FAILURE OF CRYSTALLIZATION FOR GENERALIZED LENNARD-JONES POTENTIALS AND COARSE GRAINING TO A ROTATING STARS PROBLEM IN ONE DIMENSION

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Abstract. This paper deals with ground states for systems governed by generalized Lennard-Jones potentials $LJ^{p,q}(r) := r^{-p} - r^{-q}$, for $0 < q < 1 < p$. The energy per particle diverges to $-\infty$ as the number N of particles diverges. As a consequence, the average distance between particles vanishes as $N \to +\infty$. After suitable scaling, we prove that such a model converges, as $N \to +\infty$ and in the sense of Γ-convergence, to a rotating stars model; the effective energy is given by the sum of a repulsive pressure term and an attractive nonlocal interaction functional. The ground states of such a limit energy have non constant density. As a consequence, for the generalized Lennard-Jones potentials considered here, crystallization does not occur in any reasonable sense.

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Contents

1. Introduction

The crystallization problem, in its basic form, consists in understanding periodic configurations of atoms as ground states of suitable pairwise potential interactions. Minimal assumptions on the pairwise potential are that it depends only on the distance between the particles, and that it is short range repulsive and long range attractive; the canonical reference choice for such a potential is given by the Lennard-Jones potential $LJ^{12,6}(r) := r^{-12} - r^{-6}$. At least for chains of particles in one dimension the Lennard-Jones model is able to predict crystallization: in [6] the authors prove that, for any given $N \in \mathbb{N}$, there exists a configuration $X_N = \{x_1, \dots, x_N\}$ of N particles, with $x_i < x_j$ for $i < j$, minimizing the energy $\sum_{i<j} LJ^{12,6}(|x_i - x_j|)$; moreover, as $N \to +\infty$, the particles tend to be equispaced: there is an optimal distance $\bar{r}$ such that, as $N \to +\infty$ the distance between two consecutive particles tends to $\bar{r}$, provided that the distance between such a pair of particles and both the first and the last particle of the chain diverge.

A natural question is to understand what happens for more general potentials (we refer the interested reader to the review [3]). In [8] it is proved that crystallization happens for a quite large class of short range repulsive and long range attractive potentials: roughly speaking, potentials with a single inflection point enjoy crystallization, otherwise explicit examples can be constructed where periodic but not equispaced configurations have less energy density with respect to the equispaced configuration.

The results mentioned above assume that the potential is stable, namely that the attractive part of the potential is integrable at infinity, such as $-r^{-q}$ for q greater than the dimension: such an assumption guarantees that the energy per particle is uniformly bounded with respect to N, and that, in turn, the minimal distance between particles remains positive. The last condition has always been considered as essential in order to even start talking about crystallization.

Unstable potentials are, to our knowledge, much less studied. For such systems the total energy is superlinear with respect to N, the energy per particle is unbounded, and the mutual distance between particles vanishes as $N \to +\infty$. In order to study these systems a multiscale analysis approach is mandatory.

In this paper we will focus on the so called generalized (p, q)-Lennard-Jones potentials, also referred to as Mie potentials, defined as $LJ^{p,q}(r) := r^{-p} - r^{-q}$. Specifically, we consider the case $0 < q < 1 < p$; the assumption $q < 1$ implies that the potential is not stable. For such a range of parameters we provide a complete Γ-convergence analysis as the number of particles diverges. As a byproduct of this analysis we show that crystallization does not occur.

In order to describe our results it is convenient to first detect the intrinsic scales (see (2.7)) of our model. To this purpose, given $N \in \mathbb{N}$ consider a string of equispaced particles. Optimizing with respect to the mutual distance between particles it turns out that the characteristic distance is of order $r_N := N^{\frac{q-1}{p-q}}$. This says that as N increases the distance between particles should vanish, while the total length of the chain of particles is of order $R_N := Nr_N = N^{\frac{p-1}{p-q}}$ which diverges as $N \to +\infty$. These scales are based on the ansatz that the optimal chain is made of uniformly distributed particles. As a matter of fact, even if such an ansatz turns out to be wrong, the detected intrinsic scales are correct (since configurations with uniformly distributed particles have energy comparable with that of true minimizers).

After encoding all the natural scalings in our energy functionals we compute their Γ-limit as the number of particles N diverges. The limit energy is given by the sum of a repulsive pressure term and of an attractive nonlocal term. This energy is known as governing (in three dimensions) the so-called rotating stars model [1, 2], and it has been extensively studied in [4, 5]. In this respect, our model provides a rigorous derivation in terms of Γ-convergence of such a rotating stars model, obtained by coarse graining of a discrete model for interacting particles through Lennard-Jones type potentials. By standard rearrangement arguments it is very easy to see that ground states for the rotating stars model have maximal density at the center of mass. Moreover, by computing first variations we show that the density of ground states is not constant. In terms of the approximating (p, q)-Lennard-Jones energy functionals this means that crystallization does not occur in any reasonable sense, since in fact the limit density for chains of ground states becomes non constant.

Replacing the repulsive part of the potential with an hard sphere constraint would give back in the limit problem a maximal density constraint; the corresponding ground states saturate such a maximal allowed density, restoring also crystallization properties [7].

In fact, we expect that for the generalized (p, q)-Lennard-Jones model considered here, in higher dimensions the ground states are macroscopic radial shapes, microscopically filled by optimal packing of hard spheres; in such a lattice structure the radius of the hard sphere should depend on the distance from the center of mass, with maximal density of the spheres in the center of mass. The analysis of ground states of generalized (p, q)-Lennard-Jones models in any dimension and for all values of the parameter p and q deserves, in our opinion, further investigation.

Notation of the paper In this paper we use the following notation: $\mathcal{B}(\mathbb{R})$ denotes the family of Borel sets $E \subset \mathbb{R}$, while the corresponding Lebesgue measure will be denoted by $|E|$. $\mathcal{M}_b(\mathbb{R})$ denotes the space of (non negative) finite Radon measures in $\mathbb{R}$. The Dirac delta measure centered in x_0 is denoted by δ_{x_0}, while the Lebesgue measure by $\mathcal{L}$ or dx. We denote with $C(\star, \cdots, \star)$ a constant that depends on $\star, \cdots, \star$; this constant may change in the steps of a proof.

2. The Γ-convergence result

Let p, $q > 0$ be such that $p > 1 > q$. In this paper we deal with energy functionals of the type

$$\mathcal{E}(X) = \sum_{i,j \in \{1,\ldots,N\},\, i<j} V(|x_i - x_j|), \tag{2.1}$$

where $X = \{x_1, \ldots, x_N\} \subset \mathbb{R}$ and we will focus our interest in $V : (0, +\infty) \to (0, +\infty)$ defined by (see Figure 1)

$$V(r) = LJ^{p,q}(r) := \frac{1}{r^p} - \frac{1}{r^q}. \tag{2.2}$$

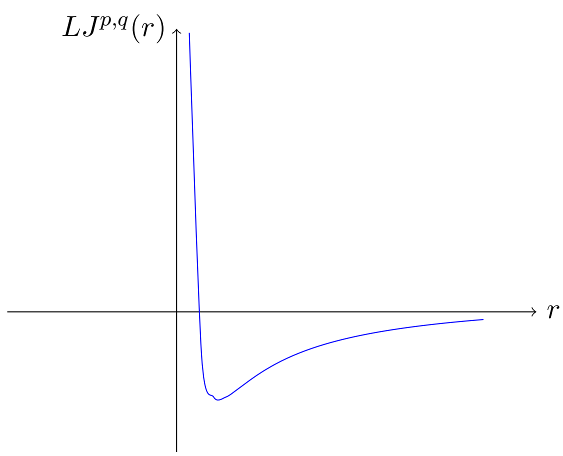

Figure 1. The function $r \to V(r)$

We will often refer to $x \in X$ as a particle, moreover from now on $N \in \mathbb{N}$ will be the number of particles, that is $N = \#X$.

Given $X = \{x_1, \dots, x_N\} \subset \mathbb{R}$, we define

$$\mathcal{E}_p(X) := \sum_{i,j \in \{1,\dots,N\},\, i<j} \frac{1}{|x_i - x_j|^p}, \quad \mathcal{E}_q(X) := \sum_{i,j \in \{1,\dots,N\},\, i<j} \frac{1}{|x_i - x_j|^q}; \tag{2.3}$$

then

$$\mathcal{E}(X) = \mathcal{E}_p(X) - \mathcal{E}_q(X). \tag{2.4}$$

It is also convenient to introduce the energies per particle

$$e_p(x_i) := \sum_{x_j \neq x_i} \frac{1}{|x_i - x_j|^p}, \quad e_q(x_i) := \sum_{x_j \neq x_i} \frac{1}{|x_i - x_j|^q}, \quad e_{p,q}(x_i) := e_p(x_i) - e_q(x_i)\,. \tag{2.5}$$

so that

$$\mathcal{E}_p(X) = \frac{1}{2}\sum_{i=1}^N e_p(x_i), \qquad \mathcal{E}_q(X) = \frac{1}{2}\sum_{i=1}^N e_q(x_i), \qquad \mathcal{E}(X) = \frac{1}{2}\sum_{i=1}^N e_{p,q}(x_i)\,. \tag{2.6}$$

As we will see, natural scaling quantities are given by

$$r_N := N^{\frac{q-1}{p-q}},\; R_N := N^{\frac{p-1}{p-q}},\; \overline{e}_N := N^{\frac{p(1-q)}{p-q}},\; e_N := N^{\frac{2p-pq-q}{p-q}}, \quad \text{for all } N \in \mathbb{N}. \tag{2.7}$$

Here r_N represents the typical distance between particles, R_N the total length of the chain of particles, e_N the order of the total energy in terms of N, and $\overline{e}_N = N^{-1}e_N$ the order of the average energy per particle. For every $N \in \mathbb{N}$, the corresponding scaled energy $\mathcal{E}_N(X)$ is defined as

$$\mathcal{E}_N(X) := \frac{\mathcal{E}(X)}{e_N}$$

where X is any finite subset of $\mathbb{R}$ with cardinality equal to N.

We denote by $\mathcal{M}_b(\mathbb{R})$ the class of bounded Radon Measures on $\mathbb{R}$. Now, we recall the tight convergence of a sequence of measures.

Definition 2.1 (Tight convergence)**.** We say that $\{\mu_N\}_{N\in\mathbb{N}} \subset \mathcal{M}_b(\mathbb{R})$ tightly converges to $\mu \in \mathcal{M}_b(\mathbb{R})$, if $\mu_N \overset{*}{\rightharpoonup} \mu$ and $\mu_N(\mathbb{R}) \to \mu(\mathbb{R})$, as $N \to +\infty$. We write $\mu_N \overset{t}{\to} \mu$ if $\{\mu_N\}_{N\in\mathbb{N}}$ tightly converges to μ.

We consider the space $\mathcal{M}_b(\mathbb{R})$ endowed by the following law of convergence.

Definition 2.2 (Law of convergence)**.** Let $\{\mu_N\}_{N\in\mathbb{N}} \subset \mathcal{M}_b(\mathbb{R})$ and $\mu \in \mathcal{M}_b(\mathbb{R})$; we say that $\mu_N \overset{L}{\to} \mu$ as $N \to +\infty$, if and only if

$$\hat{\mu}_N \to \mu, \text{ as } N \to +\infty, \text{ in the tight topology of } \mathcal{M}_b(\mathbb{R}),$$

where $\hat{\mu}_N \in \mathcal{M}_b(\mathbb{R})$ are defined by

$$\hat{\mu}_N(A) := \frac{1}{N}\mu_N\left(R_N A\right), \text{ for all borel set } A, \tag{2.8}$$

for $R_N = N^{\frac{p-1}{p-q}}$ introduced in (2.7).

Definition 2.3. We introduce the space of the empirical measures as follows

$$\mathcal{EM} := \left\{ \sum_{i=1}^N \delta_{x_i} \;:\; N \in \mathbb{N},\; x_i \neq x_j \text{ for all } i \neq j \right\} \subset \mathcal{M}_b(\mathbb{R}).$$

Moreover, given $N \in \mathbb{N}$ we define the set $\mathcal{EM}_N \subset \mathcal{EM}$ as

$$\mathcal{EM}_N := \{\mu \in \mathcal{EM} \ : \mu(\mathbb{R}) = N\}\,.$$

Clearly, there is a one to one correspondence, that we denote with $\mathcal{A}$, between the finite subsets of $\mathbb{R}$ with cardinality N and the set $\mathcal{EM}_N$. We introduce the functionals $E_N : \ \mathcal{M}_b(\mathbb{R}) \to \mathbb{R} \cup \{+\infty\}$ as follows

$$E_N(\mu) := \begin{cases} \mathcal{E}_N(\mathcal{A}(\mu)) & \text{for } \mu \in \mathcal{EM}_N\,, \\ +\infty & \text{for } \mu \in \mathcal{M}_b(\mathbb{R}) \setminus \mathcal{EM}_N\,. \end{cases} \tag{2.9}$$

We define also

$$E(\mu) := \mathcal{E}(\mathcal{A}(\mu)), \quad E_p(\mu) := \mathcal{E}_p(\mathcal{A}(\mu)), \quad E_q(\mu) := \mathcal{E}_q(\mathcal{A}(\mu)), \text{ for all } \mu \in \mathcal{EM}(\mathbb{R}),$$
$$E(\mu) := +\infty, \quad E_p(\mu) := +\infty, \quad E_q(\mu) := +\infty, \text{ for all } \mu \in \mathcal{M}_b(\mathbb{R}) \setminus \mathcal{EM}(\mathbb{R}).$$

We notice the following rescaling formula:

$$\frac{E_q(\mu_N)}{e_N} = E_q(\hat{\mu}_N) \tag{2.10}$$

which holds since $e_N = N^2(R_N)^{-q}$.

We are in a position to provide the Γ-convergence result for the functionals E_N, as $N \to +\infty$, where E_N is defined in (2.9). First, we introduce the candidate Γ-limit $F : \mathcal{M}_b(\mathbb{R}) \to \mathbb{R}\cup\{+\infty\}$ defined as

(2.11)

$$F(\mu) := \begin{cases} \zeta(p) \displaystyle\int_{\mathbb{R}} f(x)^{p+1}\,\mathrm{d}x - \frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{|x-y|^q} f(x)f(y)\,\mathrm{d}x\,\mathrm{d}y & \text{for } \mu = f\mathcal{L}^1 \in \mathfrak{D}(F)\,, \\ +\infty & \text{for } \mu \in \mathcal{M}_b(\mathbb{R}) \setminus \mathfrak{D}(F)\,, \end{cases}$$

where the set $\mathfrak{D}(F) \subset \mathcal{M}_b(\mathbb{R})$ is defined by

$$\mathfrak{D}(F) = \left\{\mu \in \mathcal{M}_b(\mathbb{R}) : \ \mu = f\mathcal{L}^1, f \in L^{p+1}(\mathbb{R}),\ f(x) \geq 0 \ \text{ a.e.}, \ \int_{\mathbb{R}} f(x)\,\mathrm{d}x = 1 \right\}, \tag{2.12}$$

and $\zeta(p) := \sum_{n=1}^{\infty} \frac{1}{n^p}$ is the Riemann zeta function evaluated at p.

Theorem 2.4. *The following Γ-convergence result holds true.*

(i) *(Compactness) Let $U \subset \mathbb{R}$ be an open bounded set and let $\{\mu_N\}_{N\in\mathbb{N}} \subset \mathcal{M}_b(\mathbb{R})$ be such that $\operatorname{supp}(\hat{\mu}_N) \subset U$, $\mu_N \in \mathcal{EM}_N$ for every $N \in \mathbb{N}$ and*

$$E_N(\mu_N) \leq M \quad \text{for every } N \in \mathbb{N}, \tag{2.13}$$

for some constant M independent of N. Then, up to a subsequence, $\mu_N \stackrel{L}{\to} \mu \in \mathcal{M}_b(\mathbb{R})$ and $\mu \in \mathfrak{D}(F)$, where $\mathfrak{D}(F)$ is the set defined in (2.12).

(ii) *(Lower bound) Let $\mu \in \mathcal{M}_b(\mathbb{R})$. For every $\{\mu_N\}_{N\in\mathbb{N}} \subset \mathcal{M}_b(\mathbb{R})$ with $\mu_N \stackrel{L}{\to} \mu$ it holds*

$$F(\mu) \leq \liminf_{N\to+\infty} E_N(\mu_N). \tag{2.14}$$

(iii) *(Upper bound) For every $\mu \in \mathcal{M}_b(\mathbb{R})$ there exists $\{\mu_N\}_{N\in\mathbb{N}} \subset \mathcal{M}_b(\mathbb{R})$ such that $\mu_N \stackrel{L}{\to} \mu$ and*

$$F(\mu) \geq \limsup_{N\to+\infty} E_N(\mu_N)\,. \tag{2.15}$$

In order to give a detailed description of this Theorem, we will divide the proof in different sections.

3. Compactness

In this section we prove that sequences of discrete measures μ_N with bounded energy $E_N(\mu_N)$ converge, up to subsequences, to absolutely continuous measures with density in L^{p+1}.

We start by estimating the energy per particle for a pair having minimal distance in a given configuration of $\tilde{N} \le N$ particles.

Lemma 3.1. *Let $\tilde{N}$, $N \in \mathbb{N}$ with $\tilde{N} \le N$ and let $X = \{x_1, \dots, x_{\tilde{N}}\} \subset \mathbb{R}^{\tilde{N}}$. Moreover, let $i \in \{1, \dots \tilde{N}-1\}$ be such that $r := x_{i+1} - x_i = \min\{x_{j+1} - x_j\}$. Then, $e_{p,q}(x_i) \ge \frac{1}{r^p} - \frac{2N^{1-q}}{1-q}\frac{1}{r^q}$.*

In particular, for all $\delta > 0$ small enough (depending only on p and q), if $r \le \delta r_N$ we have $e_{p,q}(x_i) \ge (\delta^{-p} - \frac{2}{1-q}\delta^{-q}) r_N^{-p}$, where r_N is defined in (2.7)*.*

Proof. Let Y be a configuration with $2\tilde{N}+1$ r-equispaced points. Then we have $e_p(x_i) \ge r^{-p}$, while

$$e_q(x_i) \le e_q(y_{\tilde{N}+1}) \le 2r^{-q} \sum_{i=1}^{\tilde{N}} i^{-q} \le 2r^{-q} \int_0^{\tilde{N}} t^{-q}\, dt = \frac{2}{(1-q)} \tilde{N}^{1-q} r^{-q}. \tag{3.1}$$

We conclude that

$$e_{p,q}(x_i) \ge r^{-p} - \frac{2}{1-q} \tilde{N}^{1-q} r^{-q} \ge r^{-p} - \frac{2}{1-q} N^{1-q} r^{-q}. \tag{3.2}$$

The last part of the statement follows by first applying the above estimate for $r = \delta r_N$ (notice that $N^{1-q} r_N^{-q} = r_N^{-p}$), and than observing that, for δ small enough, the quantity $(\delta^{-p} - \frac{2}{1-q}\delta^{-q})$ increases as δ decreases. $\square$

Proof of Theorem 2.4 (i). Step 1. We claim that for every δ small enough (depending only on p and q) there are k_N particles $x_{\bar{\imath}_1}, x_{\bar{\imath}_2}, \dots, x_{\bar{\imath}_{k_N}}$ with $k_N \le 4\delta^p(M + \frac{2}{1-q})N$ such that, for $C_{N-k_N} := \operatorname{supp} \mu_N \setminus \{x_{\bar{\imath}_1}, \dots, x_{\bar{\imath}_{k_N}}\}$, it holds that

$$\min_{i \ne j \in C_{N-k_N}} |x_i - x_j| > \delta r_N, \tag{3.3}$$

where M is the upper bound for the energies in (2.13). Let us denote $\Delta_{i,N} := |x_{i+1} - x_i|$ for all i, and let $\bar{\imath}_1$ be such that

$$\Delta_{\bar{\imath}_1,N} = \min_{1 \le i \le N} \Delta_{i,N} :$$

then, for the configuration $C_{N-1} := \operatorname{supp} \mu_N \setminus \{x_{\bar{\imath}_1}\}$,

$$2\mathcal{E}(X) = e_{p,q}(x_{\bar{\imath}_1}) + 2\mathcal{E}(C_{N-1})\,. \tag{3.4}$$

If $\Delta_{\bar{\imath}_1,N} \le \delta r_N$ then (3.4) and Lemma 3.1 give that (for δ small enough)

$$\mathcal{E}(X) \ge \frac{\delta^{-p}}{2} r_N^{-p} + \mathcal{E}(C_{N-1}).$$

Let now $\bar{\imath}_2$ be such that $\Delta_{\bar{\imath}_2,N}$ is the minimal distance between particles in C_{N-2}. Therefore, for $C_{N-2} := \{x_i\}_{i \notin \{\bar{\imath}_1, \bar{\imath}_2\}} = C_{N-1} \setminus \{x_{\bar{\imath}_2}\}$ we have

$$\mathcal{E}(X) \ge \frac{1}{2}(\delta r_N)^{-p} + \mathcal{E}(C_{N-1}) \ge 2\frac{1}{2}(\delta r_N)^{-p} + \mathcal{E}(C_{N-2}).$$

We may iterate this procedure until the ${k_N}^{th}$ step (with $0 \le k_N \le N-1$) when we find a configuration for which all the relative distances between particles are larger than δr_N. Recalling also the estimate (3.1), we have that

$$\begin{aligned}(3.5)\quad \frac{M\,N}{r_N^p} &\ge \mathcal{E}(X) \ge \frac{k_N}{4}(\delta r_N)^{-p} + \mathcal{E}(C_{N-k_N}) \\ &\ge \frac{k_N}{4}(\delta r_N)^{-p} - \mathcal{E}_q(C_{N-k_N}) \ge \frac{k_N}{4}(\delta r_N)^{-p} - \frac{2}{1-q}(\delta r_N)^{-q}(N-k_N)^{1-q} \\ &\ge \frac{k_N}{4}(\delta r_N)^{-p} - \frac{2}{1-q}\frac{N}{r_N^p}.\end{aligned}$$

For δ small enough we deduce that

$$\frac{k_N}{4}(\delta r_N)^{-p} \le \frac{(M+\frac{2}{1-q})\,N}{r_N^p}\,,$$

that is,

$$k_N \le 4\delta^p(M+\frac{2}{1-q})N. \tag{3.6}$$

Step 2. Since $|\hat\mu_N|(\mathbb{R}) = 1$ and $\mathrm{supp}(\hat\mu_N) \subset U$, up to a subsequence we have $\mu_N \overset{L}{\to} \mu$ for some $\mu \in \mathcal{M}_b(\mathbb{R})$ with $|\mu|(\mathbb{R}) = 1$. We have to prove that the limit measure μ is absolutely continuous with respect to the Lebesgue measure $\mathcal{L}^1$.
Let us fix $\delta > 0$ and consider the splitting

$$\mu_N = \mu^1_{N,\delta} + \mu^2_{N,\delta}, \qquad \mu^1_{N,\delta} := \mu_N \llcorner_{\{x_{\bar\imath_1},\dots,x_{\bar\imath_{k_N}}\}}, \quad \mu^2_{N,\delta} := \mu_N \llcorner_{C_{N-k_N}}, \tag{3.7}$$

where $\{x_{\bar\imath_1},\dots,x_{\bar\imath_k}\}$ have been constructed in Step 1. Moreover, let $\hat\mu^i_{N,\delta}$ be defined (according with 2.8) by $\hat\mu^i_{N,\delta}(A) := \frac{1}{N}\mu^i_{N,\delta}(R_N A)$ for every Borel set $A \subset \mathbb{R}$.

Since $\hat\mu_N \overset{t}{\to} \mu$, it easily follows that, up to a subsequence, $\hat\mu^i_{N,\delta} \overset{t}{\to} \mu^i_\delta$ for suitable nonnegative measures μ^1_δ, μ^2_δ.

By (3.3) we have that for every interval $I \subset \mathbb{R}$

$$\mu^2_{N,\delta}(R_N I) \le \frac{R_N|I|}{r_N\delta} + 1 = \frac{N|I|}{\delta} + 1 \tag{3.8}$$

and hence $\hat\mu^2_{N,\delta}(I) \le \frac{1}{\delta}|I| + \frac{1}{N}$. Then $\mu^2_\delta(I) \le \frac{1}{\delta}|I|$ for any interval $I \subset \mathbb{R}$ so that $\mu^2_\delta = f_\delta\mathcal{L}^1$, for a suitable $f_\delta \in L^\infty(U)$ with $\|f_\delta\|_\infty \le \frac{1}{\delta}$. Moreover, by (3.6) we have

$$\hat\mu^1_{N,\delta}(\mathbb{R}) = \frac{\mu^1_{N,\delta}(\mathbb{R})}{N} \le 2\delta^p(M+\frac{2}{1-q}), \qquad \mu^1_\delta(\mathbb{R}) = \lim_{N\to+\infty}\hat\mu^1_{N,\delta}(\mathbb{R}) \le 2\delta^p(M+\frac{2}{1-q}). \tag{3.9}$$

We further notice that we may assume that $\mu^2_{N,\delta_2} \ge \mu^2_{N,\delta_1}$ for any $\delta_2 < \delta_1$ (in the construction in Step 1 we pick the same particles for δ_2 and δ_1 but the procedure ends before for δ_2, then $\mu^1_{N,\delta_2} \le \mu^1_{N,\delta_1}$), so that $\mu^2_{\delta_2} \ge \mu^2_{\delta_1}$ and $f_{\delta_2} \ge f_{\delta_1}$ for every $\delta_2 < \delta_1$; then f_δ converges pointwise to a function f; since by (3.9) $\mu^1_\delta(\mathbb{R}) \to 0$ as $\delta \to 0$, by Monotone Convergence Theorem we have

$$\mu = \lim_{\delta\to0}\mu^1_\delta + \mu^2_\delta = \lim_{\delta\to0}\mu^2_\delta = f\mathcal{L}^1\,.$$

Step 3. We have to show that $f \in L^{p+1}$, so that $\mu \in \mathfrak{D}(F)$. This is in fact a consequence of the proof of the Γ-liminf inequality; for the reader's convenience we anticipate here the main estimates providing the desired summability property of f. By (4.15) below we have that, given $\varepsilon \in (0,1)$ and δ small enough,

$$E_N(\mu_N) \geq (1-\varepsilon)E_N^p(\mu_N) - E_N^q(\mu_{N,\delta}^2)$$

where $\mu_{N,\delta}^2$ is a suitable sequence of measures. By (4.16) we have $\liminf_N -E_N^q(\mu_{N,\delta}^2) =: C > -\infty$, while by (4.1) $\liminf E_N^p(\mu_N) \geq \zeta(p)\|f\|_{L^{p+1}}^{p+1}$. Therefore,

$$M \geq \liminf_N E_N(\mu_N) \geq \liminf_N (1-\varepsilon)E_N^p(\mu_N) - E_N^q(\mu_{N,\delta}^2) \geq (1-\varepsilon)\zeta(p)\|f\|_{L^{p+1}}^{p+1} - C,$$

so that $f \in L^{p+1}$. □

4. Γ-liminf inequality

Theorem 4.1. *Let $\{\mu_N\}_{N\in\mathbb{N}}$ be such that $\mu_N \in \mathcal{EM}_N$ for every $N \in \mathbb{N}$ and $\mu_N \overset{L}{\to} f\mathcal{L}^1$, with $f \in L^1$; then*

$$\liminf_{N\to+\infty} \frac{E_p(\mu_N)}{e_N} \geq \zeta(p) \int_{\mathbb{R}} f^{p+1}(x)\,\mathrm{d}x. \tag{4.1}$$

Proof. For any $L > 0$ we divide the interval $(-L, L)$ in $2L^2$ intervals $I_{k,L}$ of lenght L^{-1}; we denote by $m_{k,L}$ the average of f on $I_{k,L}$ and set $f_L := \sum_k m_{k,L}\chi_{I_{k,L}}$. We define $N_{k,L} := N\hat{\mu}_N(I_{k,L}) \in \mathbb{N}$ and we observe that

$$\lim_{N\to+\infty} \frac{N_{k,L}}{N} = \int_{I_{k,L}} f(x)\,\mathrm{d}x = \int_{I_{k,L}} f_L(x)\,\mathrm{d}x. \tag{4.2}$$

Let $\Delta_j^{k,i} := |x_{k,i} - x_{k,i+j}|$, where $x_{k,i}$ denotes the i^{th} particle in $I_{k,L}$, and let $\varphi : (0,+\infty) \to \mathbb{R}$ be the convex function $\varphi(x) := \frac{1}{x^p}$. By Jensen inequality, for all $I_{k,L}$ we have that

$$\frac{E_p(\mu_N \llcorner R_N I_{k,L})}{e_N} = \frac{1}{e_N}\sum_{j=1}^{N_{k,L}}\sum_{i=1}^{N_{k,L}-j} \varphi(\Delta_j^{k,i}) \geq \frac{1}{e_N}\sum_{j=1}^{N_{k,L}} (N_{k,L}-j)\varphi\left(\frac{\sum_i^{N_{k,L}-j}\Delta_j^{k,i}}{N_{k,L}-j}\right). \tag{4.3}$$

We observe that for all $I_{k,L}$ and for all $j \leq N_{k,L}$ we have

$$\sum_{i=1}^{N_{k,L}-j} \Delta_j^{k,i} \leq jR_N|I_{k,L}|. \tag{4.4}$$

Let $M \in \mathbb{N}$ be fixed and let $M_k := \min\{M, N_{k,L}\}$. By the formulas (4.3), (4.4) we have

$$\begin{aligned}\frac{E_p(\mu_N)}{e_N} &\geq \sum_{k=1}^{2L^2} \frac{E_p(\mu_N \llcorner R_N I_{k,L})}{e_N} \geq \frac{1}{e_N}\sum_{k=1}^{2L^2}\sum_{j=1}^{N_{k,L}} (N_{k,L}-j)\varphi\left(\frac{\sum_i^{N_{k,L}-j}\Delta_j^{k,i}}{N_{k,L}-j}\right)\\ &\geq \frac{1}{e_N}\sum_{k=1}^{2L^2}\sum_{j=1}^{N_{k,L}} (N_{k,L}-j)\varphi\left(\frac{jR_N|I_{k,L}|}{N_{k,L}-j}\right) \geq \frac{1}{e_N}\sum_{k=1}^{2L^2}\sum_{j=1}^{M_k} (N_{k,L}-j)\frac{(N_{k,L}-j)^p}{j^pR_N^p|I_{k,L}|^p}\\ &\geq \frac{1}{e_N}\sum_{k=1}^{2L^2}\sum_{j=1}^{M_k} (N_{k,L}-j)\frac{(N_{k,L}-M_k)^p}{j^pR_N^p|I_{k,L}|^p}.\end{aligned} \tag{4.5}$$

By (4.2), (4.5), since $e_N R_N^p = N^{p+1}$, and using also that, whenever $\int_{I_{k,L}} f > 0$, $M_k = M$ for N large enough, we have

$$\begin{aligned}\liminf_{N\to+\infty} \frac{E_p(\mu_N)}{e_N} &\geq \liminf_{N\to+\infty} \frac{1}{e_N} \sum_{k=1}^{2L^2} \sum_{j=1}^{M_k} (N_{k,L} - j) \frac{(N_{k,L} - M_k)^p}{j^p R_N^p |I_{k,L}|^p} \\ &= \sum_{j=1}^{M} \frac{1}{j^p} \sum_{k=1}^{2L^2} \left(\frac{1}{|I_{k,L}|} \int_{I_{k,L}} f_L(x) dx \right)^p \int_{I_{k,L}} f_L(x)\, \mathrm{d}x \\ &= \sum_{j=1}^{M} \frac{1}{j^p} \int_{\mathbb{R}} f_L^{p+1}(x)\, \mathrm{d}x.\end{aligned} \tag{4.6}$$

Then (4.1) follows by sending $L,\ M \to +\infty$, since $\sum_{j=1}^M \frac{1}{j^p} \to \zeta(p)$ as $M \to +\infty$ and $\int_{\mathbb{R}} f_L^{p+1}(x)\,\mathrm{d}x \to \int_{\mathbb{R}} f^{p+1}(x)\,\mathrm{d}x$ as $L \to +\infty$ (where $\int_{\mathbb{R}} f^{p+1}(x)\,\mathrm{d}x = +\infty$ whenever $f \notin L^{p+1}$). □

For all $R > 0$ we define the set

$$D(R) := \left\{ (x, y) \in \mathbb{R}^2 : 0 < |x - y| < R \right\}. \tag{4.7}$$

Lemma 4.2. *Let $\delta > 0$ and for all $N \in \mathbb{N}$ let $\nu_N := \sum_{i=1}^{\tilde{N}} \delta_{x_i}$ be such that $\tilde{N} \leq N$, $|x_i - x_j| \geq \frac{\delta}{N}$ for every $i \neq j$ and $\frac{1}{N}\nu_N \xrightarrow{t} f\mathcal{L}^1$ as $N \to +\infty$. Then*

$$\lim_{N\to+\infty} \int_{\mathbb{R}^2} \frac{1}{N^2 |x - y|^q}\, \mathrm{d}(\nu_N \otimes \nu_N) = \int_{\mathbb{R}^2} \frac{f(x) f(y)}{|x - y|^q}\, \mathrm{d}x\, \mathrm{d}y. \tag{4.8}$$

Proof. Since $\frac{1}{N}\nu_N \xrightarrow{t} f\mathcal{L}^1$, it holds that

$$\frac{1}{N}\nu_N \otimes \frac{1}{N}\nu_N = \sum_{i,\, j} \frac{1}{N}\delta_{x_i} \otimes \frac{1}{N}\delta_{x_j} \xrightarrow{t} f(x) f(y) \mathcal{L}^2 \tag{4.9}$$

as $N \to +\infty$, in $\mathcal{M}_b(\mathbb{R}^2)$. Since for every $x_i \neq x_j \in \operatorname{supp} \nu_N$ it holds $|x_i - x_j| > \frac{\delta}{N}$, then for every $x \in (x_i - \frac{\delta}{3N}, x_i + \frac{\delta}{3N})$ and $y \in (x_j - \frac{\delta}{3N}, x_j + \frac{\delta}{3N})$ we have $|x - y| \leq |x_i - x_j| + \frac{2\delta}{3N} < 2|x_i - x_j|$, so that

$$\frac{1}{|x_i - x_j|^q} \frac{1}{N^2} \leq 2^q \left(\frac{3}{2\delta}\right)^2 \int_{(x_i - \frac{\delta}{3N}, x_i + \frac{\delta}{3N})} \int_{(x_j - \frac{\delta}{3N}, x_j + \frac{\delta}{3N})} \frac{1}{|x - y|^q}\, \mathrm{d}x\, \mathrm{d}y.$$

Summing over the pairs $(x_i, x_j) \in D(R)$ the above inequality, we obtain that for every fixed $\varepsilon > 0$, for R small enough (depending only on ε and δ) and N large enough

(4.10)

$$\begin{aligned}\int_{D(R)} \frac{1}{N^2 |x - y|^q}\, \mathrm{d}(\nu_N \otimes \nu_N) &\leq 2^q \left(\frac{3}{2\delta}\right)^2 \sum_{i=1}^{\tilde{N}} \int_{x_i - \frac{\delta}{3N}}^{x_i + \frac{\delta}{3N}} \mathrm{d}x \sum_{|x_j - x_i| \leq R} \int_{x_j - \frac{\delta}{3N}}^{x_j + \frac{\delta}{3N}} \frac{1}{|x - y|^q}\, \mathrm{d}y \\ &\leq 2^q \left(\frac{3}{2\delta}\right)^2 \sum_{i=1}^{\tilde{N}} \int_{x_i - \frac{\delta}{3N}}^{x_i + \frac{\delta}{3N}} \mathrm{d}x \int_{x-2R}^{x+2R} \frac{1}{|x - y|^q}\, \mathrm{d}y \leq \varepsilon\,.\end{aligned}$$

Moreover, arguing as in the compactness proof (see also (4.14) below) we easily deduce that $\|f\|_{L^\infty} \leq \frac{2}{\delta}$; therefore, again for R small enough (actually for the same choice of R as before) we also have

$$\int_{D(R)} \frac{f(x)f(y)}{|x-y|^q}\,\mathrm{d}x\,\mathrm{d}y \leq \varepsilon. \tag{4.11}$$

On the other hand, using that $(x,y) \mapsto \frac{\chi_{\mathbb{R}^2\setminus D(R)}}{|x-y|^q} \in C_b(\mathbb{R}^2 \setminus D(R))$, by (4.9) we deduce that

$$\lim_{N\to+\infty} \int_{\mathbb{R}^2\setminus D(R)} \frac{1}{N^2|x-y|^q}\,\mathrm{d}(\nu_N \otimes \nu_N) = \int_{\mathbb{R}^2\setminus D(R)} \frac{f(x)f(y)}{|x-y|^q}\,\mathrm{d}x\,\mathrm{d}y. \tag{4.12}$$

By (4.10), (4.11), and (4.12), in view of the arbitrariness of ε, (4.8) follows. □

We are now in condition to prove the Γ-liminf inequality for the energy E_N.

Proof of Theorem 2.4 (ii). Fix $\varepsilon > 0$ and let $V_\varepsilon(t) := \varepsilon t^{-p} - t^{-q}$.
Step 1. For $\delta > 0$ small enough, we may split μ_N as $\mu_N = \mu^1_{N,\delta} + \mu^2_{N,\delta}$, as in (3.7) in such a way that

$$|x_i - x_j| \geq \delta r_N \quad \text{for every } x_i \neq x_j \in \operatorname{supp} \mu^2_{N,\delta}. \tag{4.13}$$

Notice that (4.13) implies

$$\hat{\mu}^2_{N,\delta}(I) \leq \frac{2}{\delta}|I| \quad \text{for every interval } I \subset U. \tag{4.14}$$

Let $x \in \mu^1_{N,\delta}$ and let $e^\varepsilon_{p,q}(x)$ be its energy corresponding to the potential V_ε. Then, recalling (3.2) we have that, for δ small enough and $r < \delta r_N$

$$e^\varepsilon_{p,q}(x_i) \geq \varepsilon r^{-p} - \frac{2}{1-q}\tilde{N}^{1-q} r^{-q} \geq \varepsilon r^{-p} - \frac{2}{1-q} N^{1-q} r^{-q} \geq 0.$$

This gives that

$$E_N(\mu_N) \geq (1-\varepsilon) E^p_N(\mu_N) - E^q_N(\mu^2_{N,\delta})\,. \tag{4.15}$$

Step 2- Conclusion. By (4.13) we may apply Lemma 4.2 with the measures ν_N replaced by the measures $\hat{\mu}^2_{N,\delta}$, defined as $\hat{\mu}^2_{N,\delta}(A) := \mu^2_{N,\delta}(R_N A)$ for all $A \subset \mathbb{R}$ Borel.

Up to a subsequence, $\hat{\mu}^2_{N,\delta} \xrightarrow{t} f^2_\delta \mathcal{L}^1$ as $N \to +\infty$ for some $f^2_\delta \in \mathrm{L}^\infty$. Therefore, in view of (4.8) (and recalling also (2.10)) we get

$$\lim_{N\to+\infty} E^q_N(\mu^2_{N,\delta}) = \lim_{N\to+\infty} \int_{\mathbb{R}^2} \frac{1}{|x-y|^q}\,\mathrm{d}\hat{\mu}^2_{N,\delta} = \int_{\mathbb{R}^2} \frac{f^2_\delta(x) f^2_\delta(y)}{|x-y|^q}\,\mathrm{d}x\,\mathrm{d}y\,. \tag{4.16}$$

By (4.15), exploiting (4.1) in Theorem 4.1 and using (4.16) we obtain

$$\liminf_{N\to+\infty} E_N(\mu_N) \geq (1-\varepsilon) \int_{\mathbb{R}} f^{p+1}\,\mathrm{d}x - \int_{\mathbb{R}^2} \frac{f^2_\delta(x) f^2_\delta(y)}{|x-y|^q}\,\mathrm{d}x\,\mathrm{d}y \tag{4.17}$$

As in the proof of the compactness property, we may assume that f_δ monotonically converges to f as $\delta \to 0$. Therefore, passing in the limit as ε, $\delta \to 0$ in (4.17), in view of the monotone convergence theorem, we deduce the Γ-liminf inequality (2.14). □

5. $\Gamma - \limsup$ INEQUALITY

In order to prove the $\Gamma - \limsup$ inequality, we treat separately the positive and the negative term of the energy. We start below with the positive term, for which we construct a recovery sequence that we adopt in the general construction. Indeed, for any sequence of measures converging with respect to $\stackrel{L}{\to}$, we have the right control for the lim sup of the negative part.

Lemma 5.1. *For every $\mu = f\mathcal{L}^1 \in \mathfrak{D}(F)$ there exists $\{\mu_N\}_{N\in\mathbb{N}} \subset \mathcal{M}_b(\mathbb{R})$ such that $\mu_N \stackrel{L}{\to} \mu$ and*

$$\limsup_{N\to+\infty} \frac{E_p(\mu_N)}{e_N} \le \zeta(p) \int_{\mathbb{R}} f(x)^{p+1}\,\mathrm{d}x. \tag{5.1}$$

Proof. By a standard diagonal argument in Γ-convergence we can assume $f = \sum_{i=1}^h a_i \chi_{I_i}$, where I_i are disjoint intervals. Consider the sets

$$X_{i,N} := \left(\frac{r_N}{a_i}\mathbb{N}\right) \cap R_N I_i, \qquad X_N = \bigcup_{i=1}^h X_{i,N},$$

and let $\tilde{\mu}_N$ be the corresponding empirical measures. Then, it is easy to see that $\tilde{\mu}_N \stackrel{L}{\to} f$. In particular, $\frac{|\tilde{\mu}_N|(\mathbb{R})}{N} \to 1$ as $N \to +\infty$. Moreover (let us denote $X_{i,N}$ by X_i below, for shortness), for $\gamma := \min_{i\neq j} \operatorname{dist}(I_i, I_j)$, for any $x_i \in X_i$ and $x_j \in X_j$ it holds $|x_i - x_j| \ge R_N\gamma$. Therefore, for N large enough

$$\sum_{i\neq j} \sum_{x_k\in X_i,\, y_l\in X_j} \frac{1}{|x_k - y_l|^p} \le \frac{2N^2}{R_N^p \gamma^p},$$

and then, using that $e_N R_N^p = N^{1+p}$ and $p > 1$ we have

$$\begin{aligned}
\lim_{N\to+\infty} \frac{E_p(\tilde{\mu}_N)}{e_N} &= \lim_{N\to+\infty} \frac{\sum_{i=1}^h \mathcal{E}_p(X_i)}{e_N} + \lim_{N\to+\infty} \frac{1}{e_N} \sum_{i\neq j} \sum_{x_k\in X_i,\, y_l\in X_j} \frac{1}{|x_k - y_l|^p} \\
&= \lim_{N\to+\infty} \frac{\sum_{i=1}^h \mathcal{E}_p(X_i)}{e_N}.
\end{aligned}$$

For every i, denoting $N_i := \#X_i$ and $X_i = \{y_1, \dots, y_{N_i}\}$, we compute

$$\mathcal{E}_p(X_i) = \sum_{k=1}^{N_i-1} \sum_{l=1}^{N_i-k} \frac{1}{|y_{l+k} - y_l|^p} = \sum_{k=1}^{N_i-1} \sum_{l=1}^{N_i-k} \frac{a_i^p}{r_N^p} \frac{1}{k^p} = \frac{a_i^p}{r_N^p} \sum_{k=1}^{N_i-1} \frac{N_i - k}{k^p}.$$

Therefore, using that $e_N = N r_N^{-p}$, we obtain

$$\begin{aligned}
\lim_{N\to+\infty} \frac{\sum_{i=1}^h \mathcal{E}_p(X_i)}{e_N} &= \sum_{i=1}^h a_i^p \lim_{N\to+\infty} \frac{1}{N} \sum_{k=1}^{N_i-1} \frac{N a_i |I_i| - k}{k^p} \\
&\le \zeta(p) \sum_{i=1}^h a_i^{p+1} |I_i| = \zeta(p) \|f\|_{L^{p+1}}.
\end{aligned}$$

We have proved that $\tilde{\mu}_N$ satisfies (5.1). Now, it remains to slightly modify $\tilde{\mu}_N$ in order to obtain a sequence μ_N that still satisfies (5.1), and such that $|\mu_N|(\mathbb{R}) = N$. This can be easily done either by removing few particles from $\tilde{\mu}_N$ (and auch a modification decreases the energy), or adding few particles to $\tilde{\mu}_N$ (that, as long as the new particles are placed far enough from each other and from the particles of $\tilde{\mu}_N$, produces an increase of the energy as small as desired). □

Now we show the desired lim sup inequality for the negative part of the energy along any sequence of measures converging in the sense of Definition 2.2.

Proposition 5.2. *Let $\{\mu_N\}_{N\in\mathbb{N}} \subset \mathcal{M}_b(\mathbb{R})$ such that $\mu_N \in \mathcal{EM}_N$ for all $N \in \mathbb{N}$ and $\mu_N \overset{L}{\to} \mu \in \mathfrak{D}(F)$ as $N \to +\infty$, where $\mathfrak{D}(F)$ is defined in* (2.12)*. Then*

$$\limsup_{N\to+\infty} -\frac{E_q(\mu_N)}{e_N} \le -\frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{|x-y|^q}\,\mathrm{d}(\mu\otimes\mu).$$

Proof. Let $\hat{\mu}_N$ be as defined in (2.8) and let $\mu := f\mathcal{L}^1 \in \mathfrak{D}(F)$. Then, setting

$$\eta_N(A) := \hat{\mu}_N \otimes \hat{\mu}_N(A \setminus \{(x,y):\ x=y\}) \qquad \text{for all } A \in \mathcal{B}(\mathbb{R}^2),$$

it is easy to see that

$$\eta_N \overset{t}{\to} f\mathcal{L}^1 \otimes f\mathcal{L}^1 \qquad \text{as } N \to +\infty. \tag{5.2}$$

We can rewrite $\frac{E_q(\mu_N)}{e_N}$ by suitably rescaling, as follows:

$$\frac{E_q(\mu_N)}{e_N} = \frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{|x-y|^q}\,\mathrm{d}\eta_N\,. \tag{5.3}$$

Notice that the functional

$$\mu \mapsto \int_{\mathbb{R}^2} \frac{1}{|x-y|^q}\,d\mu = \sup_{M>0}\int_{\mathbb{R}^2} \min\{M, \frac{1}{|x-y|^q}\}\,\mathrm{d}\mu,$$

being the supremum over M of continuous functionals, is lower semicontinuous on the family $\mathcal{M}_b^+(\mathbb{R}^2)$ of positive finite measures on $\mathbb{R}^2$ with respect to the tight convergence.

Hence by (5.2) we deduce that

$$\int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{|x-y|^q} f(x)f(y)\,\mathrm{d}x\,\mathrm{d}y \le \liminf_{N\to+\infty}\int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{|x-y|^q}\,\mathrm{d}\eta_N. \tag{5.4}$$

We then conclude by (5.3) and (5.4). □

Corollary 5.3 (Variational characterization of the harmonic series)**.** *For $p > 1$*

$$\zeta(p) = \sum_{j=1}^{+\infty}\frac{1}{j^p} = \inf\left\{\liminf_{N\to+\infty}\frac{E_p(\mu_N)}{e_N}\,\middle|\, \mu_N \overset{L}{\to} \chi_{[0,1]}\mathcal{L}^1\right\}. \tag{5.5}$$

Proof. Theorem 4.1 implies the inequality

$$\zeta(p) \le \inf\left\{\liminf_{N\to+\infty}\frac{E_p(\mu_N)}{e_N}\,\middle|\, \mu_N \overset{L}{\to} \chi_{[0,1]}\mathcal{L}^1\right\}. \tag{5.6}$$

By Lemma 5.1 we get that there exists $\{\mu_N\}_{N\in\mathbb{N}} \subset \mathcal{M}_b(\mathbb{R})$ such that $\mu_N \in \mathcal{EM}_N$ for all $N \in \mathbb{N}$ with $\mu_N \overset{L}{\to} \chi_{[0,1]}\mathcal{L}^1$ and

$$\lim_{N\to+\infty}\frac{E_p(\mu_N)}{e_N} = \zeta(p)\int_{\mathbb{R}}\chi_{[0,1]}(x)\,\mathrm{d}x = \zeta(p). \tag{5.7}$$

Therefore by (5.6) and (5.7) we obtain (5.5). □

6. Asymptotic behavior of minimizers

In this section we discuss the asymptotic behavior of (quasi) minimizers of the energy functionals E_N. This analysis relies on the Γ-convergence analysis provided by Theorem 2.4 and on some compactness properties of quasi minimizers.

First, notice that Theorem 2.4 does not provide tight convergence for general sequences with bounded energy, but only for sequences with support contained in a given bounded open set U. In fact, one may easily construct measures μ_N with bounded energy such that $\mu_N(\cdot)$ and $\mu_N(\cdot - N)$ both converge in the sense of Definition 2.2 to some measures with positive mass. As a consequence of concentrated compactness arguments [5] we will see that tight convergence holds (up to a subsequence and up to translations) for quasi minimizers.

First, we will show that the Γ-limit F admits minimizers. In the following we will consider the functional F extended also to absolutely continuous measures $\mu = f\,\mathrm{d}x$ with $\int f(x)\,\mathrm{d}x = m$ with arbitrary mass $m \geq 0$.

Proposition 6.1. *For all $m > 0$ the functional F admits a minimizer among absolutely continuous measures $\mu = f\,\mathrm{d}x$ with $f \in L^{p+1}(\mathbb{R})$ and $\int f(x)\,\mathrm{d}x = m$. Moreover, denoted by $I(m)$ the corresponding minimal value we have that $I(m) < 0$ for all $m > 0$ and that I is strictly subadditive.*

Proof. The proof is done in [5]; for the reader convenience we check that the assumptions therein are satisfied.

Assumptions (10) and (11) in [5] are satisfied for $p > q$. Moreover,

$$I(m) \leq F\big(\frac{m}{l}\mathcal{L}^1 \llcorner_{[0,l]}\big) < 0 \qquad \text{for } l \text{ large enough},$$

so that $I(m) < 0$ for all $m > 0$. Furthermore (15) in [5] holds (with the parameter m there replaced by our parameter $q \in (0, 1)$). As a consequence the assumption (S.2), that is the strictly subadditivity of I is satisfied in view of Corollary II.1, and in turn F admits minimizers for any given positive mass $m > 0$. □

The compactness property for quasi minimizers also follows by concentrated compactness arguments in [5]; next Lemma, whose proof is left to the reader, describes in a convenient formalism for our purposes the so called vanishing vs concentration dichotomy in [5].

Lemma 6.2. *Let $\{\mu_N\}$ be a sequence of probability measures. Up to a (not relabeled) subsequence, there exist sequences of translations $\{\tau_{N,k}\}_{N,k\in\mathbb{N}}$ with $|\tau_{N,k_1} - \tau_{N,k_2}| \to +\infty$ as $N \to +\infty$ for all fixed $k_1 \neq k_2$, a sequence of measures $\{\nu_k\}_{k\in\mathbb{N}}$ and $m_v \in [0, 1]$ such that:*

- (a) *There exists open sets A_N such that $\mu_N(A_N) \to m_v$, and $\mu_N(A_N \cap B_1(x_N)) \to 0$ for every sequence $\{x_N\}_{N\in\mathbb{N}}$;*
- (b) *$\mu_N(\cdot - \tau_{N,k}) \to \nu_k$ tightly;*
- (c) *Setting $m_k := \nu_k(\mathbb{R})$ we have $m_{k+1} \leq m_k$ for all $k \in \mathbb{N}$ and $\sum_k m_k = 1 - m_v$.*

Notice that it is very easy to see that, for fixed $N \in \mathbb{N}$, there exists a minimizer μ_N of E_N. Next proposition establishes that any sequence of quasi minimizers (and in particular of minimizers) up to a subsequence and up to a translation converge in the sense of Definition 2.2 to some measure μ which is a minimizer of the Γ-limit F defined in (2.11).

Proposition 6.3. *Let μ_N be such that $E_N(\mu_N) - \inf E_N \to 0$. Then, up to a subsequence, there exists a sequence of translations $\{\tau_N\}$ such that $\hat{\mu}_N(\cdot - \tau_N) \stackrel{L}{\to} \mu(\cdot) \in \mathcal{M}_b(\mathbb{R})$ and*

$\mu \in \mathfrak{D}(F)$, where $\mathfrak{D}(F)$ is the set defined in (2.12). *Moreover, μ is a minimizer of the functional F defined in* (2.11).

Proof. Let $x_{i,N}$ be the particles in μ_N with $x_{i,N} < x_{i+1,N}$ for all $i = 1, \dots N-1$ and set $\Delta_{i,N} := x_{i+1,N} - x_{i,N}$. By Lemma 3.1, arguing similarly to the proof of Theorem 2.4 (i), and taking into account the quasi minimality of μ_N we deduce that there exists $\delta > 0$ such that $\Delta_{i,N} \geq \delta r_N$ for all but K_N indices i with $K_N/N \to 0$ as $N \to +\infty$. We can assume that $\Delta_{i,N} \geq \delta r_N$ for all $1 \leq i \leq N-1$. In fact, denoting by $\{y_j\}_{j=1}^{K_N}$ the K_N particles for which $\Delta_{i,N} \leq \delta r_N$, let us consider $\lambda_N := \mu_N - \sum_{j=1}^{K_N} \delta_{y_j} + \sum_{j=1}^{K_N} \delta_{z_j}$, where $\{z_j\}_{j=1}^{K_N}$ are very far apart one from each other and from the remaining particles $\{x_i\}_{i=1}^{N} \setminus \{y_j\}_{j=1}^{K_N}$. Since $K_N/N \to 0$, still $\hat{\lambda}_N \to \mu$ and, moreover, $E_N(\lambda_N) < E_N(\mu_N)$, being the energy per particle y_j positive and the energy per particle z_j arbitrarily close to 0 for z_j sufficiently far from the other particles.

Now we apply Lemma 6.2 with μ_N replaced by $\hat{\mu}_N$. Arguing as in the proof of the Γ-liminf inequality of Theorem 2.4 (and using also that the minimal distance between the particles of μ_N is larger than δr_N) one can prove that

$$\liminf_N E_N(\mu_N) \geq \sum_k F(\nu_k) \geq \sum_k I(m_k) \geq I(1 - m_v) \geq I(1),$$

where, in view of Proposition 6.1, the last two inequalities are strict whenever $m_1 < 1$ or $m_v > 0$. Therefore, we must have $m_1 = 1$ which is equivalent to the tight convergence (up to subsequences and up to a translation) of $\hat{\mu}_N$ to $\mu := \nu_1$.

The remaining statements are easy consequences of the Γ-convergence analysis already done to prove Theorem 2.4. □

In this paper we do not study in details minimizers of F, confining our interest to the fact that homogeneous states are not minimizers.

Proposition 6.4. *Any minimizer μ of F is not of the form $t\mathcal{L}^1 \llcorner_A$, $t > 0$, $A \in \mathcal{B}(\mathbb{R})$.*

Proof. Notice that, given $t > 0$, by Riesz rearrangement inequality

$$\inf_{A \in \mathcal{B}(\mathbb{R}) : |A| = t^{-1}} F(t\mathcal{L}^1 \llcorner_A) = t^p \zeta(p) - t^2 \sup_{A \in \mathcal{B}(\mathbb{R})} \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{\chi_A(x)\chi_A(y)}{|x-y|^q} \, \mathrm{d}x \, \mathrm{d}y = F(t\mathcal{L}^1 \llcorner_{[0,t^{-1}]}). \tag{6.1}$$

Then we compute the first variation of F at $\mu = f\mathcal{L}^1$ in the direction h, with $\int_{\mathbb{R}} h \, \mathrm{d}x = 0$:

$$F'(f\mathcal{L}^1)[h] = \lim_{\varepsilon \to 0} \frac{F(f+h) - F(f)}{\varepsilon} = (p+1) \int_{\mathbb{R}} f^p(x) \, h(x) \, \mathrm{d}x - \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{f(x)h(y)}{|x-y|^q} \, \mathrm{d}x \, \mathrm{d}y.$$

For $f = t\chi_{[0,t^{-1}]}$ we will show that there exists h such that $F'(f\mathcal{L}^1)[h] < 0$. To short notation we will fix $t = 1$.

$$F'(\mathcal{L}^1 \llcorner_{[0,1]})[h] = (p+1) \int_{[0,1]} h(x) \, \mathrm{d}x - \int_{\mathbb{R}} \int_{[0,1]} \frac{h(y)}{|x-y|^q} \, \mathrm{d}x \, \mathrm{d}y.$$

Let x_1, $x_2 \in (0,1)$ and let us consider

$$h_n := \frac{\chi_{[x_1 - \frac{1}{n}, x_1 + \frac{1}{n}]}}{2n} - \frac{\chi_{[x_2 - \frac{1}{n}, x_2 + \frac{1}{n}]}}{2n}.$$

We have that $\int_{\mathbb{R}} h_n \, \mathrm{d}x = 0$ and $h_n \xrightarrow{t} \delta_{x_1} - \delta_{x_2}$ so that, by standard properties of convolution, it holds

$$\lim_{n\to+\infty} F'(\mathcal{L}^1 \llcorner_{[0,1]})[h_n] = -\int_{[0,1]} \left(\frac{1}{|x-x_1|^q} - \frac{1}{|x-x_2|^q} \right) \mathrm{d}x.$$

For $x_1 = \frac{1}{2}$ and x_2 small enough we get

$$\lim_{n\to+\infty} F'(\mathcal{L}^1 \llcorner_{[0,1]})[h_n] < 0,$$

so $\mathcal{L}^1 \llcorner_{[0,1]}$ is not a minimizer for F. □

Remark 6.5. By Proposition 6.3 and Proposition 6.4 we deduce that, for the energy $\mathcal{E}$ defined in (2.1), crystallization in any reasonable sense does not hold. In fact, for N large enough, the density of a minimal in energy chain of particles is not uniform (being in fact maximal in the middle of the chain).

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