

Research



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Author for correspondence:

José Antonio Carrillo

e-mail: carrillo@imperial.ac.uk

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

José Antonio Carrillo¹, Michel Chipot² and
Yanghong Huang¹

¹Department of Mathematics, Imperial College London,
South Kensington, London SW7 2AZ, UK

²Institut für Mathematik, Angewandte Mathematik,
Winterthurerstrasse 190, 8057 Zürich, Switzerland

We consider the minimization of the repulsive–attractive power-law interaction energies that occur in many biological and physical situations. We show the existence of global minimizers in the discrete setting and obtain bounds for their supports independently of the number of Dirac deltas in a 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 μ be a probability measure on $\mathbb{R}^d$. We are interested in minimizing the interaction potential energy defined by

$$E[\mu] = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) \, d\mu(x) \, d\mu(y). \quad (1.1)$$

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

$$W(z) = w(|z|) = \frac{|z|^\gamma}{\gamma} - \frac{|z|^\alpha}{\alpha}, \quad \gamma > \alpha, \quad (1.2)$$

with the understanding that $|z|^\eta/\eta = \log |z|$ 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

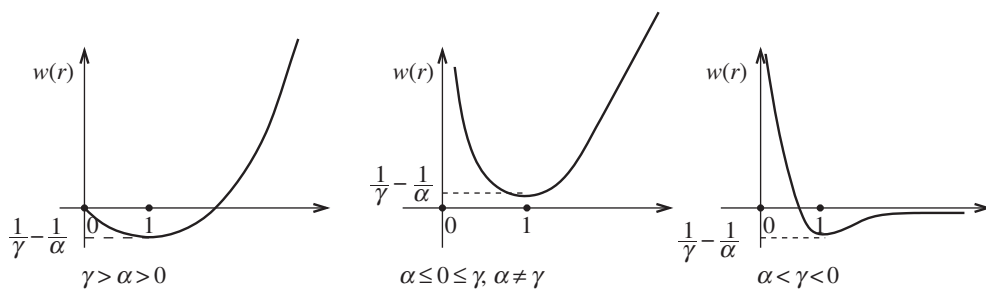


Figure 1. Three different behaviours of $w(r) = r^\gamma/\gamma - r^\alpha/\alpha$, $\gamma > \alpha$.

the signs of the exponents γ and α , the behaviour of the potential is depicted in figure 1. Because this potential W is bounded from below by $w(1) = 1/\gamma - 1/\alpha$, the energy $E[\mu]$ always makes sense, with possibly positive infinite values.

The minimizers of the energy $E[\mu]$ are related to stationary states for the aggregation equation $\rho_t = \nabla \cdot (\rho \nabla W * \rho)$ studied in [1–5] with repulsive–attractive potentials [6–12]. 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 [12,13]. In fact, it is shown in [12] 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 becomes stronger (i.e. α gets smaller) in three dimensions, 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 non-local interactions are ubiquitous in the literature. Convex attractive potentials appear in granular media [1,2,14,15]. More sophisticated potentials such as (1.2) are included to take into account short-range repulsion and long-range attraction in kinematic models of the collective behaviour of animals; see [13,16–19] and the references therein. The minimization of the interaction energy in the discrete setting is of paramount importance for the structure of virus capsids [20], for self-assembly materials in chemical engineering design [21–23] and for flock patterns in animal swarms [24–26].

Despite the efforts in understanding the qualitative behaviour of stationary solutions to the aggregation equation $\rho_t = \nabla \cdot (\rho \nabla W * \rho)$ 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 [27] for a recent analysis of this question in the more restricted set of bounded or binary densities. Here, we first try to find solutions in the restricted set of atomic measures.

The interest in understanding the global discrete minimizers of the interaction energy is not purely mathematical. The discrete global minimizers give the spatial profile of typical flocking patterns obtained in simplified models for social interaction between individuals as in [13,28] based on the famous three-zone models [29,30]. Moreover, owing to the recent nonlinear stability results in [26], we know now that the stability properties of the discrete global minimizer as the stationary solution of the first-order ordinary differential equation model

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

lead to the stability properties of the flock profiles for the second-order model in swarming introduced in [17] or additional alignment mechanisms such as the Cucker–Smale interaction [31,32]; see also [28] 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 the qualitative properties of the global minimizers in the set of equal-mass Dirac deltas. These discrete approximations are used extensively in materials science and variational calculus with hard-core potentials [33–36] in order to understand the crystallization phenomenon. However, these discrete approximations with soft potentials such as (1.2) are more difficult; apart from various properties of the minimizers [8,13,17,24], the existence as well as the convergence of these discrete minimizers are not established in general. In a certain range of exponents, we prove that the diameter of the support of the discrete minimizers does not depend on the number of Dirac deltas. This result, together with standard compactness arguments, results 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 the confinement of solutions of the aggregation equation in [37,38]. In our case, the ideas behind the proof in §2 are 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 is devoted to more refined results in one dimension. We show that, for very repulsive potentials, the bounds on the diameter are 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 one dimension. 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 first consider the discrete setting, where μ is a convex combination of Dirac deltas, i.e.

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

Setting

$$E_n(x_1, \dots, x_n) = \sum_{i \neq j}^n \left(\frac{|x_i - x_j|^\gamma}{\gamma} - \frac{|x_i - x_j|^\alpha}{\alpha} \right), \quad (2.1)$$

for such a μ , one has $E[\mu] = (1/(2n^2))E_n(x_1, \dots, x_n)$. In the definition of the energy, we can include the self-interaction for non-singular cases, $\alpha > 0$, because the two 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, owing to the translational invariance of the interaction energy, minimizers of the interaction energy $E[\mu]$ can be expected only up to translations. Moreover, when the potential is radially symmetric, as in our case, then any isometry in $\mathbb{R}^d$ also leaves invariant the interaction energy. These invariances are also inherited by the discrete counterpart $E_n(x_1, \dots, x_n)$. We first consider the minimizers of $E_n(x)$ among all $x = (x_1, \dots, x_n) \in (\mathbb{R}^d)^n$, 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,

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

which obviously vanishes for $r = 1$ and for $r = 0$ when $\alpha > 1$. We conclude, from the sign of the derivatives, that $w(r)$ always attains a global minimum at $r = 1$. There are, following the values of

$\alpha < \gamma$, three types of behaviour for w , which are shown in figure 1. In all three cases, E_n is bounded from below because

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

with the understanding that $|x|^\eta/\eta = \log |x|$ 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 $E_n(x_1, \dots, x_n)$, we can assume without loss of generality that $x_1 = 0$, which we do throughout this subsection. First, we have lemma 2.1 showing that I_n is achieved, which can be proved by discussing different ranges of the exponents γ and α .

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

Proof.

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 $x = (x_1, \dots, x_n) \in (\mathbb{R}^d)^n$ such that $x_1, \dots, x_n$ are aligned and $|x_i - x_{i+1}| = 1/n$. 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

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

Thus, because $x_1 = 0$, all the x_i have to be in the ball of centre 0 and radius $(n^2 \gamma / \alpha)^{1/(\gamma-\alpha)}$, i.e. x has to be in a compact set of $(\mathbb{R}^d)^n$. Because $E_n(x)$ 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. Because $w(r) \rightarrow +\infty$ as $r \rightarrow 0$ or $r \rightarrow \infty$, there exist $a_n, b_n > 0$ 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 pair i, j , one has

$$|x_i - x_j| < a_n \quad \text{or} \quad |x_i - x_j| > b_n, \quad (2.5)$$

then one has $E_n(x) > I_n$. Thus, the infimum (2.2) is not achieved among the points x satisfying (2.5) but among those in

$$\{x \in (\mathbb{R}^d)^n \mid a_n \leq |x_i - x_j| \leq b_n\}.$$

Because the set above is compact, being closed and contained in $(B(0, b_n))^n$ because $x_1 = 0$, 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 obtain $E_n(x) < 0$. Because $w(0^+) = +\infty$, we minimize E_n among the points x such that $x_i \neq x_j$, $i \neq j$. Thus, the summation is over $n^2 - n$ pairs (i, j) . Denote by $x^k = (x_1^k, \dots, x_n^k) \in (\mathbb{R}^d)^n$ a minimizing sequence of E_n . Because $w(r) \rightarrow +\infty$ as $r \rightarrow 0$, there exists a number $a_n < 1$ such that

$$w(a_n) > n(n-1) \left(\frac{1}{\alpha} - \frac{1}{\gamma} \right) > 0.$$

If, for a pair (i, j) , one has $|x_i^k - x_j^k| < a_n$, then

$$E(x^k) > w(a_n) + (n^2 - n - 1) \left(\frac{1}{\gamma} - \frac{1}{\alpha} \right) > \left(\frac{1}{\alpha} - \frac{1}{\gamma} \right) > 0$$

and x^k cannot be a minimizing sequence. So, without loss of generality, we may assume that $|x_i^k - x_j^k| \geq a_n$, $\forall i, j$. Let us denote by $y_1, \dots, y_d$ the coordinates in $\mathbb{R}^d$. Without loss of generality, we can assume by relabelling and isometry invariance that for every k one has

$$x_1^k = 0, \quad x_i^k \in \{y = (y_1, \dots, y_d) \mid y_d \geq 0\}.$$

Suppose that $x_i^k = (x_{i,1}^k, \dots, x_{i,d}^k)$ and the numbering of the points is done in such a way that $x_{i,d}^k \leq x_{i+1,d}^k$.

We next claim that one can assume that $x_{i+1,d}^k - x_{i,d}^k \leq 1$, $\forall i$. Indeed, if not, let i_0 be the first index such that

$$x_{i_0+1,d}^k - x_{i_0,d}^k > 1.$$

Let us leave the first x_i^k until i_0 unchanged and for $i > i_0$ replace x_i^k by

$$\tilde{x}_i^k = x_i^k - \{x_{i_0+1,d}^k - x_{i_0,d}^k - 1\}e_d,$$

where e_d is the d -vector of the canonical basis of $\mathbb{R}^d$, i.e. we shift x_i^k down in the direction e_d by $x_{i_0+1,d}^k - x_{i_0,d}^k - 1$. Denote by $\tilde{x}_i^k$, the new sequence obtained in this manner. One has

$$\begin{aligned} w(|\tilde{x}_i^k - \tilde{x}_j^k|) &< w(|x_i^k - x_j^k|), \quad \forall i \leq i_0 < j, \\ w(|\tilde{x}_i^k - \tilde{x}_j^k|) &= w(|x_i^k - x_j^k|), \quad \forall i_0 < i < j, \text{ or } i < j \leq i_0, \end{aligned}$$

and thus one has obtained a minimizing sequence with

$$\tilde{x}_{i_0+1,d}^k - \tilde{x}_{i_0,d}^k \leq 1, \quad \forall i,$$

i.e. $0 \leq x_{i,d}^k \leq n-1$, for all i .

Repeating this process in the other directions, one can assume without loss of generality that

$$x_i^k \in [0, n-1]^d \tag{2.6}$$

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 for the support of a minimizer of (2.2). However, these estimates depend on n . We 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 $x = (x_1, \dots, x_n) \in (\mathbb{R}^d)^n$ where the minimum of E_n is achieved, one has

$$0 = \nabla_{x_k} E_n(x_1, \dots, x_n) = \nabla_{x_k} \sum_{j \neq k} \left(\frac{|x_k - x_j|^\gamma}{\gamma} - \frac{|x_k - x_j|^\alpha}{\alpha} \right), \quad k = 1, 2, \dots, n.$$

Because $\nabla_x(|x|^\eta/\eta) = |x|^{\eta-2}x$, we obtain

$$\sum_{j \neq k} |x_k - x_j|^{\gamma-2}(x_k - x_j) = \sum_{j \neq k} |x_k - x_j|^{\alpha-2}(x_k - x_j), \quad k = 1, \dots, n. \quad (2.7)$$

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 obtain

$$\begin{aligned} \sum_{j \neq 1} |x_1 - x_j|^{\gamma-2}(x_1 - x_j) &= \sum_{j \neq 1} |x_1 - x_j|^{\alpha-2}(x_1 - x_j), \\ \sum_{j \neq n} |x_n - x_j|^{\gamma-2}(x_n - x_j) &= \sum_{j \neq n} |x_n - x_j|^{\alpha-2}(x_n - x_j). \end{aligned}$$

By subtraction, this leads to

$$\begin{aligned} &\sum_{j \neq 1, n} (|x_n - x_j|^{\gamma-2}(x_n - x_j) - |x_1 - x_j|^{\gamma-2}(x_1 - x_j)) + 2|x_n - x_1|^{\gamma-2}(x_n - x_1) \\ &= \sum_{j \neq n} |x_n - x_j|^{\alpha-2}(x_n - x_j) - \sum_{j \neq 1} |x_1 - x_j|^{\alpha-2}(x_1 - x_j). \end{aligned}$$

Taking the scalar product of both sides with $x_n - x_1$, we obtain

$$\begin{aligned} &\sum_{j \neq 1, n} (|x_n - x_j|^{\gamma-2}(x_n - x_j) - |x_1 - x_j|^{\gamma-2}(x_1 - x_j), x_n - x_1) + 2|x_n - x_1|^\gamma \\ &= \sum_{j \neq n} |x_n - x_j|^{\alpha-2}(x_n - x_j, x_n - x_1) - \sum_{j \neq 1} |x_1 - x_j|^{\alpha-2}(x_1 - x_j, x_n - x_1). \end{aligned}$$

For $\gamma \geq 2$, there exists a constant $C_\gamma > 0$ such that (see [39])

$$(|\eta|^{\gamma-2}\eta - |\xi|^{\gamma-2}\xi, \eta - \xi) \geq C_\gamma |\eta - \xi|^\gamma, \quad \forall \eta, \xi \in \mathbb{R}^d. \quad (2.8)$$

Note that this is nothing other than the modulus of convexity (in the sense of [2]) of the potential $|x|^\gamma$. Thus, estimating from above, we derive

$$\begin{aligned} ((n-2)C_\gamma + 2)|x_n - x_1|^\gamma &\leq \sum_{j \neq n} |x_n - x_j|^{\alpha-1}|x_n - x_1| + \sum_{j \neq 1} |x_1 - x_j|^{\alpha-1}|x_n - x_1| \\ &\leq 2(n-1)|x_n - x_1|^\alpha. \end{aligned}$$

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

$$|x_n - x_1| \leq \left(\frac{2}{C_\gamma \wedge 1} \frac{n-1}{n} \right)^{1/(\gamma-\alpha)} \leq \left(\frac{2}{C_\gamma \wedge 1} \right)^{1/(\gamma-\alpha)},$$

which proves the theorem in the case $\gamma \geq 2$. In the case where $1 < \gamma < 2$, one can replace (2.8) with

$$(|\eta|^{\gamma-2}\eta - |\xi|^{\gamma-2}\xi, \eta - \xi) \geq c_\gamma \{|\eta| + |\xi|\}^{\gamma-2} |\eta - \xi|^2, \quad \forall \eta, \xi \in \mathbb{R}^d,$$

for some constant c_γ (see [39]). We obtain, arguing as above,

$$\sum_{j \neq 1, n} c_\gamma \{|x_n - x_j| + |x_1 - x_j|\}^\gamma + 2|x_n - x_1|^\gamma \leq 2(n-1)|x_n - x_1|^\alpha.$$

Now because $\gamma - 2 < 0$, $|x_n - x_j| < |x_n - x_1|$ 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

$$|x_n - x_1| < \left\{ \frac{2}{(2^{\gamma-2}c_\gamma) \wedge 1} \right\}^{1/(\gamma-\alpha)},$$

which completes the proof of the theorem. ■

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

Theorem 2.3. *Suppose that $1 \leq \alpha < \gamma$. Then, global minimizers associated with the global minimum of $E_n(x)$ with zero centre of mass converge as $n \rightarrow \infty$ towards a global minimizer among all probability measures with bounded moments of order γ 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

$$\mu^n = \frac{1}{n} \sum_{j=1}^n \delta_{x_j^n}$$

be the associated discrete measure. From theorem 2.2, the radius of the supports of the measures μ^n is bounded uniformly in n by R , provided that the centre of the mass $\int_{\mathbb{R}^d} x \, d\mu^n$ is normalized to be the origin. By Prokhorov's theorem [40], $\{\mu^n\}$ is compact in the weak-* topology of measures and also in the metric space induced by γ -Wasserstein distance d_γ between probability measures (see [41,42] for definition and basic properties). Then, there is a measure μ^* supported on $B(0, R)$ such that

$$\mu^n \rightharpoonup \mu^* \quad \text{and} \quad d_\gamma(\mu^n, \mu^*) \rightarrow 0$$

as n goes to infinity. Note that the notion of convergence of a sequence of probability measures in d_γ is equivalent to weak convergence of the measures plus convergence of the moments of order γ ; see [42, ch. 9]. Let ν be any probability measure on $\mathbb{R}^d$ with bounded moment of order γ ; then $E[\nu] < \infty$. Moreover, there is a sequence of discrete measures ν^n of the form

$$\nu^n = \frac{1}{n} \sum_{j=1}^n \delta_{y_j^n},$$

such that $d_\gamma(\nu^n, \nu) \rightarrow 0$, and thus $\nu^n \rightharpoonup \nu$; see [41,42]. 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, because

$$d_\gamma(\mu^n \otimes \mu^n, \mu^* \otimes \mu^*) \rightarrow 0, \quad d_\gamma(\nu^n \otimes \nu^n, \nu \otimes \nu) \rightarrow 0,$$

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

$$\begin{aligned} E[\mu^*] &= \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) \, d\mu^*(x) \, d\mu^*(y) = \lim_{n \rightarrow \infty} \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) \, d\mu^n(x) \, d\mu^n(y) \\ &\leq \lim_{n \rightarrow \infty} \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) \, d\nu^n(x) \, d\nu^n(y) = E[\nu]. \end{aligned}$$

Therefore, μ^* must be a global minimizer of $E[\mu]$ in the set of probability measures with bounded moments of order γ . ■

Remark 2.4. The convergence of the minimizers of E_n can be proved also in the general framework of Γ -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 [35] and general measure quantization of power repulsion–attraction potentials [43].

Remark 2.5. 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 this 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 2.6. 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 γ th moments of the minimizers. First, if $x = (x_1, \dots, x_n) \in (\mathbb{R}^d)^n$ is a minimizer of E_n with centre of mass at the origin, then by (2.3) and Hölder inequality

$$\sum_{i,j} \frac{|x_i - x_j|^\gamma}{\gamma} < \sum_{i,j} \frac{|x_i - x_j|^\alpha}{\alpha} < \left(\sum_{i,j} \frac{|x_i - x_j|^\gamma}{\gamma} \right)^{\alpha/\gamma} \left(n^2 \gamma^{\alpha/(\gamma-\alpha)} \alpha^{-\gamma/(\gamma-\alpha)} \right)^{(\gamma-\alpha)/\gamma},$$

or equivalently

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

Because 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

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

As a consequence, we obtain a uniform bound on the γ th moment of the discrete minimizers. As a result, the minimizing sequence corresponding to the associated atomic measures is tight, leading also towards a global minimizer of $E[\mu]$.

3. Further remarks in one dimension

Here, 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 obtain 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 the global minimizers in the discrete setting does not hold. If x is a minimizer of $E_n(x)$, we always assume that the labelling of the x_i is in increasing order: $x_1 \leq x_2 \leq \dots \leq x_n$.

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,

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

holds.

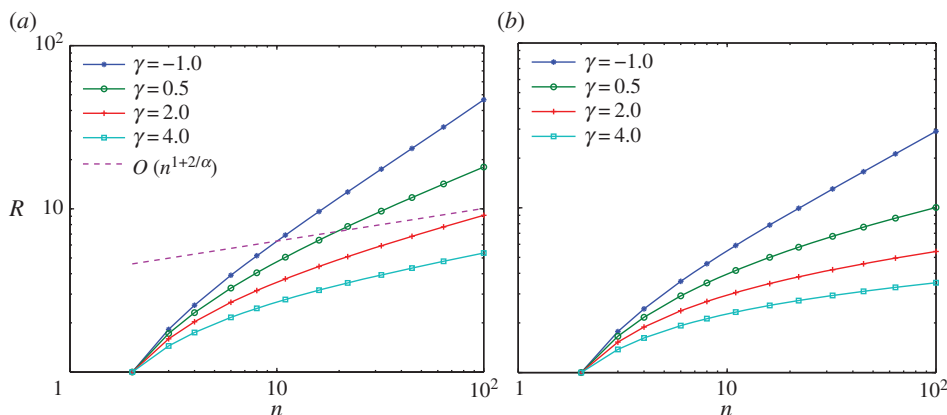


Figure 2. The dependence of the diameter $R = \max_{i,j} |x_i - x_j|$ on the number of particles n : (a) $\alpha = -2.5$; (b) $\alpha = -1.5$. (Online version in colour.)

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

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

If x is a minimizer of E_n , we claim that

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

Indeed, otherwise,

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

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

$$Cn^2 = \frac{a_n^\gamma}{\gamma} - \frac{a_n^\alpha}{\alpha} = -\frac{a_n^\alpha}{\alpha} \left(1 - \frac{\alpha}{\gamma} a_n^{\gamma-\alpha} \right) \geq -\frac{a_n^\alpha}{2\alpha},$$

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

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

Combining this with (3.2), we obtain

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

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

This property for the minimizers of this very repulsive case is similar to H-stability in statistical mechanics [44], 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 $O(n^{1+2/\alpha})$ is not sharp, which is verified in figure 2.

In fact, numerical experiments in [12,38] suggest that confinement happens for $-1 < \alpha < 1$. It is an open problem to obtain a uniform bound in the support of the discrete minimizers as in §2 in this range. In the range $\alpha \leq -1$, our numerical simulations suggest that spreading of the support happens for all γ , with a decreasing spreading rate as γ increases. For hard-core potentials considered in [33–36], 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 number of discrete minimizers (partially due to symmetries) are expected, and the uniqueness can be shown only in the macroscopic limit [35]. If x is a minimizer of $E_n(x)$, we can always assume at the expense of a translation that the centre of mass is zero, that is $(x_1 + \dots + x_n)/n = 0$. Let us recall that

$$E_n(x) = \sum_{i \neq j}^n w(|x_i - x_j|),$$

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

$$\frac{x_1 + \dots + x_n}{n} = 0, \quad x_1 \leq x_2 \leq \dots \leq x_n, \quad (3.3a)$$

and

$$\frac{y_1 + \dots + y_n}{n} = 0, \quad y_1 \leq y_2 \leq \dots \leq y_n. \quad (3.3b)$$

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 ,

$$\begin{aligned} E_n\left(\frac{x+y}{2}\right) &= \sum_{i \neq j}^n w\left(\left|\frac{x_i + y_i}{2} - \frac{x_j + y_j}{2}\right|\right) \\ &= \sum_{i \neq j}^n w\left(\left|\frac{x_i - x_j}{2} + \frac{y_i - y_j}{2}\right|\right) \\ &\leq \frac{1}{2} \left(\sum_{i \neq j}^n w(|x_i - x_j|) + \sum_{i \neq j}^n w(|y_i - y_j|) \right) = \frac{E_n(x) + E_n(y)}{2}. \end{aligned}$$

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, $x = y$. ■

As a consequence, we can now state the following result regarding the uniqueness of global discrete minimizers.

Theorem 3.3. Suppose that $\alpha \leq 1$, $\gamma \geq 1$ and $\alpha < \gamma$. Up to translations, the minimizer x of E_n is unique and symmetric with respect to its centre 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 $s(\xi) = -\xi$, $\xi \in \mathbb{R}$. If x is a minimizer of $E_n(x)$ satisfying (3.3a) then y defined by

$$y_i = s(x_{n+1-i}), \quad i = 1, \dots, n,$$

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

$$x_i = -x_{n+1-i}, \quad i = 1, \dots, n,$$

and this completes the proof of the theorem. ■

Remark 3.4 (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 McCann [45] 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 centre 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 in higher dimensions. As proved in [46], 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 centre of mass. As a consequence, the global minimizer of (1.1) in the set of probability measures is unique up to translations. Lemma 3.2 shows that this condition is equivalent to $\alpha \leq 1$, $\gamma \geq 1$ and $\alpha < \gamma$, for power-law potentials. 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 3.5 (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 [6]). When x is a minimizer of $E_n(x)$, we have by (2.7) that

$$\sum_{j \neq k} (x_k - x_j) = \sum_{j \neq k} \text{sign}(x_k - x_j) = 2k - n - 1, \quad \forall k = 1, \dots, n.$$

Replacing the index k by $k + 1$, the equation becomes

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

Subtracting the two equations above, we obtain

$$n(x_{k+1} - x_k) = 2, \quad \forall k = 1, \dots, n - 1,$$

that is $x_{k+1} - x_k = 2/n$, for all $k = 1, \dots, n - 1$.

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 $\mu = (1/n) \sum_{i=1}^n \delta_{x_i}$ 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 [6,27].

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