details.

5. CONTOURS, PEIERLS ESTIMATES

By Theorem 4.6, we will hereafter consider the functional $\mathscr{F}$ on the space $L^\infty(\mathbb{R}, [R', R''])$. In this section we will prove that the free energy cost of a density profile which "deviates" from the equilibrium values $\rho_{\beta,\pm}$ is proportional to the volume of the region where this happens. We fix β in (β_c, β_0) and often drop it from the notation. Contours are defined as regions where a "significant deviation" from equilibrium occurs. Measuring deviations by sup norm is too restrictive, an acceptable compromise is to take sup norm but after coarse graining, a procedure already used in LMP and quite common in statistical mechanics.

5.1. Block Spins

Let $\mathscr{D}^{(\ell)}$, $\ell = 2^n$, $n \in \mathbb{Z}$, be a decreasing sequence of partitions of $\mathbb{R}$ into intervals of side ℓ (i.e., $\mathscr{D}^{(\ell)}$ is coarser than $\mathscr{D}^{(\ell')}$ if $\ell \geqslant \ell'$). We also denote by $C_x^{(\ell)}$, $x \in \mathbb{R}$, the interval in $\mathscr{D}^{(\ell)}$ which contains the point x (we use the symbol C, which stands for cube, by analogy with LMP). When writing ℓ in the sequel we tacitly suppose $\ell \in \{2^n, n \in \mathbb{Z}\}$. For any such ℓ and any $\rho \in L^\infty(\mathbb{R}, [R', R''])$, we define the "coarse grained image" of ρ as

$$\mathrm{Av}^{(\ell)}(\rho; x) = \frac{1}{\ell} \int_{C_x^{(\ell)}} dx' \, \rho(x') \tag{5.1}$$

which is a bounded, $\mathscr{D}^{(\ell)}$-measurable function of x (i.e., constant on each interval of $\mathscr{D}^{(\ell)}$). We then introduce for any given $\zeta > 0$, the "block spin configuration" associated to ρ as:

$$\eta^{(\ell,\zeta)}(\rho; x) = \begin{cases} \pm 1 & \text{if } \ |\mathrm{Av}^{(\ell)}(\rho; x) - \rho_{\beta,\pm}| \leqslant \zeta \\ 0 & \text{otherwise} \end{cases} \tag{5.2}$$

Following Zahradnik,[11] we finally introduce the notion of "contours."

5.2. Contours

Given the parameters $\ell'' > \ell' > 0$ and $\zeta > 0$ we define for any $\rho \in L^\infty(\mathbb{R}; [R', R''])$ the sets of $+$ and of $-$ correct points as follows. x is $+$correct (relative to ρ) if $\eta^{(\ell',\zeta)}(\rho; y) = 1$ in the interval $C_x^{(\ell'')}$ and also in the two intervals of $\mathscr{D}^{(\ell'')}$ to the right and to the left of $C_x^{(\ell'')}$. The $-$correct points are defined analogously and the contours are the maximal connected components of the complement of the set of all (both $+$ and $-$) correct points.

To simplify notation we reduce the number of parameters by relating ℓ' and ℓ'' as follows:

$$\ell > 2; \qquad \ell_\pm = \ell^{\pm 1}, \qquad \ell' = \ell_-, \qquad \ell'' = \ell_+ \tag{5.3}$$

(recall that 2 is larger than the range of the interaction). We will often drop the suffix ℓ and ζ simply writing $\eta(\rho; r)$, when needed we will resume the old notation. The main result in this section is:

Theorem 5.1. 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 $\rho \in L^\infty(\mathbb{R}; [R', R''])$ and Γ the union of all the (ℓ, ζ)- contours of ρ, then

$$\mathscr{F}_\beta(\rho) \geqslant c\, |\Gamma| \tag{5.4}$$

($|\Gamma|$ denoting the Lebesgue measure of Γ).

Proof. Given ρ, $\ell > 2$ and ζ, we define three families of $\mathscr{D}^{(\ell_-)}$-measurable regions, $\{A_i\}$, $\{B_i\}$ and $\{I_i\}$, as follows.

$$\bigcup_i A_i = \{x\colon \eta(\rho; x) = 0\}$$

$$\bigcup_i b_i = \{x\colon \eta(\rho; x) = 1, \text{ and } \exists x' \text{ s.t. } |x' - x| = 1 \text{ and } \eta(\rho; x) = -1\}$$

A_i and B_i being intervals belonging to $\mathscr{D}^{(\ell_-)}$. The family $\mathscr{I}\{I_i\}$ is made of disjoint intervals of length $(4 + 3\ell_-)$ which are built as follows: starting from the origin, find the first interval in the collection $\{A_i, B_i\}$ which is contained in $\mathbb{R}_+$ and let I_0 be the interval of length $(4 + 3\ell_-)$ with the same center. I_1 (I_{-1}) is then constructed with the same rule, with $\mathbb{R}_+$ replaced by the half-line to the right (left) of I_0, with the further request of not intersecting I_0; same procedure defines I_k, $|k| > 1$.

We obviously have

$$\mathscr{F}_\beta(\rho) \geqslant \sum_{I \in \mathscr{I}} \mathscr{F}_{\beta, I}(\rho)$$

where, analogously to (2.3),

$$\mathscr{F}_{\beta, I}(\rho) = \int_I dx \left([F_{\beta, \lambda_\beta}(j * \rho) - F_{\beta, \lambda_\beta}(\rho_{\beta, +})] + \frac{1}{\beta} \{S(j * \rho) - j * S(\rho)\} \right) \tag{5.5}$$

By translation invariance and symmetry under reflection, we have

$$\mathscr{F}_\beta(\rho) \geqslant \text{Card}(\mathscr{I}) \inf_{\rho' \in \mathscr{M}} \mathscr{F}_{\beta, I}(\rho') \tag{5.6}$$

where I is the interval of length $4 + 3\ell_-$ centered at 0 and

$$\mathscr{M} = \{\rho \in L^\infty(\mathbb{R}; [R', R'']) : \text{either } \eta(\rho; 0) = 0 \text{ or both } \eta(\rho; 0) = 1 \\ \text{and } \eta(\rho; \ell_-) = -1\}$$

Observe that $\mathscr{F}_{\beta, I}(\rho)$ depends only on the restriction of ρ to I^*, where I^* is the interval of length $8 + 3\ell_-$ centered at 0. It is then convenient to regard the functional $\mathscr{F}_{\beta, I}$ as defined in $L^\infty(I^*; [R', R''])$. Let $\{\rho_n\}$ be a minimizing sequence for the inf in (5.6) which converges weakly in $L^2(I^*)$ to a function $\rho^* \in L^\infty(\mathbb{R}; [R', R''])$ (having used weak compactness of the balls of $L^2(I^*)$). Thus

$$\inf_{\rho' \in \mathscr{M}} \mathscr{F}_{\beta, I}(\rho') \geqslant \mathscr{F}_{\beta, I}(\rho^*)$$

by weak lower semicontinuity. Indeed by (5.5) the term

$$\int_I dx \left([F_{\beta,\lambda_\beta}(j*\rho) - F_{\beta,\lambda_\beta}(\rho_{\beta,+})] + \frac{1}{\beta} S(j*\rho) \right)$$

is continuous in the weak $L^2(I^*)$ topology, while the last term $-\int_I dx\, j*S(\rho)$ is lower semicontinuous in the same topology, by the concavity of the entropy $S(\cdot)$. Since ρ^* is a weak limit of elements of $\mathscr{M}$, ρ^* cannot be the function identically equal either to $\rho_{\beta,+}$ or $\rho_{\beta,-}$, hence $\mathscr{F}_{\beta,I}(\rho^*) > 0$ and the theorem is proved because $\text{Card}(\mathscr{I}) \geqslant c_0\, |\Gamma|$.

A more detailed analysis of the lower bound and its dependence on the parameters of the model can be found in an earlier version of this paper at the web address: http://mat.uniroma2.it/ricerca/pre-print/aree/triolo/GPTF.ps. ∎

6. EXISTENCE OF INSTANTONS

Existence of instantons (i.e., solutions of (3.5) in the space $\mathscr{N}_\beta$, defined in (3.3)) is proved in Theorem 6.3 later, where we also show that the inf in (3.4) can as well be taken on the set (subset of $\mathscr{N}_\beta$) of all instantons. We need two preliminary lemmas.

Lemma 6.1. For any $\zeta > 0$ small enough there is $\ell_1(\zeta) > 0$ so that for all $\ell \leqslant \ell_1(\zeta)$ and all pairs (ρ, N), $\rho \in L^\infty(\mathbb{R}, [R', R''])$, $N > 0$, such that $\eta^{(\ell,\zeta)}(\rho; x) = 1$ for all $x \geqslant N$,

$$\rho_{\beta,+} - \zeta < \Phi_\beta(\rho)(x) < \rho_{\beta,+} + \zeta, \qquad \text{for all} \quad x \geqslant N+2 \tag{6.1}$$

Analogously, if $\eta^{(\ell,\zeta)}(\rho; x) = -1$ for all $x \leqslant -N$, then

$$\rho_{\beta,-} - \zeta < \Phi_\beta(\rho)(x) < \rho_{\beta,-} + \zeta, \qquad \text{for all} \quad x \leqslant -N-2 \tag{6.2}$$

Finally, if $\eta^{(\ell,\zeta)}(\rho; x) = \pm 1$ for all $x \geqslant N$, resp. for all $x \leqslant -N$, and if ρ satisfies (3.5) in $x > N+2$, resp. $x < -N-2$, then in such intervals $|\rho(x) - \rho_{\beta,+}| < \zeta$ and resp. $|\rho(x) - \rho_{\beta,-}| < \zeta$.

Proof. We will use here an improved version of (4.5): let $-\infty \leqslant x_0 < x_1 \leqslant +\infty$, $a < b$ both in $[R', R'']$, then recalling (3.5) and (2.5), if $j*\rho \in L^\infty([x_0-1, x_1+1], [a, b])$,

$$\Phi_\beta(\rho; x) \in [\inf_{s\in[a,b]} \varphi_\beta(s), \sup_{s\in[a,b]} \varphi_\beta(s)], \qquad \text{for all} \quad x \in [x_0, x_1] \tag{6.3}$$

We will also use that, given any ζ small enough, there is $\epsilon > 0$ so that

$$\begin{aligned} \inf_{s \in [\rho_{\beta,+} - \zeta - \epsilon,\, \rho_{\beta,+} + \zeta + \epsilon]} \varphi_\beta(s) &\geqslant \rho_{\beta,+} - \zeta, \\ \sup_{s \in [\rho_{\beta,+} - \zeta - \epsilon,\, \rho_{\beta,+} + \zeta + \epsilon]} \varphi_\beta(s) &\leqslant \rho_{\beta,+} + \zeta \end{aligned} \tag{6.4}$$

Suppose $\eta^{(\ell,\zeta)}(\rho; x) = 1$ for all $x \geqslant N$, then for $x \geqslant N+1$,

$$\int_N^\infty dy\, j(x, y)\, \rho(y) \leqslant \int_N^\infty dy\, j^{(\ell)}(x, y)\, \rho(y) + 4c\ell R'' \leqslant \rho_{\beta,+} + \zeta + 4c\ell R''$$

where

$$j^{(\ell)}(x, y) = Av^{(\ell)}(j(x, \cdot); y), \qquad |j^{(\ell)}(x, y) - j(x, y)| \leqslant c\mathbf{1}_{|x-y| \leqslant 2}$$

with c a constant and having supposed $\ell \leqslant 1$. Analogously, for $x \geqslant N+1$

$$\int_N^\infty dy\, j(x, y)\, \rho(y) \geqslant \rho_{\beta,+} - \zeta - 4c\ell R''$$

By choosing ℓ small enough, $j * \rho(x) \in [\rho_{\beta,+} - \zeta - \epsilon, \rho_{\beta,+} + \zeta + \epsilon]$, for all $x \geqslant N+2$, hence (6.1) follows from (6.3) and (6.4) (with $x_0 = N+1$ and $x_1 = \infty$). (6.2) is proved analogously. The last statement of the lemma is trivial because $\rho = \Phi_\beta(\rho; \cdot)$ for $x > N+2$ and $x < -N-2$. The lemma is proved. ∎

Lemma 6.2. Let ℓ and $\zeta > 0$ be as in Lemma 6.1, N such that the interval $\Lambda := [N+2, \infty)$ is $\mathscr{D}^{(\ell)}$-measurable and $\rho \in L^\infty(\mathbb{R}, [R', R''])$ such that $\eta^{(\ell,\zeta)}(\rho; x) = 1$ for all $x \geqslant N$. Then

$$\eta^{(\ell,\zeta)}(T_t^\Lambda(\rho); x) = 1, \qquad \text{for all} \quad x \geqslant N+2 \text{ and all } t \geqslant 0 \tag{6.5}$$

Analogously, if $\Lambda := (-\infty, -N-2]$ is $\mathscr{D}^{(\ell)}$-measurable, $\eta^{(\ell,\zeta)}(\rho; x) = -1$ for all $x \leqslant -N$, then

$$\eta^{(\ell,\zeta)}(T_t^\Lambda(\rho); x) = -1, \qquad \text{for all} \quad x \leqslant -N-2 \text{ and all } t \geqslant 0 \tag{6.6}$$

Proof. As the two are analogous, we only prove (6.5). Call ρ_0 the function ρ of the lemma. Given $\tau > 0$, denote by $\rho(x, t)$ the elements of $C([0, \tau], L^\infty(\mathbb{R}, [R', R'']))$ and

$$\begin{aligned} X_{\tau,\rho_0} = \{&\rho \in C([0, \tau], L^\infty(\mathbb{R}, [R', R''])) : \rho(\cdot, 0) \equiv \rho_0(\cdot), \rho(\cdot, t) = \rho_0(\cdot) \\ &\text{on } \Lambda^c \times [0, \tau]\} \end{aligned}$$

Let $\mathscr{S}$ be the map from X_{τ,ρ_0} into itself defined by setting for $x \in \Lambda$ and $t \leqslant \tau$

$$\mathscr{S}\rho(x,t) = e^{-t}\rho_0(x) + \int_0^t ds\, e^{-(t-s)}\Phi_\beta(\rho(\cdot,s);x)$$

If $\tau > 0$ is small enough, $\mathscr{S}$ is a contraction on X_{τ,ρ_0} (equipped with sup norm) and the only fixed point of $\mathscr{S}$ is therefore the orbit $T_t^\Lambda(\rho_0)$. The set

$$Y = \{\rho \in X_{\tau,\rho_0} : \eta^{(\ell,\zeta)}(\rho(\cdot,t)); x) = 1 \text{ for all } x \in \Lambda\}$$

is closed and by Lemma 6.1 is invariant under $\mathscr{S}$. Then it contains the fixed point of $\mathscr{S}$ hence $(T_t^\Lambda(\rho_0))_{t\in[0,\tau]}$ is in Y, thus proving (6.5) for $t \leqslant \tau$. By induction, the validity of (6.5) extends to all t and the lemma is proved. ▮

Theorem 6.3. Let $\beta \in (\beta_c, \beta_0)$ and $\zeta > 0$, then for any $\rho \in \mathscr{N}_\beta \cap L^\infty(\mathbb{R}, [R', R''])$ such that $\mathscr{F}_\beta(\rho) < \infty$ there is an instanton $\bar\rho_\beta$ such that $\mathscr{F}_\beta(\bar\rho_\beta) \leqslant \mathscr{F}_\beta(\rho)$ and such that $|\bar\rho_\beta(x) - \rho_{\beta,\pm}| \leqslant \zeta$ definitively as $x \to \pm\infty$.

Proof. Since $\mathscr{F}_\beta(\rho) < \infty$, by Theorem 4.3, for any $t \geqslant 0$, $\mathscr{F}_\beta(T_t(\rho)) < \infty$. Let $\zeta > 0$ be as small as required by Lemma 6.1, let $\ell < \min(\ell_0(\zeta), \ell_1(\zeta))$, $\ell_0(\zeta)$ as in Theorem 5.1 and $\ell_1(\zeta)$ as in Lemma 6.1. Write $\eta = \eta^{(\ell,\zeta)}$. By Theorem 5.1, for any $t \geqslant 0$ there is N_t such that

$$\begin{aligned} &\eta(T_t(\rho);x) = \alpha_+ \neq 0, \qquad \text{for all} \quad x \geqslant N_t; \\ &\eta(T_t(\rho);x) = \alpha_- \neq 0, \qquad \text{for all} \quad x \leqslant -N_t \end{aligned} \tag{6.7}$$

We want to show that $\alpha_\pm = \pm 1$. Call $\Lambda_\pm$ the largest $\mathscr{D}^{(\ell)}$-measurable intervals in $[N_0+2, \infty)$ and $(-\infty, -N_0-2]$, N_0 the value of N_t at $t = 0$. Since $\rho \in \mathscr{N}_\beta$, $\eta(\rho;x) = \pm 1$ when $x \geqslant N_0$ and, respectively, when $x \leqslant -N_0$, then, by Lemma 6.2,

$$\begin{aligned} &\eta(T_t^{\Lambda_+}(\rho);x) = 1, \qquad \text{for all} \quad x \in \Lambda_+; \\ &\eta(T_t^{\Lambda_-}(\rho);x) = -1, \qquad \text{for all} \quad x \in \Lambda_- \end{aligned} \tag{6.8}$$

By the barrier lemma, Proposition 4.4,

$$\lim_{x\to\pm\infty} |T_t^{\Lambda_\pm}(\rho)(x) - T_t(\rho)(x)| = 0 \tag{6.9}$$

thus concluding the proof that $\alpha_\pm = \pm 1$ in (6.7).

Since $\alpha_{\pm} = \pm 1$, $T_t(\rho)$ has at least one contour. On the other hand, since it has finite free energy, $T_t(\rho)$ has finitely many contours. We call $[x_i(t), y_i(t)]$, $i = 1,..., k_t$, $k_t \geqslant 1$, the closure of the contours of $T_t(\rho)$ and notice that, by Theorem 5.1,

$$\sup_{t \geqslant 0} \sup_{i=1, k_t} |y_i(t) - x_i(t)| < \infty, \qquad \sup_{t \geqslant 0} k_t = n < \infty, \qquad (n \geqslant 1) \tag{6.10}$$

Then there is a sequence $t_j \to \infty$ with $k_{t_j} = k \in [1, n]$ for all t_j. By taking subsequences we may also suppose, without loss of generality, that $\eta(T_{t_j}(\rho); x)$ has a constant sign (for all t_j) in each interval $(y_i(t_j), x_{i+1}(t_j))$, $1 \leqslant i \leqslant k$. By possibly taking subsequences we may also suppose that

$$\liminf_{t_j \to \infty} |x_{i+1}(t_j) - y_i(t_j)| = \limsup_{t_j \to \infty} |x_{i+1}(t_j) - y_i(t_j)|, \qquad 1 \leqslant i \leqslant k-1$$

Finally, writing $D_a \rho(x) = \rho(x+a)$, by Theorem 4.8 there is a subsequence t'_j so that for any $i = 1,..., k$, $D_{x_i(t'_j)} T_{t'_j}(\rho)$, converges uniformly on the compacts of $\mathbb{R}$ to a function ρ_i. By Proposition 4.5, $\mathscr{F}_\beta(\rho_i) < \infty$ and by Theorem 4.8, ρ_i solves (3.5). Call $\alpha_{\pm, i}$ the quantities in (6.7) with ρ_i replacing $T_t(\rho)$. Then $\alpha_{-,i} = 1$ if, calling ℓ the largest integer $\leqslant i$ such that $|x_\ell(t'_j) - y_{\ell-1}(t'_j)| \to \infty$, it happens that $\eta(T_{t'_j}(\rho; \cdot) = 1$ on $[y_{\ell-1}(t'_j), x_\ell(t'_j)]$; otherwise $\alpha_{-,i} = -1$. We are using the convention that $y_0 = -\infty$ and $x_{k+1} = \infty$. Analogously, $\alpha_{+,i} = 1$ if, calling ℓ the smallest integer $> i$ such that $|x_\ell(t'_j) - y_{\ell-1}(t'_j)| \to \infty$, it happens that $\eta(T_{t'_j}(\rho; \cdot) = 1$ on $[y_{\ell-1}(t'_j), x_\ell(t'_j)]$; otherwise $\alpha_{+,i} = -1$. We want to prove that there is at least an index i such that $\alpha_{\pm, i} = \pm 1$. Let i be the smallest integer ℓ such that $\alpha_{+,\ell} = 1$, i is well defined because $\alpha_{+,k} = 1$. Then $\alpha_{-,i} = -1$, otherwise $\alpha_{+,i-1} = 1$ against the assumption of minimality of i.

We have proved so far that there is ρ, $\rho = \rho_i$, which solves (3.5) and it is such that for some $N > 0$, $\eta(\rho; x) = \pm 1$ for all $x \geqslant \pm N$. By Lemma 6.1, if ζ and ℓ are small enough, for $x > N+2$

$$\rho(x) = \Phi_\beta(\rho; x) \in [\rho_{\beta,+} - \zeta, \rho_{\beta,+} + \zeta]$$

while for $x < -N-2$

$$\rho(x) = \Phi_\beta(\rho; x) \in [\rho_{\beta,-} - \zeta, \rho_{\beta,-} + \zeta]$$

Thus $\rho \in \mathscr{N}_\beta$, hence it is an instanton. The theorem is proved. ∎

Theorem 6.4. For any $\beta \in (\beta_c, \beta_0)$ there is an instanton $\bar{\rho}_\beta$, i.e., a solution of (3.5) which is in $\mathscr{N}_\beta$, such that

$$\inf_{\rho \in \mathscr{N}_\beta} \mathscr{F}_\beta(\rho) = \mathscr{F}_\beta(\bar{\rho}_\beta) \tag{6.11}$$

Proof. Let $\rho_n \in L^\infty(\mathbb{R}, [R', R''])$ be a minimizing sequence for (3.5). By Theorem 6.3, there is a sequence $\bar{\rho}_{\beta,n}$ of instantons which is a minimizing sequence as well. By construction, there is C so that $\mathscr{F}_\beta(\bar{\rho}_{\beta,n}) \leqslant C$ for all n, while $\alpha_{\pm,n} = \pm 1$, where $\alpha_{\pm,n}$ are defined by (6.7) with $\bar{\rho}_{\beta,n}$ replacing $T_t(\rho)$. As $\bar{\rho}_{\beta,n}$ solves (3.5) its derivative is bounded (for all x and all n), thus by the Ascoli–Arzelà theorem, $\bar{\rho}_{\beta,n}$ converges uniformly on the compacts by subsequences and any limit point u satisfies (3.5) (by the continuity of $\Phi_\beta(\rho;\cdot)$ for the uniform convergence on the compacts). We can then proceed as in the proof of Theorem 6.3, thus finding a sequence n_j and reals x_{n_j} such that $D_{x_{n_j}} \bar{\rho}_{\beta,n_j} \to u$ and u is an instanton. The theorem is proved. ▮

7. ASYMPTOTIC BEHAVIOR OF INSTANTONS

We will first prove the statement in Theorem 3.1 about exponential convergence of the instantons:

Theorem 7.1. Let $\beta \in (\beta_c, \beta_0)$ and $\bar{\rho}_\beta$ an instanton such that $\mathscr{F}_\beta(\bar{\rho}_\beta) < \infty$. Then there are c and $\omega > 0$ so that

$$\begin{aligned} |\bar{\rho}(x) - \rho_{\beta,+}| &\leqslant c e^{-\omega x}, \qquad &\text{for all} \quad x \geqslant 0; \\ |\bar{\rho}(x) - \rho_{\beta,-}| &\leqslant c e^{-\omega |x|}, \qquad &\text{for all} \quad x \leqslant 0 \end{aligned} \tag{7.1}$$

Proof. Since $\bar{\rho}_\beta$ has finite free energy, it has finitely many contours (defined with $\zeta > 0$ so small to satisfy the requests below) and ℓ so large that ζ and ℓ^{-1} satisfy the assumptions of Lemma 6.1. Then by Lemma 6.1, there is N so that

$$\begin{aligned} |\rho(x) - \rho_{\beta,+}| &\leqslant \zeta, \qquad &\text{for all} \quad x \geqslant N-2; \\ |\rho(x) - \rho_{\beta,-}| &\leqslant \zeta, \qquad &\text{for all} \quad x \leqslant -N+2 \end{aligned} \tag{7.2}$$

Let us prove the statement in (7.1) relative to $\rho_{\beta,+}$, the proof of the other one is analogous and omitted. We write for $x > N$,

$$\rho(x) - \rho_{\beta,+} = \Phi_\beta(\rho; x) - \Phi_\beta(\rho_{\beta,+}; x) \tag{7.3}$$

where $\rho_{\beta,+}$ in the argument of the last term, denotes the function constantly equal to $\rho_{\beta,+}$. Calling $v(x) := |\rho(x) - \rho_{\beta,+}|$,

$$v(x) \leqslant \int_0^1 dz \left| \frac{d}{dz} \Phi_\beta(z[\rho - \rho_{\beta,+}] + \rho_{\beta,+}; x) \right| \tag{7.4}$$

By (7.2), the values of the function $z[\rho-\rho_{\beta,+}]$ involved in the computation of the last term are not larger than ζ, then, by (6.3),

$$\Phi_\beta(z[\rho-\rho_{\beta,+}]+\rho_{\beta,+};x)\leqslant \rho_{\beta,+}+\zeta$$

and

$$\left|\frac{d}{dz}\Phi_\beta(z[\rho-\rho_{\beta,+}]+\rho_{\beta,+};x)\right|$$
$$\leqslant (\rho_{\beta,+}+\zeta)\;\beta\max_{\sigma=\pm 1}\;|1-(\rho_{\beta,+}+\sigma\zeta)^2/2|\;(j*j*v)(x)$$

By (2.6) and (2.7), if $\zeta>0$ is small enough, there is $p<1$ so that, for $x\in\Lambda$,

$$v(x)\leqslant p(j*j*v)(x) \tag{7.5}$$

Then if $x-N\geqslant 2n$,

$$v(x)\leqslant p^n\,\|v\|_\infty\leqslant p^nR'' \tag{7.6}$$

An analogous argument is used for $x\leqslant 0$, the theorem is proved. ∎

Theorem 7.2. Let $\beta\in(\beta^*,\beta_0)$ and $\bar\rho_\beta$ an instanton such that $\mathscr{F}_\beta(\bar\rho_\beta)<\infty$, then the set $\{x\colon \bar\rho_\beta(x)\geqslant\rho_{\beta,+}\}$ is made of infinitely many disjoint intervals.

Proof. Writing $\rho(x)$ for $\bar\rho_\beta(x)$, since $\phi'_\beta(\rho_{\beta,+})<0$, $\rho(x)$ cannot converge to $\rho_{\beta,+}$ as $x\to\infty$ strictly from above, or strictly from below; we cannot exclude however that there is $\bar x$ so that $\rho(x)=\rho_{\beta,+}$ for all $x\geqslant\bar x$. Supposing $\bar x$ the smallest number with such a property, we want to prove that again $\rho(x)$ cannot converge to $\rho_{\beta,+}$ as $x\nearrow\bar x$, strictly from above, or strictly from below. Arguing by contradiction suppose for instance $\rho(x)<\rho_{\beta,+}$ for $x\in(\bar x-\delta,\bar x)$, $\delta>0$. Since $\rho(x)\to\rho_{\beta,+}$, there is δ' small and positive, so that $\rho(x)>\rho_{\beta,+}$ for $x\in(\bar x-\delta'+2,\bar x+2)$, against the definition of $\bar x$. The theorem is proved. ∎

Theorem 7.3. Let $\beta\in(\beta_c,\beta^*)$, then there is a unique instanton $\bar\rho_\beta$ (up to translations) and $\bar\rho'_\beta>0$.

Proof. We first observe that for any $b\in[\rho_{\beta,+},\sqrt{2})$

$$\sup_{s\leqslant b}\varphi_\beta(s)\leqslant b \tag{7.7}$$

so that, letting a as in (4.4), by (4.5) the pair (a, b) satisfies (4.2). On the other hand, restricted to $[a, b]$, the function $\varphi_\beta(s)$ is strictly increasing. For this reason, a comparison theorem is valid for (4.1) in $L^\infty(\mathbb{R}, [a, b])$, with the above values of a and b: namely if u and ρ are in $L^\infty(\mathbb{R}, [a, b])$ and $u \geqslant \rho$, then for all $t > 0$, $T_t(u) \geqslant T_t(\rho)$ and, for any measurable region Λ, $T_t^\Lambda(u) \geqslant T_t^\Lambda(\rho)$ as well. The proof is elementary and omitted.

Notice that $\rho_{\beta,\pm} \in [a, b]$, hence the restriction to $L^\infty(\mathbb{R}, [a, b])$ is inconsequential when studying instantons. Uniqueness and monotonicity of the instanton are proved as for the non-local functional arising from the ferromagnetic Ising model, as we have seen that comparison inequalities are valid for the dynamics (7.2). We just outline the argument which follows very closely that in ref. 12, to which we refer for details. The monotonicity of the instanton is proved by taking for ρ in the beginning of the proof of Theorem 6.3, an increasing function. Then $T_t(\rho)$ is still increasing, by the comparison theorem, and monotonicity is preserved in the limit. Thus the instanton $\bar{\rho}_\beta$ constructed from such ρ is non decreasing. By differentiating (3.5) we have

$$\rho' = \beta \rho j * ([1-(j*\rho)^2/2]\, j * \rho') \tag{7.8}$$

By (7.8) and observing that the square bracket is now positive, it follows that if $\bar{\rho}'_\beta(x) = 0$, then $j * j * \rho'(x) = 0$. By iterating the argument, we would find $\bar{\rho}'_\beta \equiv 0$, which contradicts the fact that $\bar{\rho}_\beta(x) \to \rho_{\beta,\pm}$ as $x \to \pm\infty$.

The proof of the uniqueness of the instanton is less elementary. It follows by proving that any orbit $T_t(\rho)$ starting from $\rho \in \mathcal{N}_\beta \cap L^\infty(\mathbb{R}, [a, b])$ is attracted by a translate of the instanton. This is done in various steps. First we study the linearization of (4.1) around the instanton $\bar{\rho}_\beta$:

$$\frac{\partial u}{\partial t} = Lu := -u + \bar{\rho}_\beta \beta j * \{[1-(j*\bar{\rho}_\beta)^2/2]\, j * u\} \tag{7.9}$$

It is convenient to regard L as an operator on $L^\infty(\mathbb{R})$. Exploiting the non negativity of the kernel of the operator $\bar{\rho}_\beta \beta j * \{[1-(j*\bar{\rho}_\beta)^2/2]\, j * u\}$ which makes L a Perron–Frobenius operator, it can be proved (following ref. 12, 13, and 14) that 0 is a simple eigenvalue with eigenvector $\bar{\rho}'_\beta$ and that there is $\omega > 0$ so that the rest of the spectrum of L is in $Re(z) < -\omega$.

It is then not too hard to prove a local stability result, namely there is $\epsilon > 0$ so that if, for some ξ, $\|\rho - D_\xi \bar{\rho}_\beta\|_\infty \leqslant \epsilon$, then there is $x_0 \in \mathbb{R}$ so that

$$\lim_{t\to\infty} T_t(\rho) = D_{x_0} \bar{\rho}_\beta \tag{7.10}$$

We then need a Fife–McLeod bound,[12] on trapping an orbit between instantons: namely, if $\rho \in \mathcal{N}_\beta$ (and with values in $[a, b]$) there are $\xi_\pm(t)$ and $\delta(t)$ so that

$$D_{\xi_-(t)}\bar{\rho}_\beta - \delta(t) \leqslant T_t(\rho) \leqslant D_{\xi_+(t)}\bar{\rho}_\beta + \delta(t) \tag{7.11}$$

with $\delta(t) \to 0$ and $\xi_\pm(t) \to \xi_\pm$, exponentially fast as $t \to \infty$. The proof uses extensively the comparison inequality stated above and, being similar to that in ref. 12, is omitted. Thus for any instanton ρ, there are $\xi_\pm$ so that

$$D_{\xi_-}\bar{\rho}_\beta \leqslant \rho \leqslant D_{\xi_+}\bar{\rho}_\beta \tag{7.12}$$

Using the local stability (proved earlier), it is shown in ref. 12 that if (7.12) holds for some $\xi_- > \xi_+$ it holds as well for $\xi'_\pm$ and $\xi'_- < \xi_-$, $\xi'_+ > \xi_+$. By iterations this proves that $\xi_- = \xi_+$, hence the uniqueness of the instanton. The above is just a sketch of the proof, which is however too long and similar to that in ref. 12 for being reported here. The theorem is proved. ∎

8. CONCLUDING REMARKS

In a paper still in preparation, Bodineau, Ioffe, and Presutti study the large deviations for the original LMP model characterizing the surface tension $\tau_{\beta,\gamma}$ of the system, when the scaling parameter γ is positive (and small). Relying on similar results for Ising systems with Kac potentials, the surface tension $\tau_{\beta,\gamma}$ should converge as $\gamma \to 0$ to the surface tension τ_β of (3.4), when $\beta \in (\beta_c, \beta^*)$. The same argument for $\beta > \beta^*$, would only indicate that the limit of $\tau_{\beta,\gamma}$ is $\leqslant \tau_\beta$.

Equality would require an extension of our analysis to cylindrical domains in $\mathbb{R}^d$, $d > 1$, of the form $\mathcal{T}_L \times \mathbb{R}$, where $\mathcal{T}_L$ denotes a torus in $\mathbb{R}^{d-1}$ of side L. One then needs to prove that there is no breaking of the planar symmetry in the variational problem (3.4) extended to these cylindrical domains, namely that the minimizers depend only on the coordinate along the axis of the cylinder and hence they are $d = 1$ instantons. There are indications, De Masi, Gobron, in preparation, that our results extend to cylindrical domains showing that the minimizers of the variational problem are d-dimensional instantons and there is numerical evidence that the minimizer is unique (up to translations) and given by the $d = 1$ instanton.

We have further results indicating that there is $\beta' \in (\beta^*, \beta_0)$ so that in the whole (β_c, β') the minimizer is unique, up to translations; on the other hand, however, we do not have examples of cases where uniqueness fails. We also have preliminary results which show that at β^* the instanton is unique and also monotone.

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REFERENCES

1. J. L. Lebowitz, A. Mazel, and E. Presutti, Liquid-vapor phase transitions for systems with finite-range interactions, *J. Stat. Phys.* **94**:955–1025 (1999).
2. M. Cassandro and E. Presutti, Phase transitions in Ising systems with long but finite range interactions, *Markov Process. Related Fields* **2**:241–262 (1996).
3. A. Bovier and M. Zahradnik, The low-temperature phase of Kac–Ising models, *J. Stat. Phys.* **87**:311–332 (1997).
4. P. Buttà, I. Merola, and E. Presutti, On the validity of the van der Waals theory in Ising systems with long range interactions, *Markov Process. Related Fields* **3**:63–88 (1997).
5. T. Bodineau, On the van der Waals theory of surface tension, Preprint, (2001).
6. G. Alberti, G. Bellettini, M. Cassandro, and E. Presutti, Surface tension in Ising systems with Kac potentials, *J. Stat. Phys.* **82**:743–796 (1996).
7. O. Benois, T. Bodineau, P. Buttà, and E. Presutti, On the validity of van der Waals theory of surface tension, *Markov Process. Related Fields* **3**:175–198 (1997).
8. O. Benois, T. Bodineau, and E. Presutti, Large deviations in the van der Waals limit, *Stochastic Process. Appl.* **75**:89–104 (1998).
9. R. Evans, R. J. F. Leote de Carvalho, J. R. Henderson, and D. C. Hoyle, Asymptotic decay of correlations in liquids and their mixtures, *J. Chem. Phys.* **100**:591–603 (1994).
10. C. A. Croxton, Atomic processes at the liquid surface, in *Progress in Liquid Physics*, pp. 41–87, Chap. 2, C. A. Croxton, ed. (Wiley, Chichester, 1978).
11. M. Zahradnik, An alternate version of Pirogov–Sinai theory, *Commun. Math. Phys.* **93**:559–581 (1984).
12. A. De Masi, E. Orlandi, E. Presutti, and L. Triolo, Uniqueness of the instanton profile and global stability in non-local evolution equations, *Rendiconti di Matematica* **14** (1993).
13. A. De Masi, T. Gobron, and E. Presutti, Travelling fronts in non-local evolution equations, *Archive Rat. Mech.* **132**:143–205 (1995).
14. P. W. Bates, P. C. Fife, X. Ren, and X. Wang, Traveling waves in a convolution model for phase transitions, *Arch. Rational Mech. Anal.* **138**:105–136 (1997).
15. C. Kipnis and C. Landim, Scaling limits of interacting particle systems, in *Grundlehren der mathematischen Wissenschaften*, Vol. 320 (Springer-Verlag, 1999).