

# EXISTENCE OF MINIMIZERS OF NONLOCAL INTERACTION ENERGIES

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ABSTRACT. We investigate nonlocal-interaction energies on the space of probability measures. We establish sharp conditions for the existence of minimizers for a broad class of nonlocal-interaction energies. The condition is closely related to the notion of  $H$ -stability of pairwise interaction potentials in statistical mechanics. Our approach uses the direct method of calculus of variations.

## 1. INTRODUCTION

We consider the minimization of the nonlocal-interaction energy

$$(1.1) \quad E[\mu] := \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} w(x-y) d\mu(x) d\mu(y)$$

over the space of probability measures  $\mathcal{P}(\mathbb{R}^N)$ . Nonlocal-interaction energies arise naturally in descriptions of systems of interacting particles, as well as continuum descriptions of systems with long-range interactions. They play an important role in statistical mechanics [34, 36] and descriptions of crystallization [1, 33]. For semi-convex interaction potentials  $w$  some systems governed by the energy  $E$  can be interpreted as a gradient flow of the energy with respect to Wasserstein metric and satisfy the nonlocal-interaction equation

$$(1.2) \quad \frac{\partial \mu}{\partial t} = 2 \operatorname{div} (\mu(\nabla w * \mu)).$$

Applications of the equation include models of collective behavior of many-agent systems [6, 32], granular media [5, 18, 38], self-assembly of nanoparticles [25, 26], and molecular dynamics simulations of matter [24].

Although the choice of the interaction potential  $w$  depends on the phenomenon modeled by either (1.1) or (1.2), the interaction between two agents/particles is often determined only by the distance between them. This yields that the interaction potential  $w$  is radially symmetric, i.e.,  $w(x) = W(|x|)$  for some  $W : [0, +\infty) \rightarrow \mathbb{R} \cup \{+\infty\}$ . Many potentials considered in the applications are repulsive at short distances ( $W'(r) < 0$  for  $r$  small) and attractive at long distances ( $W'(r) > 0$  for  $r$  large). While purely attractive potentials lead to finite-time or infinite time blow up [7] the attractive-repulsive potentials often generate finite-sized, confined aggregations [23, 28, 30]. On the other hand in statistical mechanics and in studies of crystallization it is the (attractive-repulsive) potentials that do not lead to confined states as the number of particles increases which are of interest [34, 37]. This highlights the importance of obtaining

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criteria for existence of global minimizers of the energy, for it is precisely those potentials which have a global minimizer that exhibit aggregation of particles into dense clumps.

The study of the nonlocal-interaction equation (1.2) in terms of well-posedness, finite or infinite time blow-up, and long-time behavior has attracted the interest of many research groups in the recent years [3, 4, 7, 8, 9, 10, 16, 17, 21, 23, 27, 28, 29]. The energy (1.1) plays an important role in these studies as it governs the dynamics and as its (local) minima describe the long-time asymptotics of solutions. It has been observed that even for quite simple attractive–repulsive potentials the energy minimizers are sensitive to the precise form of the potential and can exhibit a wide variety of patterns [27, 28, 40]. In [2] Balagué, Carrillo, Laurent, and Raoul obtain conditions for the dimensionality of the support of local minimizers of (1.1) in terms of the repulsive strength of the potential  $w$  at the origin. Properties of minimizers for a special class of potentials which blow up approximately like the Newtonian potential at the origin have also been studied [9, 15, 22, 23]. Particularly relevant to our study are the results obtained by Choksi, Fetecau and one of the authors [19] on the existence of minimizers of interaction energies in a certain form. There the authors consider potentials of the power-law form,  $w(x) := |x|^a/a - |x|^r/r$ , for  $-N < r < a$ , and prove the existence of minimizers in the class of probability measures when the power of repulsion  $r$  is positive. When the interaction potential has a singularity at the origin, i.e., for  $r < 0$ , on the other hand, they establish the existence of minimizers of the interaction energy in a restrictive class of uniformly bounded, radially symmetric  $L^1$ -densities satisfying a given mass constraint. Carrillo, Chipot and Huang [14] also consider the minimization of nonlocal-interaction energies defined via power-law potentials and prove the existence of a global minimizer by using a discrete to continuum approach. The minimizers and their relevance to statistical mechanics were also considered in periodic setting (and on bounded sets) by Sütö [36].

Here (Theorems 3.1 and 3.2) we obtain criteria for the existence of minimizers in a very broad class of potentials. We employ the direct method of the calculus of variations. In Lemma 2.2 we establish the weak lower-semicontinuity of the energy with respect to weak convergence of measures. When the potential  $W$  grows unbounded at infinity (case treated in Theorem 3.1) this provides enough confinement for a minimizing sequence to ensure the existence of minimizers. If  $W$  asymptotes to a finite value (case treated in Theorem 3.2) then there is a delicate interplay between repulsion at some lengths (in most applications short lengths) and attraction at other length scales (typically long) which establishes whether the repulsion wins and a minimizing sequence spreads out indefinitely and “vanishes” or the minimizing sequence is compact and has a limit. We establish a simple, sharp condition, **(HE)** on the energy that characterizes whether a global minimizer exists. To establish compactness of a minimizing sequence we use Lions’ concentration compactness lemma.

The condition **(HE)** is closely related to the notion of stability (or  $H$ -stability) used in statistical mechanics [34]. Namely stability is a necessary condition for a many body system of interacting particles to exhibit a macroscopic thermodynamical behavior. As we show in Proposition 4.1 the condition **(HE)** is almost exactly the complement of  $H$ -stability. That is if the energy (1.1) admits a global minimizer then the system of interacting particles is not expected to have a thermodynamic limit.

While the conditions **(H1)** and **(H2)** are easy-to-check conditions on the potential  $W$  itself, the condition **(HE)** is a condition on the energy and it is not always easy to verify. Due to the above connection with statistical mechanics the conditions on  $H$ -stability (or lack thereof) can be used to verify if **(HE)** is satisfied for a particular potential. We list such conditions in

Section 4. However only few general conditions are available. It is an important open problem to establish a more complete characterization of potentials  $W$  which satisfy **(HE)**.

We finally remark that as this manuscript was being completed we learned that Cañizo, Carrillo, and Patacchini [12] independently and concurrently obtained very similar conditions for the existence of minimizers, which they also show to be compactly supported. The proofs however are quite different.

## 2. HYPOTHESES AND PRELIMINARIES

The interaction potentials we consider are radially symmetric, that is,  $w(x) = W(|x|)$  for some function  $W : [0, +\infty) \rightarrow \mathbb{R} \cup \{+\infty\}$ , and they satisfy the following basic properties:

- (H1)**  $W$  is lower-semicontinuous.
- (H2)** The function  $w(x)$  is locally integrable on  $\mathbb{R}^N$ .

Beyond the basic assumptions above, the behavior of the tail of  $W$  will play an important role. We consider potentials which have a limit at infinity. If the limit is finite we can add a constant to the potential, which does not affect the existence of minimizers, and assume that the limit is zero. If the limit is infinite the proof of existence of minimizers is simpler, while if the limit is finite an additional condition is needed. Thus we split the condition on behavior at infinity into two conditions:

- (H3a)**  $W(r) \rightarrow \infty$  as  $r \rightarrow \infty$ .
- (H3b)**  $W(r) \rightarrow 0$  as  $r \rightarrow \infty$ .

*Remark 2.1.* By the assumptions **(H1)** and **(H3a)** or **(H3b)** the interaction potential  $W$  is bounded from below. Hence

$$(2.1) \quad C_W := \inf_{r \in (0, \infty)} W(r) > -\infty.$$

If **(H3a)** holds, by adding  $-C_W$  to  $W$  from now on we assume that  $W(r) \geq 0$  for all  $r \in (0, \infty)$

As noted in the introduction the assumptions **(H1)**, **(H2)** with **(H3a)** or **(H3b)** allow us to handle a quite general class of interaction potentials  $w$ . Figure 1 illustrates a set of simple examples of smooth potential profiles  $W$  that satisfy these assumptions.

In order to establish the existence of a global minimizer of  $E$ , for interaction potentials  $w$  satisfying **(H1)**, **(H2)** and **(H3b)**, the following assumption on the interaction energy  $E$  is needed:

- (HE)** There exists a measure  $\bar{\mu} \in \mathcal{P}(\mathbb{R}^N)$  such that  $E[\bar{\mu}] \leq 0$ .

We establish that the conditions **(H1)**, **(H2)** and **(H3a)** or **(H3b)** imply the lower-semicontinuity of the energy with respect to weak convergence of measures. We recall that a sequence of probability measures  $\mu_n$  converges weakly to measure  $\mu$ , and we write  $\mu_n \rightharpoonup \mu$ , if for every bounded continuous function  $\phi \in C_b(\mathbb{R}^N, \mathbb{R})$

$$\int \phi d\mu_n \rightarrow \int \phi d\mu \quad \text{as } n \rightarrow \infty.$$

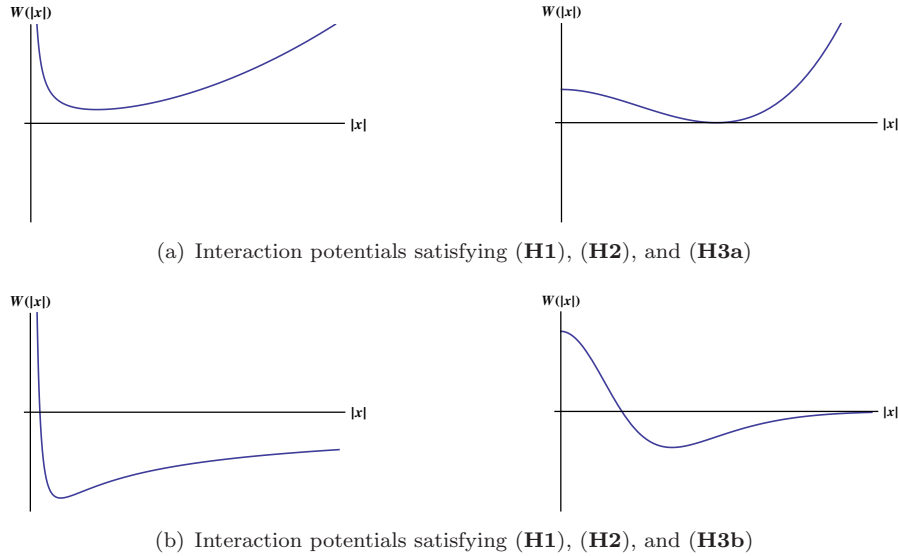


FIGURE 1. Generic examples of  $W(|x|)$ .

**Lemma 2.2** (Lower-semicontinuity of the energy). *Assume  $W : [0, \infty) \rightarrow (-\infty, \infty]$  is a lower-semicontinuous function bounded from below. Then the energy  $E : \mathcal{P}(\mathbb{R}^n) \rightarrow (-\infty, \infty]$  defined in (1.1) is weakly lower-semicontinuous with respect to weak convergence of measures.*

*Proof.* Let  $\mu_n$  be a sequence of probability measures such that  $\mu_n \rightharpoonup \mu$  as  $n \rightarrow \infty$ . Then  $\mu_n \times \mu_n \rightharpoonup \mu \times \mu$  in the set of probability measures on  $\mathbb{R}^N \times \mathbb{R}^N$ . If  $w$  is continuous and bounded

$$\int_{\mathbb{R}^N} \int_{\mathbb{R}^N} w(x-y) d\mu_n(x) d\mu_n(y) \longrightarrow \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} w(x-y) d\mu(x) d\mu(y) \quad \text{as } n \rightarrow \infty.$$

So, in fact, the energy is continuous with respect to weak convergence. On the other hand, if  $w$  is lower-semicontinuous and  $w$  is bounded from below then the weak lower-semicontinuity of the energy follows from the Portmanteau Theorem [39, Theorem 1.3.4].  $\square$

We remark that the assumption on boundedness from below is needed since if, for example,  $W(r) = -r$  then for  $\mu_n = (1 - \frac{1}{n})\delta_0 + \frac{1}{n}\delta_n$  the energy is  $E(\mu_n) = -1$  for all  $n \in \mathbb{N}$ , while  $\mu_n \rightharpoonup \delta_0$  which has energy  $E(\delta_0) = 0$ .

Finally, we state Lions' concentration compactness lemma for probability measures [31], [35, Section 4.3]. This lemma is the main tool in verifying that an energy-minimizing sequence is precompact in the sense of weak convergence of measures.

**Lemma 2.3** (Concentration-compactness lemma for measures). *Let  $\{\mu_n\}_{n \in \mathbb{N}}$  be a sequence of probability measures on  $\mathbb{R}^N$ . Then there exists a subsequence  $\{\mu_{n_k}\}_{k \in \mathbb{N}}$  satisfying one of the three following possibilities:*

- (i) (tightness up to translation) *There exists  $y_k \in \mathbb{R}^N$  such that for all  $\varepsilon > 0$  there exists  $R > 0$  with the property that*

$$\int_{B_R(y_k)} d\mu_{n_k}(x) \geq 1 - \varepsilon \quad \text{for all } k.$$

- (ii) (vanishing)  $\lim_{k \rightarrow \infty} \sup_{y \in \mathbb{R}^N} \int_{B_R(y)} d\mu_{n_k}(x) = 0$ , for all  $R > 0$ ;
- (iii) (dichotomy) *There exists  $\alpha \in (0, 1)$  such that for all  $\varepsilon > 0$ , there exist a number  $R > 0$  and a sequence  $\{x_k\}_{k \in \mathbb{N}} \subset \mathbb{R}^N$  with the following property:*

*Given any  $R' > R$  there are nonnegative measures  $\mu_k^1$  and  $\mu_k^2$  such that*

$$0 \leq \mu_k^1 + \mu_k^2 \leq \mu_{n_k},$$

$$\text{supp}(\mu_k^1) \subset B_R(x_k), \quad \text{supp}(\mu_k^2) \subset \mathbb{R}^N \setminus B_{R'}(x_k),$$

$$\limsup_{k \rightarrow \infty} \left( \left| \alpha - \int_{\mathbb{R}^N} d\mu_k^1(x) \right| + \left| (1 - \alpha) - \int_{\mathbb{R}^N} d\mu_k^2(x) \right| \right) \leq \varepsilon.$$

### 3. EXISTENCE OF MINIMIZERS

In this section we prove the existence of a global minimizer of  $E$ . We use the direct method of the calculus of variations and utilize Lemma 2.3 to eliminate the “vanishing” and “dichotomy” of an energy-minimizing sequence. The techniques in our proofs, though, depends on the behavior of the interaction potential at infinity. Thus we prove two existence theorems: one for potentials satisfying **(H3a)** and another one for those satisfying **(H3b)**.

**Theorem 3.1.** *Suppose  $W$  satisfies the assumptions **(H1)**, **(H2)** and **(H3a)**. Then the energy (1.1) admits a global minimizer in  $\mathcal{P}(\mathbb{R}^N)$ .*

*Proof.* Let  $\{\mu_n\}_{n \in \mathbb{N}}$  be a minimizing sequence, that is,  $\lim_{n \rightarrow \infty} E[\mu_n] = \inf_{\mu \in \mathcal{P}(\mathbb{R}^N)} E[\mu]$ .

Suppose  $\{\mu_k\}_{k \in \mathbb{N}}$  has a subsequence which “vanishes”. Since that subsequence is also a minimizing sequence we can assume that  $\{\mu_k\}_{k \in \mathbb{N}}$  vanishes. Then for any  $\varepsilon > 0$  and for any  $R > 0$  there exists  $K \in \mathbb{N}$  such that for all  $k > K$  and for all  $x \in \mathbb{R}^N$

$$\mu_k(\mathbb{R}^N \setminus B_R(x)) \geq 1 - \varepsilon.$$

This implies that for  $k > K$ ,

$$\iint_{|x-y| \geq R} d\mu_k(x) d\mu_k(y) = \int_{\mathbb{R}^N} \left( \int_{\mathbb{R}^N \setminus B_R(x)} d\mu_k(y) \right) d\mu_k(x) \geq 1 - \varepsilon.$$

Given  $M \in \mathbb{R}$ , by condition **(H3a)** there exists  $R > 0$  such that for all  $r \geq R$ ,  $W(r) \geq M$ . Consider  $\varepsilon \in (0, \frac{1}{2})$  and  $K$  corresponding to  $\varepsilon$  and  $R$ . Since  $W \geq 0$  by Remark 2.1,

$$\begin{aligned} E[\mu_k] &= \iint_{|x-y| \leq R} W(|x-y|) d\mu_k(x) d\mu_k(y) + \iint_{|x-y| \geq R} W(|x-y|) d\mu_k(x) d\mu_k(y) \\ &\geq \iint_{|x-y| \geq R} W(|x-y|) d\mu_k(x) d\mu_k(y) \\ &\geq (1 - \varepsilon)M. \end{aligned}$$

Letting  $M \rightarrow \infty$  implies  $E[\mu_k] \rightarrow \infty$ . This contradicts the fact that  $\mu_k$  is a subsequence of a minimizing sequence of  $E$ . Thus, “vanishing” does not occur.

Next we show that “dichotomy” is also not an option for a minimizing sequence. Suppose, that “dichotomy” occurs. As before we can assume that the subsequence along which

dichotomy occurs is the whole sequence. Let  $R$ , sequence  $x_k$  and measures

$$\mu_k^1 + \mu_k^2 \leq \mu_k.$$

be as defined in Lemma 2.3(ii). For any  $R' > R$ , using Remark 2.1, we obtain

$$\begin{aligned} \liminf_{k \rightarrow \infty} E[\mu_{n_k}] &\geq \liminf_{k \rightarrow \infty} \int_{B_R(x_{n_k})} \int_{B_{R'}^c(x_{n_k})} W(|x-y|) d\mu_k^2(x) d\mu_k^1(y) \\ &\geq \inf_{r \geq R'-R} W(r) \alpha(1-\alpha), \end{aligned}$$

where  $B_{R'}^c(x_{n_k})$  simply denotes  $\mathbb{R}^N \setminus B_{R'}(x_{n_k})$ .

By **(H3a)**, letting  $R' \rightarrow \infty$  yields that

$$\liminf_{k \rightarrow \infty} E[\mu_{n_k}] \geq \infty,$$

which contradicts the fact that  $\mu_k$  is an energy minimizing sequence.

Therefore “tightness up to translation” is the only possibility. Hence there exists  $y_k \in \mathbb{R}^N$  such that for all  $\varepsilon > 0$  there exists  $R > 0$  with the property that

$$\int_{B(y_k, R)} d\mu_{n_k}(x) \geq 1 - \varepsilon \quad \text{for all } k.$$

Let

$$\tilde{\mu}_{n_k} := \mu_{n_k}(\cdot - y_k).$$

Then the sequence of probability measures  $\{\tilde{\mu}_{n_k}\}_{k \in \mathbb{N}}$  is tight. Since the interaction energy is translation invariant we have that

$$E[\tilde{\mu}_{n_k}] = E[\mu_{n_k}].$$

Hence,  $\{\tilde{\mu}_{n_k}\}_{k \in \mathbb{N}}$  is also an energy-minimizing sequence. By the Prokhorov’s theorem (cf. [11, Theorem 4.1]) there exists a further subsequence of  $\{\tilde{\mu}_{n_k}\}_{k \in \mathbb{N}}$  which we still index by  $k$ , and a measure  $\mu_0 \in \mathcal{P}(\mathbb{R}^N)$  such that

$$\tilde{\mu}_{n_k} \rightharpoonup \mu_0$$

in  $\mathcal{P}(\mathbb{R}^N)$  as  $k \rightarrow \infty$ .

Since the energy is lower-semicontinuous with respect to weak convergence of measures, by Lemma 2.2, the measure  $\mu_0$  is a minimizer of  $E$ .  $\square$

The second existence theorem involves interaction potentials which vanish at infinity.

**Theorem 3.2.** *Suppose  $W$  satisfies the assumptions **(H1)**, **(H2)** and **(H3b)**. Then the energy  $E$ , given by (1.1), has a global minimizer in  $\mathcal{P}(\mathbb{R}^N)$  if and only if it satisfies the condition **(HE)**.*

*Proof.* Let us assume that  $E$  satisfies condition **(HE)**. As before, our proof relies on the direct method of the calculus variations for which we need to establish precompactness of a minimizing sequence.

Let  $\{\mu_n\}_{n \in \mathbb{N}}$  be a minimizing sequence and let

$$I := \inf_{\mu \in \mathcal{P}(\mathbb{R}^N)} E[\mu].$$

Condition **(HE)** implies that  $I \leq 0$ . If  $I = 0$  then by assumption **(HE)** there exists  $\bar{\mu}$  with  $E[\bar{\mu}] = 0$ , which is the desired minimizer. Thus, we focus on case that  $I < 0$ . Hence there exists  $\bar{\mu}$  for which  $E[\bar{\mu}] < 0$ . Also note that by Remark 2.1,  $I > -\infty$ .

Suppose the subsequence  $\{\mu_{n_k}\}_{k \in \mathbb{N}}$  of the minimizing sequence  $\{\mu_n\}_{n \in \mathbb{N}}$  “vanishes”. Since that subsequence is also a minimizing sequence we can assume that  $\{\mu_k\}_{k \in \mathbb{N}}$  vanishes. That is, for any  $R > 0$

$$(3.1) \quad \lim_{k \rightarrow \infty} \sup_{x \in \mathbb{R}^N} \int_{B_R(x)} d\mu_k(y) = 0.$$

Let

$$\overline{W}(R) = \inf_{r \geq R} W(r).$$

Since  $W(r) \rightarrow 0$  as  $r \rightarrow \infty$ ,  $\overline{W}(r) \rightarrow 0$  as  $r \rightarrow \infty$  and  $\overline{W}(r) \leq 0$  for all  $r \geq 0$ . Then we have that

$$\begin{aligned} E[\mu_k] &= \iint_{|x-y| \geq R} W(|x-y|) d\mu_k(x) d\mu_k(y) + \iint_{|x-y| \leq R} W(|x-y|) d\mu_k(x) d\mu_k(y) \\ &\geq \overline{W}(R) + C_W \iint_{|x-y| \leq R} d\mu_k(x) d\mu_k(y) \\ &= \overline{W}(R) + C_W \int_{\mathbb{R}^N} \left( \int_{B_R(x)} d\mu_k(y) \right) d\mu_k(x). \end{aligned}$$

Vanishing of the measures, (3.1), implies that  $\liminf_{k \rightarrow \infty} E[\mu_k] \geq \overline{W}(R)$  for all  $R > 0$ . Taking the limit as  $R \rightarrow \infty$  gives

$$\liminf_{k \rightarrow \infty} E[\mu_k] \geq 0.$$

This contradicts the fact that the infimum of the energy, namely  $I$ , is negative. Therefore “vanishing” in Lemma 2.3 does not occur.

Suppose the dichotomy occurs. Let  $\alpha$  be as in Lemma 2.3 and  $C_W$  be the constant defined in (2.1). Let  $\varepsilon > 0$  be such that

$$(3.2) \quad \varepsilon < \frac{|I|}{64|C_W|} \min \left\{ \frac{1}{\alpha} - 1, \frac{1}{1-\alpha} - 1 \right\}$$

and let  $R'$  be such that

$$(3.3) \quad |\overline{W}(R' - R)| = \left| \inf_{r \geq R' - R} W(r) \right| < \frac{|I|}{32} \min \left\{ \frac{1}{\alpha} - 1, \frac{1}{1-\alpha} - 1 \right\}.$$

As in the proof of Theorem 3.1, we can assume that dichotomy occurs along the whole sequence. Let  $\mu_k^1$  and  $\mu_k^2$  be measures described in Lemma 2.3. Let  $\nu_k = \mu_k - (\mu_k^1 + \mu_k^2)$ . Note that  $\nu_k$  is a nonnegative measure with  $|\nu_k| < \varepsilon$ , where  $|\nu_k| = \nu_k(\mathbb{R}^N)$ .

Let  $B[\cdot, \cdot]$  denote the symmetric bilinear form

$$B[\mu, \nu] := 2 \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} W(|x-y|) d\mu(x) d\nu(y).$$

By the definition of energy

$$(3.4) \quad \begin{aligned} E(\mu_k) &= E(\mu_k^1) + E(\mu_k^2) + B(\mu_k^1, \mu_k^2) + B(\mu_k^1 + \mu_k^2, \nu_k) + E(\nu_k) \\ &\geq E(\mu_k^1) + E(\mu_k^2) - |\overline{W}(R' - R)| - 2|C_W|\varepsilon \end{aligned}$$

where we used that the supports of  $\mu_k^1$  and  $\mu_k^2$  are at least  $R' - R$  apart. We can also assume, without the loss of generality, that  $E(\mu_k) < \frac{1}{2}I$  for all  $k$ . Let  $\alpha_k = |\mu_k^1|$ ,  $\beta_k = |\mu_k^2|$ .

Let us first consider the case that  $\frac{1}{\alpha_k}E(\mu_k^1) \leq \frac{1}{\beta_k}E(\mu_k^2)$ . Note that the energy has the following scaling property:

$$E[c\sigma] = c^2E[\sigma]$$

for any constant  $c > 0$  and measure  $\sigma$ . Our goal is to show that for some  $\lambda > 0$ , for all large enough  $k$ ,  $E(\frac{1}{\alpha_k}\mu_k^1) < E(\mu_k) - \lambda|I|$  which contradicts the fact that  $\mu_k$  is a minimizing sequence.

Let us consider first the subcase that  $E(\mu_k^2) \geq 0$  along a subsequence. By relabeling we can assume that the subsequence is the whole sequence. From (3.2), (3.3), and (3.4) it follows that  $\frac{1}{\alpha_k}E(\mu_k^1) < I/4$  for all  $k$ . Using the estimates again, we obtain

$$\begin{aligned} E(\mu_k) - E\left(\frac{1}{\alpha_k}\mu_k^1\right) &\geq \left(1 - \frac{1}{\alpha_k^2}\right)E(\mu_k^1) - |\overline{W}(R' - R)| - 2|C_W|\varepsilon \\ &\geq \left(\frac{1}{\alpha_k} - 1\right)\frac{|I|}{4} - |\overline{W}(R' - R)| - 2|C_W|\varepsilon \\ &\geq \left(\frac{1}{\alpha} - 1\right)\frac{|I|}{16}. \end{aligned}$$

Thus  $\mu_k$  is not a minimizing sequence. Contradiction.

Let us now consider the subcase  $E(\mu_k^2) \leq 0$  for all  $k$ . Using (3.4) and  $\frac{\beta_k}{\alpha_k}E(\mu_k^1) \leq E(\mu_k^2)$  we obtain

$$\frac{I}{2} \geq E(\mu_k) \geq \left(1 + \frac{\beta_k}{\alpha_k}\right)E(\mu_k^1) - |\overline{W}(R' - R)| - 2|C_W|\varepsilon.$$

From (3.2) and (3.3) follows that for all  $k$

$$\frac{1}{\alpha_k}E(\mu_k^1) \leq \frac{I}{8}.$$

Combining with above inequalities gives

$$\begin{aligned} E(\mu_k) - E\left(\frac{1}{\alpha_k}\mu_k^1\right) &\geq \left(1 + \frac{\beta_k}{\alpha_k} - \frac{1}{\alpha_k^2}\right)E(\mu_k^1) - |\overline{W}(R' - R)| - 2|C_W|\varepsilon \\ &\geq \left(\frac{1}{\alpha_k} - \alpha_k - \beta_k\right)\frac{|I|}{8} - \left(\frac{1}{\alpha} - 1\right)\left(\frac{|I|}{32} + \frac{|I|}{32}\right) \\ &\geq \frac{|I|}{32}\left(\frac{1}{\alpha} - 1\right) \end{aligned}$$

for  $k$  large enough. This contradicts the assumption that  $\mu_k$  is a minimizing sequence.

The case  $\frac{1}{\alpha_k}E(\mu_k^1) > \frac{1}{\beta_k}E(\mu_k^2)$  is analogous. In conclusion the dichotomy does not occur. Therefore “tightness up to translation” is the only possibility. As in the proof of Theorem 3.1, we can translate measures  $\mu_{n_k}$  to obtain a tight, energy-minimizing sequence  $\tilde{\mu}_{n_k}$ .

By Prokhorov’s theorem, there exists a further subsequence of  $\{\tilde{\mu}_{n_k}\}_{k \in \mathbb{N}}$ , still indexed by  $k$ , such that

$$\mu_{n_k} \rightharpoonup \mu_0 \quad \text{as } k \rightarrow \infty$$

for some measure  $\mu_0 \in \mathcal{P}(\mathbb{R}^N)$  in  $\mathcal{P}(\mathbb{R}^N)$  as  $k \rightarrow \infty$ . Therefore, by lower-semicontinuity of the energy,  $\mu_0$  is a minimizer of  $E$  in the class  $\mathcal{P}(\mathbb{R}^N)$ .

We now show the necessity of condition **(HE)**. Assume that  $E[\mu] > 0$  for all  $\mu \in \mathcal{P}(\mathbb{R}^N)$ . To show that the energy  $E$  does not have a minimizer consider a sequence of measures which



“vanishes” in the sense of Lemma 2.3(ii). Let

$$\rho(x) = \frac{1}{\omega_N} \chi_{B_1(0)}(x),$$

where  $\omega_N$  denotes the volume of the unit ball in  $\mathbb{R}^N$  and  $\chi_{B_R(0)}$  denotes the characteristic function of  $B_R(0)$ , the ball of radius  $R$  centered at the origin. Consider the sequence

$$\rho_n(x) = \frac{1}{n^N} \rho\left(\frac{x}{n}\right)$$

for  $n \geq 1$ . Note that  $\rho_n$  are in  $\mathcal{P}(\mathbb{R}^N)$ . We estimate

$$\begin{aligned} 0 < E[\rho_n] &= \frac{1}{\omega_N^2 n^{2N}} \int_{B_n(0)} \int_{B_n(0)} W(|x-y|) dx dy \\ &\leq \frac{1}{\omega_N^2 n^{2N}} \int_{B_n(0)} \left( \int_{B_n(y)} |W(|x|)| dx \right) dy \\ &\leq \frac{1}{\omega_N n^N} \left( \int_{B_R(0)} |W(|x|)| dx + \int_{B_{2n}(0) \setminus B_R(0)} |W(|x|)| dx \right) \\ &\leq \frac{C(R)}{\omega_N n^N} + \frac{2^N}{\omega_N} \sup_{r \geq R} |W(r)|. \end{aligned}$$

Since  $\sup_{r \geq R} |W(r)| \rightarrow 0$  as  $R \rightarrow \infty$ , for any  $\varepsilon > 0$  we can choose  $R$  so that  $\frac{2^N}{\omega_N} \sup_{r \geq R} |W(r)| < \frac{\varepsilon}{2}$ . We can then choose  $n$  large enough for  $\frac{C(R)}{\omega_N n^N} < \frac{\varepsilon}{2}$  to hold. Therefore  $\lim_{n \rightarrow \infty} E[\rho_n] = 0$ , that is,  $\inf_{\mu \in \mathcal{P}(\mathbb{R}^N)} E[\mu] = 0$ . However, since  $E[\cdot]$  is positive for any measure in  $\mathcal{P}(\mathbb{R}^N)$  the energy does not have a minimizer.  $\square$

#### 4. STABILITY AND CONDITION **(HE)**

The interaction energies of the form (1.1) have been an important object of study in statistical mechanics. For a system of interacting particles to have a macroscopic thermodynamic behavior it is needed that it does not accumulate mass on bounded regions as the number of particles goes to infinity. Ruelle called such potentials stable (a.k.a.  $H$ -stable). More precisely, a potential  $W : [0, \infty) \rightarrow (-\infty, \infty]$  is defined to be *stable* if there exists  $B \in \mathbb{R}$  such that for all  $n$  and for all sets of  $n$  distinct points  $\{x_1, \dots, x_n\}$  in  $\mathbb{R}^N$

$$(4.1) \quad \frac{1}{n^2} \sum_{1 \leq i < j \leq n} w(x_i - x_j) \geq -\frac{1}{n} B.$$

We show that for a large class of potentials the stability is equivalent with nonnegativity of energies. Our result is a continuum analogue of a part of Lemma 3.2.3 [34].

**Proposition 4.1** (Stability conditions). *Let  $W : [0, \infty) \rightarrow \mathbb{R}$  be an upper-semicontinuous function such that  $W$  is bounded from above or there exists  $\bar{R}$  such that  $W$  is nondecreasing on  $[\bar{R}, \infty)$ . Then the conditions*

- (S1)  *$w$  is a stable potential as defined by (4.1),*
- (S2) *for any probability measure  $\mu \in \mathcal{P}(\mathbb{R}^N)$ ,  $E(\mu) \geq 0$*

*are equivalent.*

Note that all potentials considered in the proposition are finite at 0. We expect that the condition can be extended to a class of potentials which converge to infinity at zero. Doing so is an open problem. We also note that condition **(S2)** is not exactly the complement of **(HE)**, as the nonnegative potentials whose minimum is zero satisfy both conditions. Such potentials indeed exist: for example consider any smooth nonnegative  $W$  such that  $W(0) = 0$ . Then the associated energy is nonnegative and  $E(\delta_0) = 0$  so any singleton is an energy minimizer. Note that  $E$  satisfies both **(HE)** and stability. To further remark on connections with statistical mechanics we note that such potentials  $W$  are not *super-stable*, but are *tempered* if  $W$  decays at infinity (both notions are defined in [34]).

*Proof.* To show that **(S2)** implies **(S1)** consider  $\mu = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$ . Then from  $E(\mu) \geq 0$  it follows that  $\frac{1}{n^2} \sum_{1 \leq i < j \leq n} w(x_i - x_j) \geq -\frac{1}{2n} W(0)$  so **(S1)** holds with  $B = \frac{1}{2} W(0)$ .

We now turn to showing that **(S1)** implies **(S2)**. Let us recall the definition of Lévy–Prokhorov metric, which metrizes the weak convergence of probability measures: Given probability measures  $\nu$  and  $\sigma$

$$d_{LP}(\nu, \sigma) = \inf\{\varepsilon > 0 : (\forall A - \text{Borel}) \nu(A) \leq \sigma(A + \varepsilon) + \varepsilon \text{ and } \sigma(A) \leq \nu(A + \varepsilon) + \varepsilon\}$$

where  $A + \varepsilon = \{x : d(x, A) < \varepsilon\}$ .

For a given measure  $\mu$ , we first show that it can be approximated in the Lévy–Prokhorov metric by an empirical measure of a finite set with arbitrarily many points. That is, we show that for any  $\varepsilon > 0$  and any  $n_0$  there exists  $n \geq n_0$  and a set of distinct points  $X = \{x_1, \dots, x_n\}$  such that the corresponding empirical measure  $\mu_X = \frac{1}{n} \sum_{j=1}^n \delta_{x_j}$  satisfies  $d_{LP}(\mu_X, \mu) < \varepsilon$ .

Let  $\varepsilon > 0$ . We can assume that  $\varepsilon < \frac{1}{2}$ . There exists  $R > 0$  such that for  $Q_R = [-R, R]^N$ ,  $\mu_X(\mathbb{R}^N \setminus Q_R) < \frac{\varepsilon}{2}$ . For integer  $l$  such that  $\sqrt{N} \frac{2R}{l} < \varepsilon$  divide  $Q_R$  into  $l^N$  disjoint cubes  $Q_i$ ,  $i = 1, \dots, l^N$  with sides of length  $2R/l$ . While cubes have the same interiors, they are not required to be identical, namely some may contain different parts of their boundaries, as needed to make them disjoint. Note that the diameter of each cube,  $\sqrt{N} \frac{2R}{l}$ , is less than  $\varepsilon$ . Let  $n > n_0$  be such that  $\frac{l^N}{n} < \frac{\varepsilon}{2}$ . Let  $p = \frac{1}{n}$ . For  $i = 1, \dots, l^N$  let  $p_i = \mu(Q_i)$ ,  $n_i = \lfloor p_i n \rfloor$ , and  $q_i = n_i p$ . Note that  $0 \leq p_i - q_i \leq p$  and thus  $s_q = \sum_i q_i \geq \sum_i p_i - l^N p > 1 - \frac{\varepsilon}{2}$ . In each cube  $Q_i$  place  $n_i$  distinct points and let  $\tilde{X}$  be the set of all such points. Note that  $\tilde{n} = \sum_i n_i = s_q n > (1 - \varepsilon)n$ . Let  $\hat{X}$  be an arbitrary set of  $n - \tilde{n}$  distinct points in  $Q_{2R} \setminus Q_R$ . Let  $X = \tilde{X} \cup \hat{X}$ . Note that  $X$  is a set of  $n$  distinct points. Then for any Borel set  $A$

$$\mu(A) \leq \sum_{i: \mu(A \cap Q_i) > 0} \mu(Q_i) + \frac{\varepsilon}{2} \leq \sum_{i: \mu(A \cap Q_i) > 0} (\mu_X(Q_i) + p) + \frac{\varepsilon}{2} \leq \mu_X(A + \varepsilon) + \varepsilon.$$

Similarly

$$\mu_X(A) \leq \mu(A + \varepsilon) + \varepsilon.$$

Therefore  $d_{LP}(\mu, \mu_X) \leq \varepsilon$ .

Consequently there exists a sequence of sets  $X_m$  with  $n(m)$  points satisfying  $n(m) \rightarrow \infty$  as  $m \rightarrow \infty$  for which the empirical measure  $\mu_m = \mu_{X_m}$  converges weakly  $\mu_m \rightarrow \mu$  as  $m \rightarrow \infty$ . By assumption **(S1)**

$$\iint_{x \neq y} W(x - y) d\mu_m(x) d\mu_{X_m}(y) \geq -\frac{1}{n(m)} B.$$

Let us first consider the case that  $W$  is an upper-semicontinuous function bounded from above. It follows from Lemma 2.2 that the energy  $E$  is an upper-semicontinuous functional. Therefore

$$E(\mu) \geq \limsup_{m \rightarrow \infty} E(\mu_m) \geq \limsup_{m \rightarrow \infty} -\frac{1}{n(m)}(B - W(0)) = 0$$

as desired.

If  $W$  is an upper-semicontinuous function such that there exists  $\bar{R}$  such that  $W$  is nondecreasing on  $[\bar{R}, \infty)$  we first note that we can assume that  $W(r) \rightarrow \infty$  as  $r \rightarrow \infty$ , since otherwise  $W$  is bounded from above which is covered by the case above. If  $\mu$  is a compactly supported probability measure then there exists  $L$  such that for all  $m$ ,  $\text{supp } \mu_m \subseteq [-L, L]^N$ . Since  $W$  is upper-semicontinuous it is bounded from above on compact sets and thus upper-semicontinuity of the energy holds. That is  $E(\mu) \geq \limsup_{m \rightarrow \infty} E(\mu_m) \geq 0$  as before.

If  $\mu$  is not compactly supported it suffices to show that there exists a compactly supported measure  $\tilde{\mu}$  such that  $E(\mu) \geq E(\tilde{\mu})$ , since by above we know that  $E(\tilde{\mu}) \geq 0$ . Note that since  $E(\frac{1}{2}(\delta_x + \delta_0)) \geq 0$ ,  $W(|x|) \geq -W(0)$ . Therefore  $W$  is bounded from below by  $-W(0)$  and  $W(0) \geq 0$ .

Since  $W(r) \rightarrow \infty$  as  $r \rightarrow \infty$  there exists  $R_1 \geq \bar{R}$  such that  $W(R_1) \geq \max\{1, \max_{r \leq R_1} W(r)\}$  and  $m_1 = \mu(\bar{B}_{R_1}(0)) > \frac{7}{8}$ . Let  $R_2$  be such that  $W(R_2) > 2W(R_1)$ , and define the constants  $m_2 = \mu(\bar{B}_{R_2}(0) \setminus \bar{B}_{R_1}(0))$  and  $m_3 = \mu(\mathbb{R}^N \setminus \bar{B}_{R_2}(0))$ . Note that  $m_1 + m_2 + m_3 = 1$ . Consider the mapping

$$P(x) = \begin{cases} x & \text{if } |x| \leq R_2 \\ 0 & \text{if } |x| > R_2. \end{cases}$$

Let  $\tilde{\mu} = P_{\#}\mu$ . Estimating the interaction of particles between the regions provides:

$$\begin{aligned} E(\tilde{\mu}) &\leq E(\mu) + 2W(0)m_3^2 + 2(W(R_2) + W(0))m_2m_3 - 2(W(R_2) - W(R_1))m_1m_3 \\ &\leq E(\mu) + W(R_2)m_3(m_3 + 4m_2 - m_1) < E(\mu). \end{aligned}$$

□

As we showed in Theorem 3.2 the property **(HE)** is necessary and sufficient for the existence of a global minimizer when  $E$  is defined via an interaction potential satisfying **(H1)**, **(H2)** and **(H3b)**. The property **(HE)** is posed as a condition directly on the energy  $E$ , and can be difficult to verify for a given  $W$ . It is then natural to ask what conditions the interaction potential  $W$  needs to satisfy so that the energy  $E$  has the property **(HE)**. In other words, how can one characterize interaction potentials  $w$  for which  $E$  admits a global minimizer? We do not address that question in detail, but just comment on the partial results established in the context of  $H$ -stability of statistical mechanics and how they apply to the minimization of the nonlocal-interaction energy.

Perhaps the first condition which appeared in the statistical mechanics literature states that absolutely integrable potentials which integrate to a negative number over the ambient space are not stable (cf. [20, Theorem 2] or [34, Proposition 3.2.4]). In our language these results translate to the following proposition.

**Proposition 4.2.** *Consider an interaction potential  $w(x) = W(|x|)$  where  $W$  satisfies the hypotheses **(H1)**, **(H2)** and **(H3b)**. If  $w$  is absolutely integrable on  $\mathbb{R}^N$  and*

$$\int_{\mathbb{R}^N} W(|x|) dx < 0,$$

then the energy  $E$  defined by (1.1) satisfies the condition **(HE)**.

*Proof.* Since  $\int_{\mathbb{R}^N} W(|x|) dx < 0$ , given  $\varepsilon > 0$  there exists a constant  $R > 0$  such that

$$\int_{B_R(0)} W(|x|) dx < \varepsilon.$$

Consider the function  $\rho(x) := \frac{1}{\omega_N R^N} \chi_{B_R(0)}(x)$ , i.e., the scaled characteristic function of the ball of radius  $R$ . Since  $\rho \in L^1(\mathbb{R}^N)$  with  $\|\rho\|_{L^1(\mathbb{R}^N)} = 1$  it defines a probability measure. Estimating at the energy of  $\rho$  we obtain

$$\begin{aligned} E[\rho] &= \frac{1}{\omega_N^2 R^{2N}} \int_{B_R(0)} \int_{B_R(0)} W(|x-y|) dx dy \\ &= \frac{1}{\omega_N^2 R^{2N}} \int_{B_R(0)} \left( \int_{B_R(y)} W(|x|) dx \right) dy < \varepsilon. \end{aligned}$$

Letting  $\varepsilon \rightarrow 0$  shows that the energy  $E$  satisfies **(HE)**.  $\square$

An alternative condition for instability of interaction potential is given in [13, Section II]. This condition, which we state and prove in the following proposition, extends the result of Proposition 4.2 to interaction potentials which are not absolutely integrable.

**Proposition 4.3.** *Suppose the interaction potential  $W$  satisfies the hypotheses **(H1)**, **(H2)** and **(H3b)**. If there exists  $p \geq 0$  for which*

$$(4.2) \quad \int_{\mathbb{R}^N} W(|x|) e^{-p^2|x|^2} dx < 0,$$

then the energy  $E$  defined by (1.1) satisfies the condition **(HE)**.

*Proof.* Let  $p \geq 0$  be given such that the inequality (4.2) holds. Since the case  $p = 0$  has been considered in Proposition 4.2 we can assume  $p > 0$ . Consider the function

$$\rho(x) = \frac{p^N}{\pi^{N/2}} e^{-2p^2|x|^2}.$$

Clearly  $\rho \in L^1(\mathbb{R}^N)$  and  $\|\rho\|_{L^1(\mathbb{R}^N)} = 1$ ; hence, it defines a probability measure on  $\mathbb{R}^N$ . Using the linear transformation on  $\mathbb{R}^{2N}$  given by

$$u = x - y, \quad v = x + y$$

for  $x$  and  $y$  in  $\mathbb{R}^N$  and denoting by  $C$  the Jacobian of this transformation we get that

$$\begin{aligned} E[\rho] &= \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} W(|x-y|) e^{-2p^2|x|^2} e^{-2p^2|y|^2} dx dy \\ &= C \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} W(|u|) e^{-p^2|u+v|^2/2} e^{-p^2|u-v|^2/2} dudv \\ &= C \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} W(|u|) e^{-p^2(|u|^2+|v|^2)} dudv \\ &= C \int_{\mathbb{R}^N} \left( \int_{\mathbb{R}^N} W(|u|) e^{-p^2|u|^2} du \right) e^{-p^2|v|^2} dv < 0. \end{aligned}$$

Hence, the energy  $E$  satisfies **(HE)**.  $\square$

*Remark 4.4.* Another useful criterion can be obtained by using the Fourier transform, as also noted in [34]. Namely if  $w \in L^2(\mathbb{R}^N)$ , for measure  $\mu$  that has a density  $\rho \in L^2(\mathbb{R}^N)$ , by Plancharel's theorem

$$E(\mu) = \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} w(x-y) d\mu(x) d\mu(y) = \int_{\mathbb{R}^N} \hat{w}(\xi) |\hat{\rho}(\xi)|^2 d\xi.$$

So if real part of  $\hat{w}$  is positive, the energy does not have a minimizer.

This criterion can be refined. By Bochner's theorem the Fourier transforms of finite non-negative measures are precisely the positive definite functions. Thus we know which family of functions,  $\hat{\rho}$  belongs to. Hence we can formulate the following criterion:

If  $w \in L^2(\mathbb{R}^N)$  and there exists a positive definite complex valued function  $\psi$  such that  $\int \hat{w}(\xi) |\psi^2(\xi)| d\xi \leq 0$  then the energy  $E$  satisfies the condition **(HE)**.

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