On global minimizers of repulsive-attractive power-law interaction energies

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We consider the minimisation of power-law repulsive-attractive interaction energies which occur in many biological and physical situations. We show existence of global minimizers in the discrete setting and get bounds for their supports independently of the number of Dirac Deltas in certain range of exponents. These global discrete minimizers correspond to the stable spatial profiles of flock patterns in swarming models. Global minimizers of the continuum problem are obtained by compactness. We also illustrate our results through numerical simulations.
1. Introduction

Let $\mu$ be a probability measure on $\mathbb{R}^d$. We are interested in minimizing the interaction potential energy defined by

$$E[\mu] = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y)d\mu(x)d\mu(y).$$

(1.1)

Here, $W$ is a repulsive-attractive power-law potential

$$W(z) = w(|z|) = \frac{|z|^\gamma}{\gamma} - \frac{|z|^\alpha}{\alpha}, \quad \gamma > \alpha,$$

(1.2)

with the understanding that $\frac{\log |z|}{\eta}$ for $\eta = 0$. Moreover, we define $W(0) = +\infty$ if $\alpha \leq 0$. This is the simplest possible potential that is repulsive in the short range and attractive in the long range. Depending on the signs of the exponents $\gamma$ and $\alpha$, the behaviour of the potential is depicted in Figure 1. Since this potential $W$ is bounded from below by $w(1) = \frac{1}{\gamma} - \frac{1}{\alpha}$, the energy $E[\mu]$ always makes sense, with possibly positive infinite values.

![Figure 1: Three different behaviours of $w(r) = \frac{r^\gamma}{\gamma} - \frac{r^\alpha}{\alpha}, \gamma > \alpha$.](image)

The minimizers of the energy $E[\mu]$ are related to stationary states for the aggregation equation $\rho_t = \nabla \cdot (\rho \nabla W \ast \rho)$ studied in [8–10,14,15] with repulsive-attractive potentials [4,5,23–26,39]. The set of local minimizers of the interaction energy, in both the discrete setting of empirical measures (equal mass Dirac Deltas) and the continuum setting of general probability measures, can exhibit rich complicated structure as studied numerically in [5,32]. In fact, it is shown in [5] that the dimensionality of the support of local minimizers of (1.1) depends on the strength of the repulsion at zero of the potential $W$. For instance, as the repulsion at the origin gets stronger (i.e., $\alpha$ gets smaller) in three dimension, the support of the local minimizer is concentrated on points, curves, surfaces and eventually some sets of non-zero Lebesgue measure.

From the viewpoint of applications, these models with nonlocal interactions are ubiquitous in the literature. Convex attractive potentials appear in granular media [7,14,15,33]. More sophisticated potentials like (1.2) are included to take into account short range repulsion and long range attraction in kinetic models of collective behaviour of animals, see [20,31,32,36,37] and the references therein. The minimization of the interaction energy in the discrete settings is of paramount importance for the structure of virus capsides [29], for self-assembly materials in chemical engineering design [21,40,46], and for flock patterns in animal swarms [13,44,45].

Despite the efforts in understanding the qualitative behaviour of stationary solutions to the aggregation equation $\rho_t = \nabla \cdot (\rho \nabla W \ast \rho)$ and the structure of local minimizers of the interaction energy $E[\mu]$, there are no general results addressing the global minimization of $E[\mu]$ in the natural framework of probability measures. See [17] for a recent analysis of this question in the more restricted set of bounded or binary densities. Here, we will first try to find solutions in the restricted set of atomic measures.
The interest of understanding the global discrete minimizers of the interaction energy is not purely mathematical. The discrete global minimizers will give the spatial profile of typical flocking patterns obtained in simplified models for social interaction between individuals as in [2,32] based on the famous 3-zones models, see for instance [30,34]. Moreover, due to the recent nonlinear stability results in [13], we know now that the stability properties of the discrete global minimizer as stationary solution of the first order ODE model

$$\dot{x}_i = -\sum_{j \neq i} n \nabla W (x_i - x_j), \quad i = 1, \ldots, n,$$

lead to stability properties of the flock profiles for the second order model in swarming introduced in [20] or with additional alignment mechanisms as the Cucker-Smale interaction [18,19], see also [2] and the discussion therein.

Our objective is to show the existence of global minimizers of the interaction energy defined on probability measures under some conditions on the exponents. Our approach starts with the discrete setting by showing qualitative properties about the global minimizers in the set of equal mass Dirac Deltas. These discrete approximations are used extensively in material science and variational calculus with hardcore potentials [1,3,22,42] in order to understand the crystallization phenomena. However, these discrete approximations with soft potentials as (1.2) are more difficult; apart from various properties of the minimizers [20,25,32,45], the existence as well as the convergence of these discrete minimizers is not established in general. In a certain range of exponents, we will prove that the diameter of the support of discrete minimizers does not depend on the number of Dirac Deltas. This result together with standard compactness arguments will result in our desired global minimizers among probability measures.

In fact, our strategy to show the confinement of discrete minimizers is in the same spirit as the proof of confinement of solutions of the aggregation equation in [6,11]. In our case, the ideas of the proof in Section 2 will be based on convexity-type arguments in the range of exponents \(\gamma > \alpha \geq 1\) to show the uniform bound in the diameter of global minimizers in the discrete setting. Section 3 will be devoted to more refined results in one dimension. We show that for very repulsive potentials, the bounds on the diameter is not uniform in the number of Dirac Deltas, complemented by numerical simulations; in the range of exponents \(\gamma > 1 > \alpha\), the minimizers turn out to be unique (up to translation), analogous to the simplified displacement convexity in 1D; in the special case \(\gamma = 2\) and \(\alpha = 1\), we can find the minimizers and show the convergence to the continuous minimizer explicitly.

### 2. Existence of Global minimizers

We will first consider the discrete setting where \(\mu\) is a convex combinations of Dirac Deltas, i.e.,

$$\mu = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}, \quad x_i \in \mathbb{R}^d.$$  

Setting

$$E_n(x_1, \ldots, x_n) = \sum_{i \neq j} \left( \frac{|x_i - x_j|^{\gamma}}{\gamma} - \frac{|x_i - x_j|^{\alpha}}{\alpha} \right),$$

for such a \(\mu\) one has \(E[\mu] = \frac{1}{n^2} E_n(x_1, \ldots, x_n)\). In the definition of the energy, we can include the self-interaction for non singular cases, \(\alpha > 0\), since both definitions coincide. Fixing \(W(0) = +\infty\) for singular kernels makes \(W\) upper semi-continuous, and the self-interaction must be excluded to have finite energy configurations.

Let us remark that due to translational invariance of the interaction energy, minimizers of the interaction energy \(E[\mu]\) can only be expected up to translations. Moreover, when the potential is radially symmetric, as in our case, then any isometry in \(\mathbb{R}^d\) will also leave invariant the interaction energy. These invariances are also inherited by the discrete counterpart \(E_n(x_1, \ldots, x_n)\). We
will first consider the minimizers of $E_n(x)$ among all $x = (x_1, \cdots, x_n) \in (\mathbb{R}^d)^n$, and then the convergence to the global minimizers of $E[\mu]$ as $n$ goes to infinity.

(a) Existence of minimizer: Discrete setting

Let us consider for $\alpha < \gamma$, the derivative of the radial potential

$$w'(r) = r^{\gamma-1} - r^{\alpha-1} = r^{\alpha-1} \left( r^{\gamma-\alpha} - 1 \right),$$

which obviously vanishes for $r = 1$ and for $r = 0$ when $\alpha > 1$. We conclude from the sign of derivatives, that $w(r)$ attains always a global minimum at $r = 1$. There are, following the values of $\alpha < \gamma$, three types of behaviours for $w$ that are shown in Figure 1. In all the three cases, $E_n$ is bounded from below since

$$E_n(x) \geq n^2 \left( \frac{1}{\gamma} - \frac{1}{\alpha} \right),$$

with the understanding that $|x|^\eta = \log |x|$ for $\eta = 0$. We set

$$I_n = \inf_{x \in (\mathbb{R}^d)^n} E_n(x). \quad (2.2)$$

Using the translational invariance of $E_n(x_1, \cdots, x_n)$, we can assume without loss of generality that $x_1 = 0$ what we do along this subsection. First we have the following lemma showing that $I_n$ is achieved, which can be proved by discussing different ranges of the exponents $\gamma$ and $\alpha$.

**Lemma 2.1.** For any finite $n \geq 2$, the minimum value $I_n$ is obtained for some discrete minimizers in $(\mathbb{R}^d)^n$.

The case $0 < \alpha < \gamma$. We claim that

$$n^2 \left( \frac{1}{\gamma} - \frac{1}{\alpha} \right) \leq I_n < 0. \quad (2.3)$$

Indeed consider $x = (x_1, \cdots, x_n) \in (\mathbb{R}^d)^n$ such that $x_1, \cdots, x_n$ are aligned and $|x_i - x_{i+1}| = \frac{1}{\pi}$. Then for any $i, j$ one has $0 < |x_i - x_j| \leq 1$ and $w(|x_i - x_j|) < 0$. Therefore (2.3) follows.

Let us show that the infimum $I_n$ is achieved. Let $x \in (\mathbb{R}^d)^n$. Set $R = \max_{i,j} |x_i - x_j|$. A minimizer is sought among the points such that $E_n(x) < 0$ and one has for such a point

$$\frac{R^\gamma}{\gamma} \leq \sum_{i,j} \frac{|x_i - x_j|^\gamma}{\gamma} < \sum_{i,j} \frac{|x_i - x_j|^{\alpha}}{\alpha} \leq n^2 \frac{R^\alpha}{\alpha}.$$

This implies the upper bound

$$R \leq \left( \frac{n^2 \gamma}{\alpha} \right)^{\frac{1}{\gamma-\alpha}}. \quad (2.4)$$

Thus, since $x_1 = 0$, all the $x_i$’s have to be in the ball of center 0 and radius $\left( \frac{n^2 \gamma}{\alpha} \right)^{\frac{1}{\gamma-\alpha}}$, i.e., $x$ has to be in a compact set of $(\mathbb{R}^d)^n$. Since $E_n(x)$ is continuous, the infimum $I_n$ is achieved. Note that the bound on the radius, where all Dirac Deltas are contained, depends a priori on $n$.

The case $\alpha \leq 0 \leq \gamma$ and $\alpha \neq \gamma$. In this case $w(0^+) = -\infty$ and $w(\infty) = +\infty$. We minimize among all $x$ such that $x_i \neq x_j$ for $i \neq j$. Note that $w$ and $I_n$ are both positive. Since $w(r) \to +\infty$ as $r \to 0$...
or \( r \to \infty \), there exists \( a_n, b_n > 0 \) such that
\[
    a_n < 1 < b_n, \quad w(a_n) = w(b_n) > I_n.
\]
Let \( x \in (\mathbb{R}^d)^n \). If for a couple \( i, j \), one has
\[
    |x_i - x_j| < a_n \quad \text{or} \quad |x_i - x_j| > b_n
\]
then one has \( E_n(x) > I_n \). Thus the infimum (2.2) will not be achieved among the points \( x \) satisfying (2.5) but among those in
\[
    \{ x \in (\mathbb{R}^d)^n \mid a_n \leq |x_i - x_j| \leq b_n \}
\]
Since the set above is compact, being closed and contained in \((B(0, b_n))^n\) due to \( x_1 = 0 \), the infimum \( I_n \) is achieved.

The case \( \alpha < \gamma < 0 \). In this case \( I_n < 0 \). Indeed it is enough to choose
\[
    |x_i - x_j| > 1 \quad \forall i, j
\]
to get \( E_n(x) < 0 \). Since \( w(0^+) = +\infty \), we minimize \( E_n \) among the points \( x \) such that \( x_i \neq x_j, i \neq j \). Thus the summation is on \( n^2 - n \) couples \((i, j)\). Denote by \( x^k = (x^k_1, \cdots, x^k_n) \in (\mathbb{R}^d)^n \) a minimizing sequence of \( E_n \). Since \( w(r) \to +\infty \) as \( r \to 0 \), there exists a number \( a_0 < 1 \) such that
\[
    w(a_0) > n(n - 1) \left( \frac{1}{\alpha} - \frac{1}{\gamma} \right) > 0.
\]
If for a couple \((i, j)\) one has \( |x^k_i - x^k_j| < a_0 \) then
\[
    E(x^k) > w(a_0) + (n^2 - n - 1) \left( \frac{1}{\gamma} - \frac{1}{\alpha} \right) > 0
\]
and \( x^k \) cannot be a minimizing sequence. So without loss of generality, we may assume that
\[
    |x^k_i - x^k_j| \geq a_0, \quad \forall i, j.
\]
Let us denote by \( y_1, \cdots, y_d \) the coordinates in \( \mathbb{R}^d \). Without loss of generality, we can assume by relabelling and isometry invariance that for every \( k \) one has
\[
    x^k_1 = 0, \quad x^k_i \in \{ y = (y_1, \cdots, y_d) \mid y_d \geq 0 \}.
\]
Suppose that \( x^k_i = (x^k_{i,1}, \cdots, x^k_{i,d}) \) and the numbering of the points is done in such a way that
\[
    x^k_{i,d} \leq x^k_{i+1,d}.
\]
We next claim that one can assume that \( x^k_{i+1,d} - x^k_{i,d} \leq 1, \forall i \). Indeed if not, let \( i_0 \) be the first index such that
\[
    x^k_{i_0+1,d} - x^k_{i_0,d} > 1.
\]
Let us leave the first \( x^k \) until \( i_0 \) unchanged and replace for \( i > i_0 \), \( x^k_i \) by
\[
    x^k_i = x^k_i - (x^k_{i+1,d} - x^k_{i,d} - 1) e_d
\]
where \( e_d \) is the \( d \)-vector of the the canonical basis of \( \mathbb{R}^d \), i.e., we shift \( x^k_i \) down in the direction \( e_d \) by \( x^k_{i+1,d} - x^k_{i,d} - 1 \). Denote by \( \tilde{x}^k_i \) the new sequence obtained in this manner. One has
\[
    w(|\tilde{x}^k_i - x^k_i|) < w(|x^k_i - x^k_j|), \quad \forall i \leq i_0 < j,
\]
\[
    w(|\tilde{x}^k_i - x^k_i|) = w(|x^k_i - x^k_j|), \quad \forall i_0 < i < j, \text{ or } i < j \leq i_0
\]
and thus one has obtained a minimizing sequence with
\[
    \tilde{x}^k_{i_0+1,d} - \tilde{x}^k_{i_0,d} \leq 1, \quad \forall i
\]
i.e., \( 0 \leq \tilde{x}^k_{i,d} \leq n - 1 \), for all \( i \).
Repeating this process in the other directions one can assume without loss of generality that

\[ x^k_i \in [0, n-1]^d \]  

(2.6)

for all \( k \), i.e., that \( x^k \) is in a compact subset of \((\mathbb{R}^d)^n\), and extracting a convergent subsequence, we obtain our desired minimizer in \([0, n-1]^d\).

(b) Existence of minimizer: General measures

The estimates (2.4) and (2.6) give estimates on the support of a minimizer of (2.2). However, these estimates depend on \( n \). We will show now that the diameter of any minimizer of (2.2) can sometimes be bounded independently of \( n \).

**Theorem 2.2.** Suppose that \( 1 \leq \alpha < \gamma \). Then the diameter of any global minimizer of \( E_n \) achieving the infimum in (2.2) is bounded independently of \( n \).

**Proof.** At a point \( x = (x_1, \ldots, x_n) \in (\mathbb{R}^d)^n \) where the minimum of \( E_n \) is achieved one has

\[ 0 = \nabla x E_n(x_1, \ldots, x_n) = \nabla x \sum_{j \neq k} \left( \frac{|x_k - x_j|^\gamma}{\gamma} - \frac{|x_k - x_j|^\alpha}{\alpha} \right), \quad k = 1, 2, \ldots, n. \]

Since \( \nabla x (|x|^\gamma/\gamma) = |x|^{\gamma-2}x \), we obtain

\[ \sum_{j \neq k} |x_k - x_j|^{\gamma-2}(x_k - x_j) = \sum_{j \neq k} |x_k - x_j|^{\alpha-2}(x_k - x_j), \quad k = 1, \ldots, n. \]  

(2.7)

Suppose the points are labelled in such a way that

\[ |x_n - x_1| = \max_{i,j} |x_i - x_j|. \]

Then for \( k = 1 \) and \( n \) in (2.7), we get

\[ \sum_{j \neq 1} |x_1 - x_j|^{\gamma-2}(x_1 - x_j) = \sum_{j \neq 1} |x_1 - x_j|^{\alpha-2}(x_1 - x_j), \]

\[ \sum_{j \neq n} |x_n - x_j|^{\gamma-2}(x_n - x_j) = \sum_{j \neq n} |x_n - x_j|^{\alpha-2}(x_n - x_j). \]

By subtraction, this leads to

\[ \sum_{j \neq 1, n} \left( |x_n - x_j|^{\gamma-2}(x_n - x_j) - |x_1 - x_j|^{\gamma-2}(x_1 - x_j) \right) + 2|x_n - x_1|^{\gamma-2}(x_n - x_1) \]

\[ = \sum_{j \neq n} |x_n - x_j|^{\alpha-2}(x_n - x_j) - \sum_{j \neq 1} |x_n - x_j|^{\alpha-2}(x_1 - x_j). \]

Taking the scalar product of both sides with \( x_n - x_1 \) we obtain

\[ \sum_{j \neq 1, n} \left( |x_n - x_j|^{\gamma-2}(x_n - x_j) - |x_1 - x_j|^{\gamma-2}(x_1 - x_j), x_n - x_1 \right) + 2|x_n - x_1|^{\gamma} \]

\[ = \sum_{j \neq n} |x_n - x_j|^{\alpha-2}(x_n - x_j, x_n - x_1) - \sum_{j \neq 1} |x_n - x_j|^{\alpha-2}(x_1 - x_j, x_n - x_1). \]

For \( \gamma \geq 2 \), there exists a constant \( C_\gamma > 0 \) such that (see [16])

\[ \langle |\eta|^{\gamma-2}\eta - |\xi|^{\gamma-2}\xi, \eta - \xi \rangle \geq C_\gamma |\eta - \xi|^{\gamma}, \quad \forall \eta, \xi \in \mathbb{R}^d. \]  

(2.8)
Note that this is nothing else that the modulus of convexity (in the sense of [15]) of the potential \(|x|^{\gamma}\). Thus estimating from above, we derive
\[
((n - 2)C_\gamma + 2)|x_n - x_1|^\gamma \leq \sum_{j \neq n} |x_n - x_j|^\alpha - 1|x_n - x_1| + \sum_{j \neq 1} |x_1 - x_j|^\alpha - 1|x_n - x_1|
\]
\[
\leq 2(n - 1)|x_n - x_1|^\alpha.
\]
Thus if \(a \wedge b\) denotes the minimum of two numbers \(a\) and \(b\), we derive
\[
(C_\gamma \wedge 1)n|x_n - x_1|^\gamma \leq 2(n - 1)|x_n - x_1|^\alpha.
\]
That is
\[
|x_n - x_1| \leq \left( \frac{2}{C_\gamma \wedge 1} \frac{n - 1}{n} \right)^{\frac{1}{\gamma - \alpha}} \leq \left( \frac{2}{C_\gamma \wedge 1} \right)^{\frac{1}{\gamma - \alpha}},
\]
which proves the theorem in the case \(\gamma \geq 2\). In the case where \(1 < \gamma < 2\), one can replace (2.8) with
\[
(|\eta|^{\gamma - 2} - |\xi|^{\gamma - 2})|\eta - \xi| \geq c_\gamma (|\eta| + |\xi|)^{\gamma - 2}|\eta - \xi|^2, \quad \forall \eta, \xi \in \mathbb{R}^d,
\]
for some constant \(c_\gamma\), (see [16]). We get, arguing as above,
\[
\sum_{j \neq 1, n} c_\gamma \left( |x_n - x_j| + |x_1 - x_j| \right)^{\gamma - 1} + 2|x_n - x_1|^\gamma \leq 2(n - 1)|x_n - x_1|^\alpha.
\]
No since \(\gamma - 1 < 0\), \(|x_n - x_j| < |x_n - x_1|\) and \(|x_1 - x_j| < |x_n - x_1|\), we derive that
\[
((n - 2)c_\gamma 2^{\gamma - 2} + 2)|x_n - x_1|^\gamma \leq 2(n - 1)|x_n - x_1|^\alpha.
\]
We thus obtain the bound
\[
|x_n - x_1| < \left( \frac{2}{(2^{\gamma - 2}c_\gamma) \wedge 1} \right)^{\frac{1}{\gamma - \alpha}},
\]
which completes the proof of the theorem.

As a direct consequence of this bound independent of the number of Dirac Deltas, we can prove existence of global minimizers in the continuous setting.

**Theorem 2.3.** Suppose that \(1 < \alpha < \gamma\). Then global minimizers associated to the global minimum of \(E_n(x)\) with zero center of mass converge as \(n \to \infty\) toward a global minimizer among all probability measures with bounded moments of order \(\gamma\) of the interaction energy \(E[\mu]\) in (1.1).

**Proof.** Let \(x^n \in (\mathbb{R}^d)^n\) be a minimizer of (2.1) and
\[
\mu^n = \frac{1}{n} \sum_{j} \delta_{x^n_j}
\]
be the associated discrete measure. From Theorem 2.2, the radius of the supports of the measures \(\mu^n\) are bounded uniformly in \(n\) by \(R\) provided that the center of the mass \(\int_{\mathbb{R}^d} x d\mu^n\) is normalized to be the origin. By Prokhorov’s theorem [38], \(\mu^n\) is compact in the weak-\(\ast\) topology of measures and also in the metric space induced by \(\gamma\)-Wasserstein distance \(d_\gamma\) between probability measures (see [28,43] for definition and basic properties). Then there is a measured \(\mu^*\) supported on \(B(0, R)\) such that
\[
\mu^n \rightharpoonup \mu^* \quad \text{and} \quad d_\gamma(\mu^n, \mu^*) \to 0
\]
as \(n\) goes to infinity. Note that the notion of convergence of a sequence of probability measures in \(d_\gamma\) is equivalent to weak convergence of the measures plus convergence of the moments of order
\( \gamma \), see [43, Chapter 9]. Let \( \nu \) be any probability measure on \( \mathbb{R}^d \) with bounded moment of order \( \gamma \), then \( E[\nu] < \infty \). Moreover, there is a sequence of discrete measures \( \nu_n \) of the form

\[
\nu_n = \frac{1}{n} \sum_{j=1}^{n} \delta_{y^n_j},
\]

such that \( d_\gamma (\nu^n, \nu) \to 0 \), and thus \( \nu_n \to \nu \), see [28,43]. By the definition of \( E_n \) in (2.2), we deduce

\[
E[\nu^n] = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) d\nu^n(x) d\nu^n(y) \geq \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) d\mu^n(x) d\mu^n(y) = E[\mu^n].
\]

On the other hand, since

\[
d_\gamma (\mu^n \otimes \mu^n, \mu^* \otimes \mu^*) \to 0, \quad d_\gamma (\nu^n \otimes \nu^n, \nu \otimes \nu) \to 0,
\]

as \( n \to \infty \), and the function \( w(x-y) = |x-y|^{\gamma}/|x-y|^\alpha \) is Lipschitz continuous on bounded sets in \( \mathbb{R}^d \times \mathbb{R}^d \) with growth of order \( \gamma \) at infinity, then

\[
E[\mu^*] = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) d\mu^*(x) d\mu^*(y) = \lim_{n \to \infty} \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) d\mu^n(x) d\mu^n(y)
\]

\[
\leq \lim_{n \to \infty} \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) d\nu^n(x) d\nu^n(y) = E[\nu].
\]

Therefore, \( \mu^* \) must be a global minimizer of \( E[\mu] \) in the set of probability measures with bounded moments of order \( \gamma \).

**Remark.** The convergence of the minimizers of \( E_n \) can be proved also in the general framework of \( \Gamma \)-convergence, a well-known technique of variational convergence of sequences of functionals. This approach was implemented successfully to show the rescaled configurations to the Wulff shape [3] and general measure quantization of power repulsion-attraction potentials [27].

**Remark.** Global minimizers of the energy in the continuum setting might be a convex combination of a finite number of Dirac Deltas. Numerical experiments suggest that it is always the case in the range \( 2 < \alpha < \gamma \). It is an open problem in this range to show that global minimizers in the discrete case do not change (except symmetries) for \( n \) large enough and coincide with global minimizers of the continuum setting.

**Remark.** The range of exponents \( 1 \leq \alpha < \gamma \) in Theorem 2.3 can be extended to \( \gamma \geq 1 \) and \( \gamma > \alpha > 0 \), using uniform bounds on the \( \gamma \)-th moments of the minimizers. First, if \( x = (x_1, \ldots, x_n) \in (\mathbb{R}^d)^n \) is a minimizer of \( E_n \) with center of mass at the origin, then by (2.3) and Hölder inequality

\[
\sum_{i,j} \frac{|x_i - x_j|}{\gamma} \leq \sum_{i,j} \frac{|x_i - x_j|^\alpha}{\alpha} \leq \left( \sum_{i,j} \frac{|x_i - x_j|^\gamma}{\gamma} \right)^{\alpha/\gamma} \left( \frac{1}{n^2} \sum_{i,j} |x_i - x_j|^\gamma \right)^{\gamma-\alpha}/\gamma,
\]

or equivalently

\[
\frac{1}{n^2} \sum_{i,j} |x_i - x_j|^\gamma \leq \frac{\gamma^{\alpha/\gamma}}{\alpha^{\gamma-\alpha}}.
\]

Since the function \( \Phi(x) = |x-y|^\gamma \) is convex for any \( \gamma \geq 1 \) and \( y \in \mathbb{R}^d \), Jensen’s inequality implies that

\[
\frac{1}{n^2} \sum_{i,j} |x_i - x_j|^\gamma \geq \frac{1}{n} \sum_i \left( \frac{1}{n} \sum_j |x_i - x_j|^\gamma \right) \geq \frac{1}{n} \sum_i \frac{1}{n} \sum_j |x_i - x_j|^\gamma = \frac{1}{n} \sum_i |x_i|^\gamma.
\]

As a consequence, we get a uniform bound on the \( \gamma \)-th moment of the discrete minimizers. As a result, the minimizing sequence corresponding to the associated atomic measures is tight, leading also toward a global minimizer of \( E[\mu] \).
3. Further Remarks in one dimension

In this section, we concentrate on the one dimensional case ($d = 1$) for more refined properties.

(a) Confinement of Discrete Global Minimizers

We check first how sharp are the conditions on the exponents of the potential to get the confinement of global discrete minimizers independently of $n$. In fact, when the potential is very repulsive at the origin, we can show that a uniform bound in $n$ of the diameter of global minimizers of the discrete setting does not hold. If $x$ is a minimizer of $E_n(x)$, we will always assume that the labelling of $x_i$s is in increasing order: $x_1 \leq x_2 \cdots \leq x_n$.

**Theorem 3.1.** Suppose $\alpha < \gamma < 0$ and $\alpha < -2$. If $x$ is a minimizer of $E_n$, then there exists a constant $C_{\alpha, \gamma}$ such that for $n$ large enough

$$x_n - x_1 \geq C_{\alpha, \gamma} n^{1 + \frac{\alpha}{2}}$$

holds.

**Proof.** Set $C = \frac{1}{\alpha} - \frac{1}{\gamma} > 0$. Denote by $a_n$ the unique element of $\mathbb{R}$ such that

$$w(a_n) = C n^2. \quad (3.1)$$

If $x$ is a minimizer of $E_n$, we claim that

$$x_{i+1} - x_i \geq a_n, \quad \forall i = 1, \ldots, n. \quad (3.2)$$

Indeed otherwise,

$$E_n(x) \geq w(x_{i+1} - x_i) - (n^2 - n - 1)C > C n^2 - (n^2 - n - 1)C = (n + 1)C > 0$$

and we know that in this case $E_n < 0$. From (3.1) we derive

$$C n^2 = \frac{a_n^\gamma}{\gamma} - \frac{a_n^\alpha}{\alpha} = -\frac{a_n^\alpha}{\alpha} (1 - \frac{\alpha}{\gamma} a_n^{\gamma - \alpha}) \geq -\frac{a_n^\alpha}{2\alpha},$$

for $n$ large enough (recall that $a_n \to 0$ when $n \to \infty$). It follows that

$$a_n \geq (2\alpha C n^2)^{\frac{\alpha}{\gamma}} = (-2\alpha C)^{\frac{1}{\alpha}} n^{\frac{\alpha}{\gamma}}.$$

Combining this with (3.2) we get

$$x_n - x_1 \geq (n - 1)a_n \geq \frac{n}{2} (-2\alpha C)^{\frac{1}{\alpha}} n^{\frac{\alpha}{\gamma}} = \frac{(-2\alpha C)^{\frac{1}{\alpha}}}{2} n^{1 + \frac{\alpha}{2}}$$

for $n$ large enough, proving the desired estimate with $C_{\alpha, \gamma} = (-2\alpha C)^{\frac{1}{\alpha}} / 2$. \qed

This property for the minimizers of this very repulsive case is similar to H-stability in statistical mechanics [41], where the minimal distance between two particles is expected to be constant when $n$ is large, and crystallization occurs. This also suggests that the lower bound $O(n^{1 + \frac{\alpha}{2}})$ is not sharp, which is verified in Figure 2.

In fact, numerical experiments in [5,6] suggest that confinement happens for $-1 < \alpha < 1$. It is an open problem to get a uniform bound in the support of the discrete minimizers as in Section 2 in this range. In the range $\alpha \leq -1$, our numerical simulations suggest that spreading of the support happens for all $\gamma$ with a decreasing spreading rate as $\gamma$ increases. For hardcore potentials considered in [1,3,22,42], the crystallization can be rescaled to a macroscopic cluster with uniform density; however, the scaling relation seems to have a more delicate dependence on the parameters when $\alpha \leq 2$.
(b) Uniqueness of global minimizers

We turn now to the issue of uniqueness (up to isometry) of global discrete and continuum minimizers. In general, a large amount of discrete minimizers (partially due to symmetries) are expected, and the uniqueness can be shown only in the macroscopic limit [3]. If \( x \) is a minimizer of \( E_n(x) \), we can always assume at the expense of a translation that the center of mass is zero, that is \( x_1 + \cdots + x_n = 0 \). Let us recall that

\[
E_n(x) = \sum_{i \neq j} w(|x_i - x_j|)
\]

with the convention that \( x_i \neq x_j \) when \( i \neq j \), \( \alpha < 0 \).

**Lemma 3.2.** Suppose that \( \alpha \leq 1, \gamma \geq 1, \) and \( \alpha < \gamma \). Let \( x, y \) be two points of \( \mathbb{R}^n \) such that

\[
\frac{x_1 + \cdots + x_n}{n} = 0, \ x_1 \leq x_2 \leq \cdots \leq x_n, \tag{3.3a}
\]

\[
\frac{y_1 + \cdots + y_n}{n} = 0, \ y_1 \leq y_2 \leq \cdots \leq y_n. \tag{3.3b}
\]

then

\[
E_n\left(\frac{x + y}{2}\right) < \frac{E_n(x) + E_n(y)}{2}
\]

unless \( x = y \).

**Proof.** One has \( w''(r) = (\gamma - 1)r^{\gamma-2} - (\alpha - 1)r^{\alpha-2} > 0 \), for all \( r > 0 \). Thus \( w \) is strictly convex. Then one has by the strict convexity of \( w \),

\[
E_n\left(\frac{x + y}{2}\right) = \sum_{i \neq j} w\left(\frac{x_i + y_i}{2} - \frac{x_j + y_j}{2}\right)
\]

\[
= \sum_{i \neq j} w\left(\frac{x_i - x_j}{2} + \frac{y_i - y_j}{2}\right)
\]

\[
\leq \frac{1}{2} \left( \sum_{i \neq j} w(|x_i - x_j|) + \sum_{i \neq j} w(|y_i - y_j|) \right) = \frac{E_n(x) + E_n(y)}{2}
\]

The equality above is strict unless \( x_i - x_j = y_i - y_j \) for all \( i, j \), that is \( x_{i+1} - x_i = y_{i+1} - y_i \). Therefore \( x = y \). \( \square \)
As a consequence, we can now state the following result regarding the uniqueness of global discrete minimizers.

**Theorem 3.3.** Suppose \( \alpha \leq 1, \gamma \geq 1, \) and \( \alpha < \gamma. \) Up to translations, the minimizer \( x \) of \( E_n \) is unique and symmetric with respect to its center of mass.

**Proof.** Let \( x, y \) be two minimizers of \( E_n \) satisfying (3.3). If \( x \neq y, \) by Lemma 3.2, one has

\[
E_n\left(\frac{x + y}{2}\right) < \frac{E_n(x) + E_n(y)}{2} = I_n
\]

and a contradiction. This shows the uniqueness of a minimizer satisfying (3.3a). Denote now by \( s \) the symmetry defined by \( s(\xi) = -\zeta, \xi \in \mathbb{R}. \) If \( x \) is a minimizer of \( E_n(x) \) satisfying (3.3a) then \( y \) defined by

\[
y_i = s(x_{n+1-i}) \quad i = 1, \ldots, n
\]

is also a minimizer satisfying (3.3b). Thus by uniqueness

\[
x_i = -x_{n+1-i} \quad i = 1, \ldots, n,
\]

and this completes the proof of the theorem. \( \square \)

**Remark** (Uniqueness and displacement convexity in one dimension). Lemma 3.2 and Theorem 3.3 are just discrete versions of uniqueness results for the continuum interaction functional (1.1). In the seminal work of R. McCann [35] that introduces the notion of displacement convexity, he already dealt with the uniqueness (up to translation) of the interaction energy functional (1.1) using the theory of optimal transportation: if \( W \) is strictly convex in \( \mathbb{R}^d, \) then the global minimizer is unique among probability measures by fixing the center of mass, as the energy \( E[\mu] \) is (strictly) displacement convex. However, the displacement convexity of a functional is less strict in one dimension than that in higher dimensions. As proven in [12], to check the displacement convexity of the energy \( E[\mu] \) in one dimension, it is enough to check the convexity of the function \( w(r) \) for \( r > 0. \) Therefore, if \( w(r) \) is strictly convex in \((0, \infty), \) then the energy functional (1.1) is strictly displacement convex for probability measures with zero center of mass. As a consequence, the global minimizer of (1.1) in the set of probability measures is unique up to translations. Finally, the convexity of \( E_n \) in Lemma 3.2 is just the displacement convexity of the energy functional (1.1) restricted to discrete measures. We included the proofs of the convexity and uniqueness because they are quite straightforward in this case, without appealing to more involved concepts in optimal transportation.

**Remark** (Explicit convergence to uniform density). As a final example we consider the case where \( \gamma = 2, \alpha = 1, \) which corresponds to quadratic attraction and Newtonian repulsion in one dimension (see [23]). When \( x \) is a minimizer of \( E_n(x), \) we have by (2.7) that

\[
\sum_{j \neq k} (x_k - x_j) = \sum_{j \neq k} \text{sign}(x_k - x_j) = k - n - 1, \quad \forall \ k = 1, \ldots, n.
\]

Replacing the index \( k \) by \( k + 1, \) the equation becomes

\[
\sum_{j \neq k+1} (x_{k+1} - x_j) = \sum_{j \neq k+1} \text{sign}(x_{k+1} - x_j) = 2k - n + 1, \quad \forall \ k = 1, \ldots, n - 1.
\]

Subtracting the two equations above, we get

\[
n(x_{k+1} - x_k) = 2, \quad \forall \ k = 1, \ldots, n - 1,
\]

that is \( x_{k+1} - x_k = \frac{2}{n}, \) for all \( k = 1, \ldots, n - 1. \)

This shows that in the case \( \gamma = 2 \) and \( \alpha = 1, \) the points \( x_i \) are uniformly distributed; as \( n \) goes to infinity, the corresponding discrete measure \( \mu = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} \) converges to the uniform probability
measure on the interval \([-1, 1]\). This uniform density is known to be the global minimizer of the energy \(E[\mu]\) in the continuum setting, see \([17,23]\).

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