CLASSIFYING MINIMUM ENERGY STATES FOR INTERACTING PARTICLES (II) — REGULAR SIMPLICES

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Abstract. Consider densities of particles on $\mathbf{R}^n$ which interact pairwise through an attractive-repulsive power-law potential $W_{\alpha,\beta}(x) = |x|^\alpha/\alpha - |x|^\beta/\beta$ in the mildly repulsive regime $\alpha \geq \beta \geq 2$. For $n \geq 2$, we show there exists $\beta_n \in (2, 4)$ and a decreasing homeomorphism α_{Δ^n} of $[2, \beta_n]$ onto $[\beta_n, 4]$ which can be extended (non-homeomorphically) by setting $\alpha_{\Delta^n}(\beta) = \beta$ for $\beta > \beta_n$ such that: distributing the particles uniformly over the vertices of a regular unit diameter n-simplex minimizes the potential energy if and only if $\alpha \geq \alpha_{\Delta^n}(\beta)$. Moreover this minimum is uniquely attained up to rigid motions when $\alpha > \alpha_{\Delta^n}(\beta)$. We estimate $\alpha_{\Delta^n}(\beta)$ above and below, and identify its limit as the dimension grows large. These results are derived from a new northeast comparison principle in the space of exponents. At the endpoint $(\alpha, \beta) = (4, 2)$ of this transition curve, we characterize all minimizers by showing they lie on a sphere and share all first and second moments with the spherical shell. Suitably modified versions of these statements are also established for $n = 1$, and for the attractive-repulsive potentials $D_\alpha(x) = |x|^\alpha(\alpha \log |x| - 1)$ that arise in the limit $\beta \nearrow \alpha$.

Keywords: attractive-repulsive power-law potential, pattern formation, interaction energy, simplex, unique minimum, symmetry breaking, mild repulsion, aggregation dynamics, infinite-dimensional quadratic program, L^∞-Kantorovich-Rubinstein-Wasserstein, d_∞-local
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1. Introduction

Particles interacting through long-range attraction and short-range repulsion given by differences of power-laws have been used to model a range of physical [20] [15] and biological [26] [5] [18] systems, to predict or explain many of

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the patterns they display [1] [4] [19] [30]. For very few values of the attractive and repulsive exponents (α, β) are the energy minimizing configurations of particles explicitly known; see however [6] [9] [10] [11] [12] [13] [14] [23]. Here we complement these results, which apart from [23] concern $\beta \geq 2$, by showing that for a region containing the intersection of the infinite rectangle $(\alpha, \beta) \in [4, \infty) \times [2, \infty) \setminus \{(4, 2)\}$ with the triangle $\alpha > \beta$, the minimizer consists precisely of those configurations which equidistribute their particles over the vertices of an appropriately sized simplex, i.e. an equilateral triangle in two dimensions and a regular tetrahedron in three. We are able to give a detailed description the region in question, and explain precisely how uniqueness of these minimizers fails at its corner $(\alpha, \beta) = (4, 2)$.

Let us recall the setting and notation from our companion work [12]: The self-interaction energy of a collection of particles with mass distribution $d\mu(x) \geq 0$ on $\mathbf{R}^n$ is given by

$$\mathcal{E}_W(\mu) = \frac{1}{2} \iint_{\mathbf{R}^n \times \mathbf{R}^n} W(x - y) d\mu(x) d\mu(y), \tag{1.1}$$

assuming the particles interact with each other through a pair potential $W(x)$. Normalizing the distribution to have unit mass ensures that μ belongs to the space $\mathcal{P}(\mathbf{R}^n)$ of Borel probability measures on $\mathbf{R}^n$.

Our goal is to identify global energy minimizers of $\mathcal{E}_W(\mu)$ on $\mathcal{P}(\mathbf{R}^n)$, for *power-law* potentials $W = W_{\alpha,\beta}$ where

$$W_\alpha(x) := |x|^\alpha / \alpha \quad \text{and} \tag{1.2}$$

$$W_{\alpha,\beta}(x) := W_\alpha(x) - W_\beta(x) \quad \alpha > \beta > -n, \tag{1.3}$$

with the appropriate convention if $\alpha = 0$ or $\beta = 0$ [3]. In this paper we focus exclusively on the mildly repulsive regime $\beta \geq 2$ of [8], and its frontier $\beta = 2$. The latter is called the centrifugal line in [23], since, at least on $\mathbf{R}^2$, the potential $-W_2$ induces the outward force which particles rotating uniformly around their common center of mass seem to experience in a corotating reference frame; see e.g. [25]. On this frontier the energy also acts as a Lyapunov function of the rescaled dynamics of the purely attractive Patlak-Keller-Segel [26] [18] model in self-similar variables around the time of blow-up [28]. On the segment $(\alpha, \beta) \in (2, 4) \times \{2\}$, our companion paper shows the minimizer is uniquely given (up to translations) by a spherical shell — i.e. the uniform probability measure on a spherical hypersurface — at least if $n \geq 2$.

For $\alpha \geq 4$ and $\alpha > \beta \geq 2$ but $(\alpha, \beta) \neq (4, 2)$, we now show that the minimizer is uniquely given (apart from rotations and translations) by the measure $\nu = \nu_1$ which equidistributes its mass over the vertices of a regular, unit diameter, n-simplex, defined below, i.e. an equilateral triangle if $n = 2$ and a regular tetrahedron if $n = 3$. These results answer a question of Sun, Uminsky and Bertozzi, by showing that the linear stability of selfsimilar blow-up which they found for the aggregation dynamics in these two complementary regimes can be improved to a nonlinear stability result. This improvement is explained in [12]; for spherically symmetric perturbations of the spherical shell, such an improvement was already found by Balagué et al [2], while asymptotic stability of measures on the simplex vertices was addressed by Simione [27]. On the other hand, at the threshold exponent separating these two regimes, we will show that although all centered convex combinations of the configurations mentioned above remain mimimizers, there are many additional minimizers as well: indeed for $(\alpha, \beta) = (4, 2)$ the centered minimizers consist precisely of all measures supported on the minimizing spherical shell which share its moments up to order 2. When $n \geq 2$, this case is distinguished from $\alpha \neq 4$ by the fact that the attractor formed by global energy minimizers becomes infinite-dimensional.

In the mildly repulsive region $\alpha > \beta \geq 2$, two of us recently showed the existence of a finite threshold $\alpha_{\Delta^n}(\beta) < \infty$ above which the energy is uniquely minimized by ν_1 and its rotates and translates [23]. In the current manuscript, we estimate $\alpha_{\Delta^n}(\beta) \leq \max\{\beta, 4\}$ concretely, showing equality holds when $\beta = 2 \leq n$ and finding the high dimensional limiting threshold explicitly in the broader range $\beta > 2$. We also show it is impossible for ν_1 to minimize $\mathcal{E}_{W_{\alpha,\beta}}$ for any $\alpha < \alpha_{\Delta^n}(\beta)$. Further results concerning α_{Δ^n} are established in §4 below and summarized in Remark 1.5.

To describe our conclusions, it will be convenient to recall the following class of sets and measures which were the main object of study in [22] [23]. We say that a set $K \subseteq \mathbf{R}^n$ is called a regular k-simplex if it is the convex hull of $k+1$ points $\{x_0, x_1, ..., x_k\}$ in $\mathbf{R}^n$ satisfying $|x_i - x_j| = d$ for some $d > 0$ and all $0 \leq i < j \leq k$. The points $\{x_0, x_1, ..., x_k\}$ are called *vertices* of the simplex. In particular, it is called a *unit k-simplex* if $d = 1$. We also define the following set of measures:

$$\begin{aligned} \mathcal{P}_{\Delta^n} := \{\nu \in \mathcal{P}(\mathbf{R}^n) \mid \nu &\text{ is uniformly distributed over} \\ &\text{the vertices of a unit } n\text{-simplex.}\} \end{aligned} \tag{1.4}$$

In particular $\mathcal{P}_{\Delta^1} = \{\frac{1}{2}(\delta_a + \delta_{a+1}) \mid a \in \mathbf{R}\}$. Let $\mathcal{P}^0_{\Delta^n} = \mathcal{P}_{\Delta^n} \cap \mathcal{P}_0(\mathbf{R}^n)$ where $\mathcal{P}_0(\mathbf{R}^n)$ denotes the centered probability measures on $\mathbf{R}^n$ — meaning those having finite first moments and satisfying

$$\int_{\mathbf{R}^n} x \, d\mu(x) = 0. \tag{1.5}$$

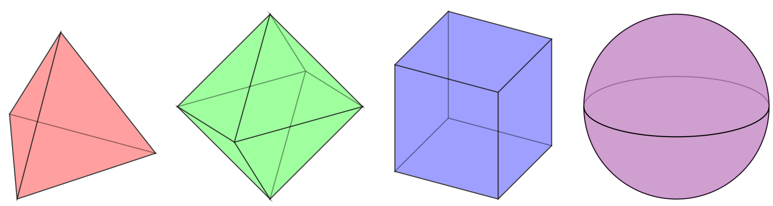
We can now present our results. Let Id denote the $n \times n$ identity matrix.

Theorem 1.1 (Characterizing energy minimizers at $(\alpha, \beta) = (4, 2)$)**.** *A measure $\mu \in \mathcal{P}_0(\mathbf{R}^n)$ minimizes $\mathcal{E}_{W_{4,2}}$ in* (1.1) *if and only if μ is concentrated on the centered sphere of radius $\sqrt{\frac{n}{2n+2}}$ and has*

$$\int x \otimes x \, d\mu(x) = \left(\int x_i x_j d\mu(x) \right)_{1 \leq i,j \leq n} = \frac{1}{2n+2} \mathrm{Id}. \tag{1.6}$$

Notice, if $n=1$, $\frac{\delta_{-1/2}+\delta_{1/2}}{2} \in \mathcal{P}_{\Delta^1}$ is the only minimizer in $\mathcal{P}_0(\mathbf{R})$. For $n=3$, several inequivalent minimizers are illustrated in Figure 1.

FIGURE 1. Convex hulls of supports of sample minimizers of $\mathcal{E}_{W_{4,2}}$ in $\mathcal{P}_0(\mathbf{R}^3)$. Each of these four minimizers is inscribed in the sphere of radius $\sqrt{3/8}$ and has mass uniformly distributed over the set of extreme points of the convex hull of its support. Moreover, rotates and convex combinations of any of these minimizers are also minimizers. This implies that general minimizers of $\mathcal{E}_{W_{4,2}}$ need not have any rotational symmetries.



Now for each $\alpha > \beta$, let

$$A_{\alpha,\beta} = \{(\alpha', \beta') \in \mathbf{R}^2 \mid \alpha' > \beta',\ \alpha' \geq \alpha,\ \beta' \geq \beta,\ (\alpha', \beta') \neq (\alpha, \beta)\}$$

denote the region of parameters lying north, east, or northeast of (α, β).

Theorem 1.2 (Northeast comparison of simplex energies and potentials)**.** *Let $\alpha > \beta > 0$. If $\nu \in \mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{W_{\alpha,\beta}}$ on $\mathcal{P}(\mathbf{R}^n)$, then for $(\alpha', \beta') \in A_{\alpha,\beta}$,*

$$\mathcal{P}_{\Delta^n} = \operatorname*{argmin}_{\mathcal{P}(\mathbf{R}^n)} \mathcal{E}_{W_{\alpha',\beta'}} \quad \text{and} \quad \operatorname{spt} \nu = \operatorname*{argmin}_{\mathbf{R}^n} (\nu * W_{\alpha',\beta'}). \tag{1.7}$$

Remark 1.3 (One dimension)**.** *If $n=1$, our companion paper [12] shows $\mathcal{P}_{\Delta^1}$ uniquely minimizes $\mathcal{E}_{W_{\alpha,2}}$ for all $\alpha \geq 3$. Kang, Kim, Lim and Seo [16, Theorem 2] on the other hand showed $\mathcal{P}_{\Delta^1}$ is not a d_∞-local minimizer, hence not a global minimizer, in the range $\beta = 2 < \alpha < 3$.*

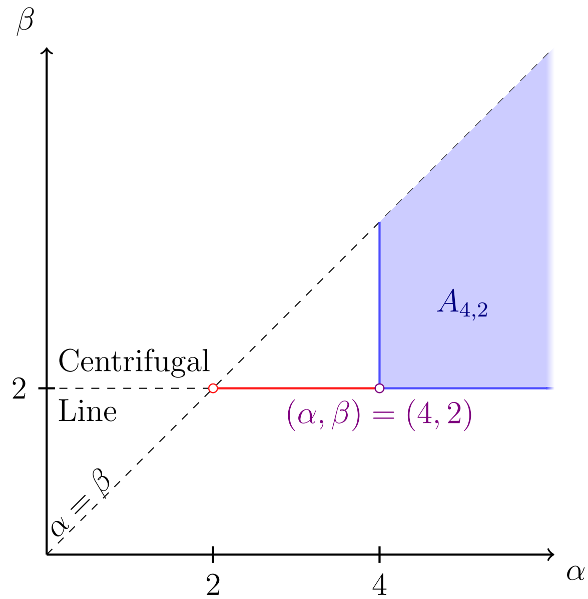
Set

$$4^* := \begin{cases} 3 & \text{if } n=1 \\ 4 & \text{otherwise.} \end{cases} \tag{1.8}$$

Notice Theorems 1.1, 1.2 and Remark 1.3 imply the following corollary; see also Figure 2.

Corollary 1.4 (Simplices minimize for $\alpha \geq \max\{4^*, \beta\}$)**.** *For each $(\alpha, \beta) \in A_{4^*,2}$, $\mathcal{P}_{\Delta^n}$ uniquely minimizes $\mathcal{E}_{W_{\alpha,\beta}}$ on $\mathcal{P}(\mathbf{R}^n)$.*

FIGURE 2. Partial phase diagram of the mildly repulsive region $\alpha > \beta \geq 2$ for $n \geq 2$: on the red segment linking $(2,2)$ to $(4,2)$, energy is uniquely minimized by a spherical shell [12]. In the blue region, $A_{4,2}$, it is minimized precisely by the elements in $\mathcal{P}_{\Delta^n}$. At $(\alpha, \beta) = (4,2)$, the energy is minimized by any convex combination of the above configurations, but also admits other minimizers.



Remark 1.5 (Transition threshold). *Our theorems imply that for each $\beta \geq 2$ there exists a transition threshold $\alpha_{\Delta^n}(\beta) \in [\beta, \infty)$ in the sense that $\mathcal{P}_{\Delta^n}$ uniquely minimizes $\mathcal{E}_{W_{\alpha,\beta}}$ for all $\alpha > \alpha_{\Delta^n}(\beta)$, while $\mathcal{P}_{\Delta^n}$ fails to be a minimizer for all $\alpha \in (\beta, \alpha_{\Delta^n}(\beta))$. Also, $\alpha_{\Delta^n}(2) = 4^*$ and there exists $\beta_n \in (2, 4^*]$ such that $\alpha_{\Delta^n}(\beta) = \beta$ for $\beta > \beta_n$, and $\alpha_{\Delta^n} : [2, \beta_n] \longrightarrow [\beta_n, 4^*]$ is nonincreasing. Theorem 4.1 improves this by showing $\alpha_{\Delta^n} : [2, \beta_n] \longrightarrow [\beta_n, 4^*]$ is continuous and strictly decreasing, with $\alpha_{\Delta^n}(\beta_n) = \beta_n \in (2, 4^*)$. In addition, Propositions 4.8 and 4.13 provide dimension-dependent lower bounds $\underline{\alpha}_{\Delta^n} \leq \underline{\alpha}^+_{\Delta^n}$ for α_{Δ^n}, and Proposition 4.6 provides an upper bound α^*_∞ for α_{Δ^n}, which is dimension independent for all $n \geq 2$. These bounds become sharp in the limit $n \to \infty$, and also provide estimates for β_n. Even so, it would be interesting to know the value of β_n and of $\alpha_{\Delta^n}(\beta)$ in the range $\beta \in (2, \beta_n)$ more precisely. For example, might $\alpha_{\Delta^n} \equiv \underline{\alpha}^+_{\Delta^n}$?*

Remark 1.6 (Open global minimization problems). *An interesting open problem is to determine the structure of minimizers of $\mathcal{E}_{W_{\alpha,\beta}}$ for $2 < \beta < \alpha < \alpha_{\Delta^n}(\beta)$. Carrillo, Figalli, and Patacchini showed the supports of such minimizers must have finite cardinality, and placed a bound on this cardinality, but little else is known about this subregime [8]. If $n = 1$ and $\beta = 2$, global minimizers of $\mathcal{E}_{W_{\alpha,2}}$*

remain elusive even along the segment $(\alpha, \beta) \in (2,3) \times \{2\}$ of the centrifugal line, as neither [8] nor the present work treat that regime.

Finally, taking the limit $\beta \to \alpha$ for the rescaled potential $\overline{W}_{\alpha,\beta} = \frac{\alpha\beta}{\alpha-\beta} W_{\alpha,\beta}$ (which has minimum value -1), leads us to introduce the following new class of interaction kernels,

$$D_\alpha(x) := \alpha^2 \frac{\partial}{\partial \alpha} W_{\alpha,\beta}(x) = |x|^\alpha (\alpha \log |x| - 1), \quad \alpha \in \mathbf{R} \setminus \{0\} \tag{1.9}$$

which form another intriguing one-parameter family of attractive-repulsive potentials uniquely minimized at $|x| = 1$. Taking $W = D_\alpha$ in (1.1), we can relate the minimizers of $\mathcal{E}_{W_{\alpha,\beta}}$ to those of $\mathcal{E}_{D_\alpha}$ by the following corollary to the proof of Theorem 1.2.

Corollary 1.7 (Relation to minimizers of limiting potential). *If $\mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{W_{\alpha,\beta}}$ for some $\alpha > \beta > 0$, then $\mathcal{P}_{\Delta^n}$ uniquely minimizes $\mathcal{E}_{D_\gamma}$ on $\mathcal{P}(\mathbf{R}^n)$ for all $\gamma \geq \alpha$. Conversely, if $\mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{D_\beta}$ for some $\beta > 0$, then $\mathcal{P}_{\Delta^n}$ uniquely minimizes $\mathcal{E}_{W_{\alpha,\beta}}$ on $\mathcal{P}(\mathbf{R}^n)$ for all $\alpha > \beta$. Thus from Remark 1.5, $\mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{D_\alpha}$ uniquely if $\alpha > \beta_n$, and fails to minimize $\mathcal{E}_{D_\alpha}$ if $0 < \alpha < \beta_n$.*

2. Classifying minimizers at $(\alpha, \beta) = (4, 2)$

Our first task is to adapt Lopes' proof [21] of energetic convexity from densities to measures in Lemma 2.2, extracting conditions for strict convexity; see [7] and [12] for the analogous extension in the interval $(\alpha, \beta) \in (2, 4) \times \{2\}$, whose endpoint we now analyze.

Definition 2.1 (Second moment tensor). *The second moment tensor for $\mu \in \mathcal{P}(\mathbf{R}^n)$ is the $n \times n$ matrix given by*

$$I(\mu) = \int x \otimes x \, d\mu(x) = \left(\int x_i x_j d\mu(x) \right)_{i,j \in \{1,\dots,n\}}. \tag{2.1}$$

Lemma 2.2 (Moment criteria for strict convexity). *For any $\mu_0, \mu_1 \in \mathcal{P}_0(\mathbf{R}^n)$ having finite fourth moments, set $a(t) := \mathcal{E}_{W_4}(\mu_t)$ where $\mu_t := (1-t)\mu_0 + t\mu_1$. Then $a(t)$ is convex, and depends affinely on $t \in [0,1]$ if and only if $I(\mu_0) = I(\mu_1)$.*

Proof. Fix $\mu_0, \mu_1 \in \mathcal{P}_0(\mathbf{R}^n)$ with fourth moments. Since $\mathcal{E}_{W_4}(\mu)$ is a quadratic function of μ, we see $a''(t) = 2\mathcal{E}_{W_4}(\mu_0 - \mu_1)$. Thus convexity and affinity of $a(t)$ on $t \in [0,1]$ depend on the sign of

$$8\mathcal{E}_{W_4}(\mu_0 - \mu_1) = \iint_{\mathbb{R}^n \times \mathbb{R}^n} |x - y|^4 d(\mu_0 - \mu_1)(x) d(\mu_0 - \mu_1)(y).$$

Vanishing of the zeroth and first moments of $\eta := \mu_0 - \mu_1$ allows us to express $\mathcal{E}_{W_4}(\eta)$ as the following sum of squares involving the second moment tensors $I(\eta) := I(\mu_0) - I(\mu_1)$ from (2.1)

$$\begin{aligned}8\mathcal{E}_{W_4}(\eta) &= \iint_{\mathbf{R}^n\times\mathbf{R}^n}[4(x\cdot y)^2+2|x|^2|y|^2]d\eta(x)d\eta(y)\\ &= 4\operatorname{Tr}(I(\eta)^2)+2(\operatorname{Tr} I(\eta))^2.\end{aligned}$$

Thus $\mathcal{E}_{W_4}(\eta)\geq 0$ with equality if and only if $I(\mu_0)=I(\mu_1)$, as desired. □

Lemma 2.3 (Second moments for measures on centered spheres)**.** *Let $\mathbf{S}_r$ be the centered sphere of radius r in $\mathbf{R}^n$, and let $\mu\in\mathcal{P}(\mathbf{S}_r)$. If $I(\mu)=\lambda\mathrm{Id}$ for some $\lambda>0$, then $I(\mu)=I(\sigma_r)$ where σ_r is the uniform probability on $\mathbf{S}_r$.*

Proof. If $I(\mu)=\lambda\mathrm{Id}$, any rotation $R\mu$ of μ has the same second moment tensor $I(R\mu)=I(\mu)$. Now if we uniformize μ by averaging over its rotations, the resulting measure σ_r will have the same second moment tensor as μ due to the linearity of I. □

It is plausible that the following lemma is known, but lacking a reference we provide a proof for the sake of clarity and completeness.

Lemma 2.4 (Minimizing moments under moment constraints)**.** *Let $0<p<q<\infty$, $C>0$ and $\mu_0\in\mathcal{P}(\mathbf{R}^n)$. Then*

$$\mu_0\in\operatorname{argmin}\left\{\int|x|^q d\mu(x)\;\middle|\;\mu\in\mathcal{P}(\mathbf{R}^n),\ \int|x|^p d\mu(x)=C\right\}$$

if and only if μ_0 is concentrated on the centered sphere of radius $C^{1/p}$.

Proof. Let $m(x)=|x|$ be the modulus map for $x\in\mathbf{R}^n$, and let $\eta:=m_\#(\mu)\in\mathcal{P}(\mathbf{R}_+)$ be the push-forward of $\mu\in\mathcal{P}(\mathbf{R}^n)$ by the map m. Then $\int_{\mathbf{R}^n}|x|^p d\mu(x)=\int_0^\infty r^p d\eta(r)$ for any $p>0$. Hence from now on we assume $\eta\in\mathcal{P}(\mathbf{R}_+)$ and $\int r^p d\eta(r)=C$. Recall Jensen's inequality, which states that if $f:\mathbf{R}\to\mathbf{R}$ is convex and X is a real-valued random variable with average value $E[X]$, then $E[f(X)]\geq f(E[X])$, and equality holds if and only if f is linear on the interval $[\inf X,\sup X]$. With $f(r)=r^{q/p}$, Jensen's inequality yields $\int r^q d\eta(x)\geq\left(\int r^p d\eta(x)\right)^{q/p}=C^{q/p}$, and moreover equality holds if and only if η is supported at a point in $\mathbf{R}_+$, since f is strictly convex on $\mathbf{R}_+$. This proves the lemma. □

Proof of Theorem 1.1. Define

$$F(\mu)=\frac{1}{4}\iint|x-y|^4d\mu(x)d\mu(y),\ G(\mu)=\frac{1}{2}\iint|x-y|^2d\mu(x)d\mu(y)$$

so that $2E=F-G$. Then for $\mu\in\mathcal{P}_0(\mathbf{R}^n)$,

$$G(\mu)=\int|x|^2d\mu(x)=\operatorname{Tr} I(\mu)$$

is no longer quadratic, but depends linearly on μ instead. Applying the calculation from the proof of Lemma 2.2, modified slightly to account for the fact that $\int d\mu = 1$ whereas $\int d\eta = 0$, we get:

$$F(\mu) = \frac{1}{2}\int |x|^4 d\mu(x) + \frac{1}{2}(\mathrm{Tr}\, I(\mu))^2 + \mathrm{Tr}(I(\mu)^2).$$

Thus the energy $\mathcal{E}_{W_{4,2}}$ is convex, and by Lemma 2.2 its minimizers must all share the same second moment tensor. Convexity also implies $\mathcal{E}_{W_{4,2}}$ admits a spherically symmetric minimizer. This yields that this common second moment tensor must be $\lambda\mathrm{Id}$ for some $\lambda > 0$ to be determined. This leads us to define

$$A_\lambda = \{\mu \in \mathcal{P}_0(\mathbf{R}^n) \mid I(\mu) = \lambda \mathrm{Id}\}.$$

For the correct choice of λ, A_λ contains all minimizers of (1.1), and moreover by the above formulas for F and G, for every $\mu \in A_\lambda$ we have

$$2E(\mu) = \frac{1}{2}\int |x|^4 d\mu(x) + \frac{1}{2}n^2\lambda^2 + n\lambda^2 - n\lambda. \tag{2.2}$$

This leads us to consider minimizing the fourth moment over A_λ. Set

$$B_\lambda = \{\mu \in \mathcal{P}_0(\mathbf{R}^n) \mid \mathrm{Tr}\, I(\mu) = n\lambda\}.$$

Notice $A_\lambda \subseteq B_\lambda$. Now Lemma 2.4 asserts that μ minimizes $\int |x|^4 d\mu(x)$ over B_λ if and only if μ is concentrated on the centered sphere of radius $r := \sqrt{n\lambda}$. But observe that σ_r, the uniform probability on the sphere of radius r, also belongs to A_λ. This yields that the set of minimizers $X \subseteq \mathcal{P}_0(\mathbf{R}^n)$ for (1.1) is precisely the following:

$$\begin{aligned} X &:= \{\mu \in \mathcal{P}_0(\mathbf{R}^n) \cap \mathcal{P}(\mathbf{S}_{\sqrt{n\lambda}}) \mid I(\mu) = \lambda\mathrm{Id}\} \\ &= \{\mu \in \mathcal{P}_0(\mathbf{R}^n) \cap \mathcal{P}(\mathbf{S}_{\sqrt{n\lambda}}) \mid I(\mu) = c\mathrm{Id} \ \text{ for some } c > 0\} \end{aligned} \tag{2.3}$$

where $\mathbf{S}_r$ is the centered sphere of radius r in $\mathbf{R}^n$, and the second equality is due to Lemma 2.3. Notice X is convex since I is linear in μ.

Finally let us determine the optimal λ. By (2.2), $2E(\mu) = n^2\lambda^2 + n\lambda^2 - n\lambda$ for any $\mu \in X$, and $\frac{dE}{d\lambda} = 0$ gives $\lambda = \frac{1}{2n+2}$, hence $r = \sqrt{n\lambda} = \sqrt{\frac{n}{2n+2}}$ as claimed. $\square$

Example 2.5 (Infinite-dimensional attractor at transition threshold)**.** *If $(\alpha, \beta) = (4, 2)$, then the spherical shell σ_r of radius $r := \sqrt{\frac{n}{2n+2}}$ is a minimizer. For others, let $\{e_i\}$ be the standard basis of $\mathbf{R}^n$. Then the probability $\frac{1}{2n}\sum_{i=1}^n (\delta_{re_i} + \delta_{-re_i})$ clearly belongs to the set $X \subseteq \mathcal{P}_0(\mathbf{R}^n)$ of minimizers from (2.3), which can be also seen by Lemma 2.3. And any rotation and convex combination of these is a minimizer due to the convexity of X, which shows the set of minimizers is infinite dimensional. In particular, the minimizers do not need to coincide with each other even up to rotation and translation. The uniform measure on the vertices of the regular simplex inscribed in $\mathbf{S}_r$ is also a minimizer, by the following standard observation.*

Remark 2.6 (Second moments for the uniform measure on the vertices of a regular simplex)**.** *Let $\nu_d \in \mathcal{P}_0(\mathbf{R}^n)$ denote the uniform measure on the $n+1$ vertices of a regular simplex with center of mass at the origin and diameter d. Then $I(\nu_d) = \frac{d^2}{2n+2}\,\mathrm{Id}$.*

Proof. Let $\mathbb{1} = (1, 1, \ldots, 1) \in \mathbf{R}^{n+1}$. The standard simplex is $\Delta^n := \{x \in [0,\infty)^{n+1} \mid \mathbb{1} \cdot x = 1\}$. Its vertices coincide with the standard basis vectors $e_0, \ldots, e_n$ for $\mathbf{R}^{n+1}$. Note that its diameter is $\sqrt{2}$. We compute the second moments $I(\nu)$ of the uniform measure $\nu = \frac{1}{n+1}\sum_{i=0}^n \delta_{e_i}$ over these vertices, and its translation $T_\lambda \nu = \frac{1}{n+1}\sum_{i=0}^n \delta_{e_i - \lambda\mathbb{1}}$ along the principal diagonal $\mathbb{1}$ for each $\lambda \in \mathbf{R}$:

$$\begin{aligned} I_{jk}(T_\lambda \nu) &= \frac{1}{n+1}\sum_{i=0}^{n}(e_i - \lambda\mathbb{1})_j (e_i - \lambda\mathbb{1})_k \\ &= \frac{1}{n+1}(\delta_{jk} - 2\lambda + (n+1)\lambda^2), \end{aligned}$$

i.e. $I(T_\lambda\nu) = \frac{1}{n+1}\,\mathrm{Id} + \lambda(\lambda - \frac{2}{n+1})\mathbb{1}\otimes\mathbb{1}$. Note that the choice $\lambda = \frac{1}{n+1}$ makes $\nu_{\sqrt{2}} = T_\lambda \nu$ centered at the origin and lie in the subspace $\mathbb{1}^\perp$, and since $I(T_\lambda\nu)\, v = \frac{1}{n+1} v$ for any $v \in \mathbb{1}^\perp$, we have $v_i \cdot I(T_\lambda \nu)\, v_j = \frac{1}{n+1}\delta_{ij}$ for any orthonormal basis $\{v_i\}$ of $\mathbb{1}^\perp$, as desired. For general diameter d we multiply $(d/\sqrt{2})^2$. $\square$

Remark 2.7 (Concerning d_∞-local energy minimizers)**.** *For $2 < \beta < \alpha$ or $2\beta = 4 < \alpha$, two of us showed the measure ν_1 of unit diameter in Remark 2.6 minimizes the energy uniquely (up to rotations and translations) d_∞-locally [23]; see also Simione [27]. Example 2.5 shows that for $n \geq 2$ the uniqueness part of this statement no longer holds true at the endpoint $(\beta, \alpha) = (2, 4)$ of the latter regime, since $\frac{1}{2}(\nu_1 + R_\theta \nu_1)$ is also minimizing, and lies as d_∞-close to ν_1 as we like when θ is sufficiently small.*

3. Identifying mildly repulsive minimizers for $\alpha \geq 4^*$

For $\alpha\beta > 0$, let w_α and $w_{\alpha,\beta}$ be defined on $\mathbf{R}_+$ by

$$w_\alpha(r) = \frac{r^\alpha}{\alpha}, \qquad w_{\alpha,\beta}(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta},$$

so that $W_{\alpha,\beta}(x) = w_{\alpha,\beta}(|x|)$. If $\alpha \neq \beta$, the rescaled potential

$$\overline{w}_{\alpha,\beta}(r) = \frac{w_{\alpha,\beta}(r)}{-w_{\alpha,\beta}(1)} = \frac{\beta r^\alpha - \alpha r^\beta}{\alpha - \beta} = \overline{w}_{\beta,\alpha}(r)$$

then satisfies $\overline{w}_{\alpha,\beta}(r) \geq -1$ on $r \geq 0$ with equality if and only if $r = 1$. Define $\overline{W}_{\alpha,\beta}(x) = \overline{w}_{\alpha,\beta}(|x|)$. Obviously $\mathcal{E}_{W_{\alpha,\beta}}$ and $\mathcal{E}_{\overline{W}_{\alpha,\beta}}$ share the same minimizers on $\mathcal{P}(\mathbf{R}^n)$ as long as $\alpha > \beta$. The crux of the proof of Theorem 1.2 is the following monotonicity:

Lemma 3.1 (Rescaled potential increases with either exponent)**.** *For each $\alpha \neq 0$, $\beta \neq \alpha$, $r > 0$, we have $\alpha \frac{\partial}{\partial \beta} \overline{w}_{\alpha,\beta}(r) \geq 0$ with equality holding if and only if $r = 1$.*

Proof. Direct computation yields

$$\alpha \frac{\partial}{\partial \beta} \overline{w}_{\alpha,\beta}(r) = \frac{\alpha^2 r^\beta}{(\alpha - \beta)^2} (r^{\alpha-\beta} - 1 - \log r^{\alpha-\beta}).$$

From this, the lemma follows from the fact that the function $t \mapsto t - 1 - \log t \geq 0$ for $t > 0$ with equality holding only if $t = 1$. □

Proof of Theorem 1.2. Assume $\alpha > \beta > 0$ and $\mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{W_{\alpha,\beta}}$. It is enough to prove $\mathcal{P}_{\Delta^n}$ uniquely minimizes both $\mathcal{E}_{W_{\alpha+\epsilon,\beta}}$ and $\mathcal{E}_{W_{\alpha,\beta+\epsilon}}$ on $\mathcal{P}(\mathbf{R}^n)$ for all $\epsilon \in (0, \alpha - \beta)$, and that the support of $\nu \in \mathcal{P}_{\Delta^n}$ uniquely minimizes both $\nu * W_{\alpha+\epsilon,\beta}$ and $\nu * W_{\alpha,\beta+\epsilon}$ on $\mathbf{R}^n$. Let $\rho(x, y) = |x - y|$. For $\mu \in \mathcal{P}(\mathbf{R}^n)$, observe the push-forward $\tilde{\mu} := \rho_\#(\mu \otimes \mu) \in \mathcal{P}(\mathbf{R}_+)$ via the map ρ satisfies, since $W(x) = w(|x|)$,

$$\mathcal{E}_{\overline{W}_{\alpha,\beta}}(\mu) = \frac{1}{2} \int_0^\infty \overline{w}_{\alpha,\beta}(r) d\tilde{\mu}(r). \tag{3.1}$$

Let $\nu \in \mathcal{P}_{\Delta^n}$. By assumption $\int \overline{w}_{\alpha,\beta}(r) d\tilde{\mu}(r) \geq \int \overline{w}_{\alpha,\beta}(r) d\tilde{\nu}(r)$. Since $\operatorname{spt}(\tilde{\nu}) = \{0, 1\}$ and $\overline{w}_{\alpha,\beta}(r)$ is constant in $\alpha > \beta > 0$ at $r = 0$ and 1,

$$\int \overline{w}_{\alpha,\beta}(r) d\tilde{\nu}(r) = \int \overline{w}_{\alpha+\epsilon,\beta}(r) d\tilde{\nu}(r) = \int \overline{w}_{\alpha,\beta+\epsilon}(r) d\tilde{\nu}(r)$$

for all $0 < \epsilon < \alpha - \beta$. On the other hand, by Lemma 3.1 (and the symmetry of $\overline{w}$ in α, β), $\epsilon > 0$ implies

$$\int \overline{w}_{\alpha,\beta}(r) d\tilde{\mu}(r) \leq \int \overline{w}_{\alpha+\epsilon,\beta}(r) d\tilde{\mu}(r), \quad \int \overline{w}_{\alpha,\beta}(r) d\tilde{\mu}(r) \leq \int \overline{w}_{\alpha,\beta+\epsilon}(r) d\tilde{\mu}(r)$$

with equality holding only if $\operatorname{spt}(\tilde{\mu}) \subseteq \{0, 1\}$, i.e. only if μ is concentrated on the set of vertices of a unit simplex. Now if μ minimizes $\mathcal{E}_{\overline{W}_{\alpha+\epsilon,\beta}}$ or $\mathcal{E}_{\overline{W}_{\alpha,\beta+\epsilon}}$ then we must have $\operatorname{spt}(\tilde{\mu}) \subseteq \{0, 1\}$, and hence by e.g. the Perron-Frobenius theorem, we conclude μ must also uniformly distribute its mass over the vertices of a unit simplex, i.e. $\mu \in \mathcal{P}_{\Delta^n}$. This proves the first identity (1.7).

Observe that the Euler-Lagrange equation from e.g. [12] asserts

$$\operatorname{spt} \nu \subseteq \operatorname{argmin}(\nu * W_{\alpha,\beta}). \tag{3.2}$$

Since the vertices of a unit simplex, $\operatorname{spt} \nu$, is characterized as the maximal set of points at distance one from each other, Lemma 3.1 shows

$$\nu * W_{\alpha,\beta} \leq \nu * W_{\alpha+\epsilon,\beta} \quad \text{and} \quad \nu * W_{\alpha,\beta} \leq \nu * W_{\alpha,\beta+\epsilon}$$

with equalities holding precisely on $\operatorname{spt} \nu$. This implies the second identity (1.7) to establish Theorem 1.2. □

Proof of Corollary 1.7. Lemma 3.1 shows $\overline{w}_{\alpha,\beta}(r)$ is a nondecreasing function of $\beta \in (0,\alpha)$, and strictly increasing unless $r \in \{0,1\}$. Also $\lim_{\beta\to\alpha} \overline{w}_{\alpha,\beta}(r) = r^\alpha(\alpha \log r - 1)$, so $\lim_{\beta\to\alpha} \overline{W}_{\alpha,\beta}(x) = D_\alpha(x)$. As in the preceding proof, if $\mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{W_{\alpha,\beta}}$, comparison shows it then minimizes $\mathcal{E}_{D_\alpha}$ uniquely. Conversely if $\mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{D_\beta}$, then minimizes $\mathcal{E}_{W_{\alpha,\beta}}$ uniquely for all $\alpha > \beta$. □

Proof of Corollary 1.4. Theorems 1.1–1.2 and Remarks 1.3 and 2.6 yield Corollary 1.4. □

4. The transition threshold

In this section, we establish the existence of a transition threshold $\alpha_{\Delta^n}(\beta)$ which separates the part of the mildly repulsive region $\beta \geq 2$ on which equidistribution $\mathcal{P}_{\Delta^n}$ over the vertices of the unit simplex minimizes the energy $\mathcal{E}_{W_{\alpha,\beta}}$ from the part on which it does not. Above the threshold, these minimizers are unique up to rigid motions. We also establish that this threshold lies in the range $[\underline{\alpha}^+_{\Delta^n}(\beta), \alpha^*_\infty(\beta)] \subseteq [\underline{\alpha}_{\Delta^n}(\beta), \alpha^*_\infty(\beta)]$ given by Definitions 4.2, 4.7 and 4.10, which collapses to the point $\{\alpha^*_\infty(\beta)\}$ in the high dimensional limit (Proposition 4.14).

Theorem 4.1 (Transition threshold)**.** *For each $\beta \geq 2$ there exists $\alpha_{\Delta^n}(\beta) \in [\beta,\infty)$ such that*

$$\mathcal{P}_{\Delta^n} = \operatorname*{argmin}_{\mathcal{P}(\mathbf{R}^n)} \mathcal{E}_{W_{\alpha,\beta}} \text{ if } \alpha > \alpha_{\Delta^n}(\beta), \tag{4.1}$$

$$\emptyset = \mathcal{P}_{\Delta^n} \cap \operatorname*{argmin}_{\mathcal{P}(\mathbf{R}^n)} \mathcal{E}_{W_{\alpha,\beta}} \text{ if } \beta < \alpha < \alpha_{\Delta^n}(\beta). \tag{4.2}$$

If $\alpha = \alpha_{\Delta^n}(\beta)$ and $\nu \in \mathcal{P}_{\Delta^n}$, then at least one of the following two containments is strict:

$$\mathcal{P}_{\Delta^n} \subsetneq \operatorname*{argmin}_{\mathcal{P}(\mathbf{R}^n)} \mathcal{E}_{W_{\alpha,\beta}} \quad \text{or} \quad \operatorname{spt}\nu \subsetneq \operatorname*{argmin}_{\mathbf{R}^n}(W_{\alpha,\beta} * \nu). \tag{4.3}$$

Moreover, $\alpha_{\Delta^n}(2) = 4^*$ from (1.8)*, and we have $\beta_n \in (2, 4^*)$ such that $\alpha_{\Delta^n}(\beta) = \beta$ for $\beta \geq \beta_n$, and $\alpha_{\Delta^n} : [2, \beta_n] \longrightarrow [\beta_n, 4^*]$ is continuous and strictly decreasing.*

Proof. For $\beta \geq 2$, the existence of $\alpha_{\Delta^n}(\beta) \in [\beta,\infty]$ satisfying (4.1) and (4.2) follow from Theorem 1.2; also $\alpha_{\Delta^n}(\beta) < \infty$ is asserted in [23]. The fact that $\alpha_{\Delta^n}(2) \leq 4^*$, existence of a minimal $\beta_n \in [2, 4^*]$ such that $\alpha_{\Delta^n}(\beta) = \beta$ for $\beta > \beta_n$, and (nonstrict) monotonicity of $\alpha_{\Delta^n} : [2, \beta_n] \longrightarrow [\beta_n, 4^*]$ are consequences of Corollary 1.4. The centrifugal value $\alpha_{\Delta^n}(2) = 4^*$ follows from Theorem 1.1 and Remark 1.3. We next establish that at least one of the containments (4.3) is strict by combining results from [23] with the strategy used to provide an analogous statement for a related problem in [24].

For $p \in [1,\infty]$, recall that the Kantorovich-Rubinstein-Wasserstein distance between $\mu, \mu' \in \mathcal{P}(\mathbf{R}^n)$ is defined by

$$d_p(\mu,\mu') := \inf_{X\sim\mu, Y\sim\mu'} \|X - Y\|_{L^p}, \tag{4.4}$$

where the infimum is taken over arbitrary couplings of random vectors X and Y in $\mathbf{R}^n$ whose laws are given by μ and μ' respectively. The metrics d_p are well-known to metrize weak convergence of measures on compact subsets $K \subseteq \mathbf{R}^n$ unless $p = \infty$ [29]. Given such a compact set $K \subseteq \mathbf{R}^n$ and $\alpha > \beta \geq 2$, we first claim that if $(\alpha, \beta) = \lim_{k\to\infty}(\alpha(k), \beta(k))$ for a sequence $\alpha(k) > \beta(k) \geq 2$, then the functionals $\mathcal{E}_{W_{\alpha(k),\beta(k)}}$ Γ-converge to $\mathcal{E}_{\alpha,\beta}$ on $(\mathcal{P}(K), d_2)$. Since the potentials $\{W_{\alpha(k),\beta(k)}\}_k$ are uniformly equicontinuous on $K \times K$, this is easy to prove using the argument, e.g., from Lemma 3.2 of [24], so we do not give more details here. Now Proposition 1.1 of [12] ensures the minimizers of $\mathcal{E}_{W_{\alpha,\beta}}$ on $\mathcal{P}(\mathbf{R}^n)$ exist and can all be translated to lie in a centered ball of radius $e^{1/\beta}$; as $k \to \infty$ it follows from this Γ-convergence that d_2-accumulation points of minimizers of $\mathcal{E}_{\alpha(k),\beta(k)}$ therefore minimize $\mathcal{E}_{\alpha,\beta}$ on $\mathcal{P}(\mathbf{R}^n)$. Taking $\beta(k) = \beta$ and $\alpha(k) \searrow \alpha_{\Delta^n}(\beta)$ then shows that the (nonstrict) first containment of (4.3) is a consequence of (4.1). When $\alpha_{\Delta^n}(\beta) = \beta$, strict containment becomes trivial. We may therefore assume $\alpha_{\Delta^n}(\beta) =: \alpha > \beta$, and let $\beta(k) = \beta$ and $\alpha(k) \nearrow \alpha$. We also assume $\beta > 2$ because for $\beta = 2 \leq n$ strict containment follows from Theorem 1.1, while for $(\beta, n) = (2, 1)$ it is easy to check $\operatorname{spt}\psi = \{-\frac{1}{2}, \frac{1}{2}\} \subsetneq [-\frac{1}{2}, \frac{1}{2}] = \operatorname{argmin}(W_{3,2} * \psi)$. Since there exist minimizers μ_k of $\mathcal{E}_{\alpha(k),\beta}$ on $\mathcal{P}(\mathbf{R}^n)$ whose support lies in the centered ball of radius $e^{1/\beta}$, weak compactness of the probability measures on this ball yields a subsequential limit $d_2(\mu_k, \mu_\infty) \to 0$ (the subsequence having been relabelled μ_k); Γ-convergence then ensures μ_∞ minimizes $\mathcal{E}_{W_{\alpha,\beta}}$ on $\mathcal{P}\Big(\overline{B_{e^{1/\beta}}(0)}\Big)$, hence on $\mathcal{P}(\mathbf{R}^n)$ by [12, Proposition 2.1].

The second containment in (4.3) follows from the first and the Euler-Lagrange equation described e.g. in Proposition 1.1 of [12]. To derive a contradiction, assume neither containment in (4.3) is strict, so that $\mu_\infty \in \mathcal{P}_{\Delta^n}$ and

$$\operatorname{spt}\mu_\infty = \operatorname*{argmin}_{\mathbf{R}^n} W_{\alpha,\beta} * \mu_\infty. \tag{4.5}$$

Set $\operatorname{spt}\mu_\infty = \{x_0, \ldots, x_n\}$ and $0 < R < 1/2$. Since $d_2(\mu_k, \mu_\infty) \to 0$ and the Euler-Lagrange equation applied to μ_k, and the uniform convergence on every ball of $W_{\alpha(k),\beta} * \mu_k$ to $W_{\alpha,\beta} * \mu_\infty$ together with (4.5) yields

$$1 = \mu_k[\cup_{i=0}^n B_R(x_i)], \quad \text{while} \quad \mu_k[B_R(x_i)] \in (\frac{1}{n+2}, \frac{1}{n})$$

for k sufficiently large; c.f. Lemma 4.3 of [24] or Corollary 3.6 of [23]. Setting

$$\mu_k' := \sum_{i=0}^n \mu_k[B_R(x_i)]\delta_{x_i} \tag{4.6}$$

ensures $d_\infty(\mu_k, \mu_k') < R$. On the other hand, if $\alpha(k) > \beta^* := \frac{1}{3}(\alpha + 2\beta)$, Corollary 4.3 of [23] provides $r = r(\beta, \beta^*, n)$ such that μ_k' (and its rotates and translates) uniquely minimize $\mathcal{E}_{W_{\alpha(k),\beta}}$ on a d_∞-ball of radius r around μ_k'. But μ_k was chosen to minimize $\mathcal{E}_{W_{\alpha(k),\beta}}$ globally on $\mathcal{P}(\mathbf{R}^n)$. Taking $R < r$ and k correspondingly large therefore forces μ_k to be a rotate or translate of μ'_k. From e.g. the Perron-Frobenius theorem, μ_k then assigns equal mass to each point in $\operatorname{spt}\mu_k$, hence $\mu_k \in \mathcal{P}_{\Delta^n}$. Since $\alpha(k) < \alpha_{\Delta^n}(\beta)$ by construction, (4.2) produces the desired contradiction $\mu_k \notin \mathcal{P}_{\Delta^n}$, to establish that at least one of the containments in (4.3) is strict. From this, notice the monotonicity of $\alpha_{\Delta^n} : [2, \beta_n] \longrightarrow [\beta_n, 4^*]$ must be strict in view of (1.7), and implies $\beta_n \in (2, 4^*)$.

It remains to deduce continuity of α_{Δ^n} at each $\beta \in [2, \beta_n]$. Set

$$\alpha_{\Delta^n}(\beta\pm) := \lim_{\epsilon \downarrow 0} \alpha_{\Delta^n}(\beta \pm \epsilon).$$

If $\alpha \in (\alpha_{\Delta^n}(\beta), \alpha_{\Delta^n}(\beta-))$ for some $\beta \in (2, \beta_n]$, then choosing μ_k to minimize $\mathcal{E}_{W_{\alpha,\beta-1/k}}$ on $\mathcal{P}(\mathbf{R}^n)$, after translation into a centered ball of radius $e^{1/(\beta-1)}$ we can extract a subsequential d_2-limit μ_∞ of μ_k. Notice $\mu_k \notin \mathcal{P}_{\Delta^n}$, while Γ-convergence implies μ_∞ minimizes $\mathcal{E}_{\alpha,\beta}$ hence $\mu_\infty \in \mathcal{P}_{\Delta^n}$ by Theorem 1.2. But then as above, this contradicts the d_∞-unique local minimality of μ'_k from (4.6) for R sufficiently small and k correspondingly large. On the other hand, if $\alpha \in (\alpha_{\Delta^n}(\beta+), \alpha_{\Delta^n}(\beta))$ for some $\beta \in [2, \beta_n]$, then choosing μ_k to minimize $\mathcal{E}_{W_{\alpha,\beta+1/k}}$ on $\mathcal{P}(\mathbf{R}^n)$, we can extract a subsequential d_2-limit μ_∞ of μ_k. This time $\mu_k \in \mathcal{P}_{\Delta^n}$, while Γ-convergence and $\alpha < \alpha_{\Delta^n}(\beta)$ imply $\mu_\infty \notin \mathcal{P}_{\Delta^n}$, contradicting the fact that $\mathcal{P}_{\Delta^n}$ is d_2-closed. We conclude the desired continuity $\alpha_{\Delta^n}(\beta) = \alpha_{\Delta^n}(\beta\pm)$, which also implies $\alpha_{\Delta^n}(\beta_n) = \beta_n$. $\square$

4.1. **Threshold upper bound independent of dimension $n \geq 2$.**

We now establish an upper bound $\alpha^*_\infty(\beta)$ for the threshold $\alpha_{\Delta^n}(\beta)$. Note that this upper bound and the quantities β^*_∞ and $f^*_\infty(\beta)$ defining it become independent of dimension as soon as $n \geq 2$. The asterisk on these quantities reminds us of their implicit dependence on $\min\{n, 2\}$, however.

Definition 4.2 (Threshold upper bound)**.** *Set*

$$\beta^*_\infty := \frac{4^* - 2}{\log(4^*/2)} = \begin{cases} \frac{1}{\log(3/2)} & \text{if } n = 1, \\ \frac{2}{\log 2} & \text{if } n \geq 2. \end{cases}$$

For $\beta \geq 2$, define $\alpha^*_\infty = \alpha^*_\infty(\beta)$ as the largest solution of

$$\frac{e^{\alpha/\beta^*_\infty}}{\alpha} = \frac{e^{\beta/\beta^*_\infty}}{\beta}. \tag{4.7}$$

Remark 4.3 (Number of solutions)**.** *For any given $\beta \geq 2$ and $n \in \{1, 2\}$, there are at most two solutions to equation (4.7), which follows from the fact that $f^*_\infty(t) := -\frac{e^{t/\beta^*_\infty}}{t}$ is unimodal on $(0, \infty)$, i.e. has a unique global maximum and no local minima. In particular, we see $t^2 \beta^*_\infty e^{-t/\beta^*_\infty} \frac{df^*_\infty}{dt} = t - \beta^*_\infty$ is positive on $(0, \beta^*_\infty)$, zero at β^*_∞, and negative on (β^*_∞, ∞). Thus $\alpha^*_\infty(\beta) = \beta$ if and only if $\beta \geq \beta^*_\infty$.*

Remark 4.4 (Alternative interpretation)**.** *Set*

$$\bar{w}_{\beta,\beta}(r) := \lim_{\alpha\to\beta} \bar{w}_{\alpha,\beta}(r) = r^\beta(\beta \log r - 1),$$

and let $z_{\alpha,\beta}$ denote the positive zero of $\bar{w}_{\alpha,\beta}$, where $z_{\alpha,\beta} = (\frac{\alpha}{\beta})^{\frac{1}{\alpha-\beta}}$ for $\alpha \neq \beta$ and $z_{\beta,\beta} := e^{1/\beta}$. Notice that $z_{4^*,2} = \frac{3}{2}$, if $n = 1$, and $z_{4^*,2} = \sqrt{2}$, if $n \geq 2$. Hence, after some rearranging, we obtain β^*_∞ from the equation $z_{\beta^*_\infty,\beta^*_\infty} = z_{4^*,2}$ and α^*_∞ as the largest solution of $z_{\alpha,\beta} = z_{4^*,2}$, or rather $w_{\alpha,\beta}(z_{4^*,2}) = 0$.

The following lemma and corollary demonstrate that α^*_∞ is indeed an upper bound for the threshold function:

Lemma 4.5 (Comparing pair potentials)**.** *Let $2 < \beta < \alpha < 4^*$. Then $\bar{w}_{4^*,2}(r) \leq \bar{w}_{\alpha,\beta}(r)$ for all $r \in [0, z_{\alpha,\beta}]$ if and only if $z_{\alpha,\beta} \leq z_{4^*,2}$.*

Proof. One direction is trivial, as if $\bar{w}_{4^*,2}(r) \leq \bar{w}_{\alpha,\beta}(r)$ for all $r \in [0, z_{\alpha,\beta}]$, then in particular $\bar{w}_{4^*,2}(z_{\alpha,\beta}) \leq \bar{w}_{\alpha,\beta}(z_{\alpha,\beta}) = 0$, hence $z_{\alpha,\beta} \leq z_{4^*,2}$. For the proof of the other direction, we begin by defining

$$g(r) := \bar{w}_{4^*,2}(r) - \bar{w}_{\alpha,\beta}(r) = \frac{2r^{4^*} - 4^* r^2}{4^* - 2} - \frac{\beta r^\alpha - \alpha r^\beta}{\alpha - \beta}.$$

We may divine the behaviour of g from its fifth derivative

$$g^{(5)}(r) = \frac{\alpha\beta r^{\beta-5}}{\alpha-\beta}\left[-r^{\alpha-\beta}\prod_{i=1}^{4}(\alpha - i) + \prod_{i=1}^{4}(\beta - i)\right]$$

for $r \in (0,\infty)$. Written in this form, we see that $g^{(5)}(r)$ is monotone and hence has at most one sign change. Thus, $g^{(3)}(r)$ is either convex-concave, concave-convex, or strictly convex on $(0,\infty)$. Moreover, we may write

$$g^{(3)}(r) = 2\cdot 4^*(4^*-1)r^{4^*-3} + \frac{\alpha\beta}{\alpha-\beta}\left[-(\alpha-1)(\alpha-2)r^{\alpha-3} + (\beta-1)(\beta-2)r^{\beta-3}\right].$$

Here, both the highest order term r^{4^*-3} and the lowest order term $r^{\beta-3}$ have positive coefficients, which implies that $g^{(3)}$ is positive outside a compact subinterval of $(0,\infty)$. This, combined with the convex/concave structure of $g^{(3)}$, implies that $g^{(3)}$ can have at most two zeros on $(0,\infty)$ and, in particular, may change signs at most twice — from positive to negative to positive.

This implies either g' is convex-concave-convex on $(0,\infty)$ or just convex. We may assume g' is convex-concave-convex as, if it is simply convex, an easier argument than what follows will yield the desired conclusion. Notice that

$$g'(r) = \frac{4^*\cdot 2}{4^*-2}(r^{4^*-1} - r) - \frac{\alpha\beta}{\alpha-\beta}(r^{\alpha-1} - r^{\beta-1})$$

is negative near zero and hence, the convex-concave-convexity implies g' changes sign at most thrice on $(0,\infty)$. Note $g'(0) = g'(1) = 0 = g(0) = g(1)$. Since

g' is negative near zero, we see that g' must change from negative to positive somewhere in $(0,1)$, implying the existence of a zero of g' on this interval. Hence g' has at most one zero on $(1,\infty)$. But if there is no zero on $(1,\infty)$, then the shape of g' and $g(1)=g'(1)=0$ implies $g'>0$ hence $g>0$ on $(1,\infty)$, yielding $z_{\alpha,\beta}>z_{4^*,2}$, a contradiction. Hence we deduce that, on $(1,\infty)$, g' changes sign from negative to positive. With $g(1)=0$, this implies g also changes sign from negative to positive on $(1,\infty)$. Now since the condition $z_{\alpha,\beta}\le z_{4^*,2}$ clearly implies $g(z_{\alpha,\beta})\le 0$, this allows us to conclude that $g\le 0$ on $[1,z_{\alpha,\beta}]$.

It remains to show $g\le 0$ on $[0,1]$. Assume g is positive somewhere in $(0,1)$. Then g' would have to change signs (at least) twice on the interval $(0,1)$, from negative to positive to negative. With $g'(1)=0$ all three zeros of g' are in $(0,1]$, thus no zero on $(1,\infty)$, contradiction as before. This concludes the proof. □

Corollary 4.6 (Threshold upper bound)**.** *If $\beta\ge 2$ then $\alpha_{\Delta^n}(\beta)\le\alpha^*_\infty(\beta)$.*

Proof. Recall $\mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{W_{4^*,2}}$ from Corollary 1.4. The fact from Lemma 4.5, namely $\bar w_{4^*,2}(r)\le\bar w_{\alpha^*_\infty,\beta}(r)$ on $r\in[0,z_{\alpha^*_\infty,\beta}]$ with equality at $r=1$, shows $\mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{W_{\alpha^*_\infty,\beta}}$, since any minimizer of $\mathcal{E}_{W_{\alpha^*_\infty,\beta}}$ has its diameter no greater than $z_{\alpha^*_\infty,\beta}$, by [16, Lemma 1]. □

4.2. **Threshold lower bound for each dimension.** We now derive a dimension dependent lower bound $\underline{\alpha}^+_{\Delta^n}$ for α_{Δ^n} from the Euler-Lagrange equation (3.2) for minimizers.

Definition 4.7 (Threshold lower bound)**.** *Let $\nu\in\mathcal{P}_{\Delta^n}$. For each $\beta\ge 2$, define $\underline{\alpha}^+_{\Delta^n}(\beta)\in[\beta,\infty)$ to be*

$$\begin{aligned}\underline{\alpha}^+_{\Delta^n}(\beta) &:= \inf\{\alpha>\beta \mid \operatorname{spt}\nu\subseteq \operatorname*{argmin}_{\mathbf{R}^n}(W_{\alpha,\beta}*\nu)\}\\ &= \sup\{\alpha\in\mathbf{R} \mid \operatorname{spt}\nu\not\subseteq \operatorname*{argmin}_{\mathbf{R}^n}(W_{\alpha,\beta}*\nu)\}.\end{aligned}\tag{4.8}$$

Proposition 4.8 (Threshold lower bound)**.** *Let $\nu\in\mathcal{P}_{\Delta^n}$. If $\alpha>\underline{\alpha}^+_{\Delta^n}(\beta)$ for some $\beta\ge 2$, then $\operatorname{spt}\nu=\operatorname{argmin}_{\mathbf{R}^n}(W_{\alpha,\beta}*\nu)$. In particular,*

$$\underline{\alpha}^+_{\Delta^n}(\beta)=\inf\{\alpha>\beta \mid \operatorname{spt}\nu=\operatorname*{argmin}_{\mathbf{R}^n}(W_{\alpha,\beta}*\nu)\},\tag{4.9}$$

and $\underline{\alpha}^+_{\Delta^n}\le\alpha_{\Delta^n}$.

Proof. For any $\alpha>\underline{\alpha}^+_{\Delta^n}(\beta)$, notice Lemma 3.1 yields $\operatorname{spt}\nu=\operatorname{argmin}_{\mathbf{R}^n}(W_{\alpha,\beta}*\nu)$, which gives (4.9). The fact that $\underline{\alpha}^+_{\Delta^n}\le\alpha_{\Delta^n}$ is a direct consequence of the Euler-Lagrange equation satisfied by a minimizer: i.e. if $\alpha\ge\alpha_{\Delta^n}$, so that $\nu\in\mathcal{P}_{\Delta^n}$ minimizes $\mathcal{E}_{W_{\alpha,\beta}}$, then ν satisfies (3.2) hence $\alpha\ge\underline{\alpha}^+_{\Delta^n}$. □

Although the value of $\underline{\alpha}^+_{\Delta^n}(\beta)$ is not very explicit, it is possible to estimate it explicitly from below by evaluating the potential $W_{\alpha,\beta}*\nu$ at points chosen judiciously to expose potential violations of the Euler-Lagrange equation. The resulting estimates $\underline{\alpha}_{\Delta^n} \leq \underline{\alpha}^+_{\Delta^n}$ provide weaker but explicit lower bounds for the threshold. This requires the following family of functions and their unimodality:

Definition 4.9 (A family of unimodal functions)**.** *Define $f_n : (0,\infty) \to \mathbf{R}$ by*

$$f_n(t) := \begin{cases} \frac{2^{-1}-2^{-t}}{t} & \text{if } n = 1 \\ \frac{n-(\frac{2n}{n+1})^{t/2}-n(\frac{n-1}{n+1})^{t/2}}{t} & \text{if } n \geq 2. \end{cases} \tag{4.10}$$

Using this family of functions, we define a new family of lower bounds:

Definition 4.10 (A weaker threshold lower bound)**.** *For $\beta \geq 2$, define $\underline{\alpha}_{\Delta^n}(\beta)$ by*

$$\underline{\alpha}_{\Delta^n}(\beta) = \max\{\alpha \geq 2 \mid f_n(\alpha) = f_n(\beta)\}. \tag{4.11}$$

In particular, the set over which we take the maximum in the previous definition has at most two elements, as the following lemma shows:

Lemma 4.11 (Unimodality of f_n)**.** *For any $n \geq 1$, the function $f_n(t)$ is unimodal on $t \in (0,\infty)$. Indeed, f_n admits a unique global maximum $\underline{\beta}_n := \operatorname{argmax}_{t>0} f_n(t)$ and no other critical points.*

Proof. We first treat the case $n = 1$ separately. Here, notice that $f_1'(t)$ has the same sign as $g_1(t) := t^2 f_1'(t) = (t \log 2 + 1)2^{-t} - 2^{-1}$. Since $g_1'(t) = -t2^{-t}\log^2 2$ is always negative, and since $g_1(0) = \frac{1}{2}$ and $\lim_{t\to\infty} g_1(t) = -\frac{1}{2}$, we conclude that f_1' switches sign from positive to negative at its unique zero in $(0,\infty)$, and has no other sign changes. We denote the unique zero of f_1' by $\underline{\beta}_1$.

The $n \geq 2$ case proceeds in a similar manner. Here, we notice that

$$\begin{aligned} g_n(t) := t^2 f_n'(t) = -\frac{t}{2}\left[\left(\frac{2n}{n+1}\right)^{t/2} \log\frac{2n}{n+1} + n\left(\frac{n-1}{n+1}\right)^{t/2} \log\frac{n-1}{n+1}\right] \\ - n + \left(\frac{2n}{n+1}\right)^{t/2} + n\left(\frac{n-1}{n+1}\right)^{t/2}, \end{aligned}$$

and compute

$$g_n'(t) = -\frac{t}{4}\left[\left(\frac{2n}{n+1}\right)^{t/2} \log^2\frac{2n}{n+1} + n\left(\frac{n-1}{n+1}\right)^{t/2} \log^2\frac{n-1}{n+1}\right].$$

Since $g_n'(t)$ is negative everywhere, $g_n(0) = 1$, and $\lim_{t\to\infty} g_n(t) = -\infty$, we may apply an identical argument to the one employed in the $n = 1$ case to show the existence of $\underline{\beta}_n$ with all desired properties. $\square$

Remark 4.12 (Diagonal intersects bound)**.** *Notice $\underline{\alpha}_{\Delta^n}(\beta) > \beta$ if and only if $\beta < \underline{\beta}_n$. That is, the graph of $\underline{\alpha}_{\Delta^n}$ intersects the line $\alpha = \beta$ at the point $(\underline{\beta}_n, \underline{\beta}_n)$.*

Proposition 4.13 (Estimating threshold lower bound)**.** *For $\beta \geq 2$, the thresholds of Definitions 4.10, 4.7 and Theorem 4.1 satisfy $\underline{\alpha}_{\Delta^n}(\beta) \leq \underline{\alpha}^+_{\Delta^n}(\beta) \leq \alpha_{\Delta^n}(\beta)$.*

Proof. In view of Proposition 4.8 we need only show $\underline{\alpha}_{\Delta^n}(\beta) \leq \underline{\alpha}^+_{\Delta^n}(\beta)$. We proceed by relating the defining equations for $\underline{\alpha}_{\Delta^n}$ to the Euler-Lagrange equation for a unit simplex $\nu \in \mathcal{P}_{\Delta^n}$. As in the introduction, we denote the vertices of the unit n-simplex by $\{x_0, ..., x_n\}$. We divide the proof into two cases, $n = 1$ and $n \geq 2$. Notice that, in either case, the inequality is trivial for any β for which $\underline{\alpha}_{\Delta^n}(\beta) = \beta$, so we are free to assume that $\underline{\alpha}_{\Delta^n}(\beta) > \beta$.

If $n = 1$, notice that the Euler-Lagrange equation requires that

$$(W_{\alpha,\beta} * \nu)(x_0) \leq (W_{\alpha,\beta} * \nu)(0).$$

More explicitly, as $\nu = \frac{\delta_{x_0}+\delta_{x_1}}{2}$, this inequality reads $\frac{1}{2}\left[\frac{1}{\alpha} - \frac{1}{\beta}\right] \leq \frac{1}{\alpha 2^\alpha} - \frac{1}{\beta 2^\beta}$, or,

$$f_1(\alpha) = \frac{2^{-1} - 2^{-\alpha}}{\alpha} \leq \frac{2^{-1} - 2^{-\beta}}{\beta} = f_1(\beta). \tag{4.12}$$

By definition, $\alpha = \underline{\alpha}_{\Delta^1}(\beta)$ saturates this inequality. Our assumption $\underline{\alpha}_{\Delta^1}(\beta) > \beta$ with the unimodality of f_1 from Lemma 4.11 ensure that for any $\gamma \in (\beta, \underline{\alpha}_{\Delta^1}(\beta))$,

$$f_1(\gamma) > f_1(\beta) = f_1(\underline{\alpha}_{\Delta^1}(\beta)).$$

This implies that the simplex ν violates the Euler-Lagrange equation for $\mathcal{E}_{W_{\gamma,\beta}}$, and hence that $\gamma \leq \underline{\alpha}^+_{\Delta^1}(\beta)$. Of course, since this inequality holds for all $\gamma \in (\beta, \underline{\alpha}_{\Delta^1}(\beta))$, this proves that $\underline{\alpha}_{\Delta^1}(\beta) \leq \underline{\alpha}^+_{\Delta^1}(\beta)$ for any $\beta \geq 2$.

Our proof proceeds analogously for $n \geq 2$, with the key difference being that the definition (4.10) of f_n is derived from the inequality

$$(W_{\alpha,\beta} * \psi)(x_0) \leq (W_{\alpha,\beta} * \psi)(-x_0),$$

which again is a necessary condition for the Euler-Lagrange equation to hold for ν. Since the simplex geometry yields $|x_0|^2 = \frac{n}{2n+2}$ and $|x_0 + x_1|^2 = \frac{n-1}{n+1}$ (c.f. Theorem 1.1 and Remark 2.6), this inequality can be re-expressed as:

$$\frac{n}{n+1}\left(\frac{1}{\alpha} - \frac{1}{\beta}\right) \leq \frac{1}{n+1}\left(\frac{\left(\frac{2n}{n+1}\right)^{\alpha/2}}{\alpha} - \frac{\left(\frac{2n}{n+1}\right)^{\beta/2}}{\beta}\right) + \frac{n}{n+1}\left(\frac{\left(\frac{n-1}{n+1}\right)^{\alpha/2}}{\alpha} - \frac{\left(\frac{n-1}{n+1}\right)^{\beta/2}}{\beta}\right),$$

or equivalently,

$$f_n(\alpha) = \frac{n - \left(\frac{2n}{n+1}\right)^{\alpha/2} - n\left(\frac{n-1}{n+1}\right)^{\alpha/2}}{\alpha} \leq \frac{n - \left(\frac{2n}{n+1}\right)^{\beta/2} - n\left(\frac{n-1}{n+1}\right)^{\beta/2}}{\beta} = f_n(\beta).$$

Since f_n is still unimodal for $n \geq 2$, the remainder of the proof proceeds in an identical manner to the proof for $n = 1$ following (4.12), hence is omitted. □

We summarize our findings for $n = 2$ and $n = 1$ in Figures 3 and 4 respectively.

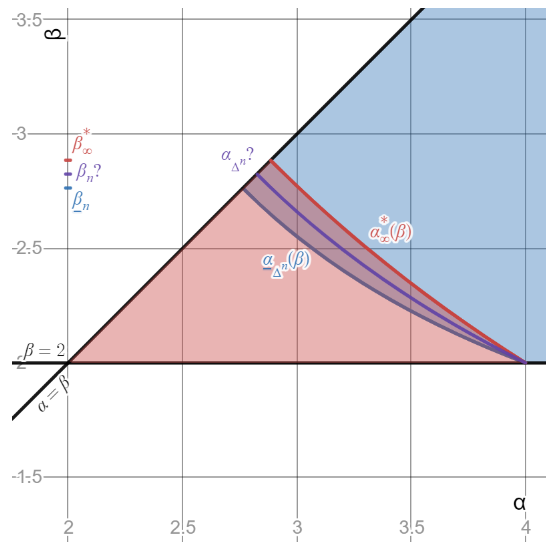


FIGURE 3. The mildly repulsive regime for, e.g., $n = 2$. In the red region to the left of the blue curve $\alpha = \underline{\alpha}_{\Delta^2}(\beta)$, the simplex does not minimize $\mathcal{E}_{W_{\alpha,\beta}}$. Conversely, in the rightmost blue region, the simplex uniquely minimizes $\mathcal{E}_{W_{\alpha,\beta}}$. In the intermediate region, it is not entirely known where the simplex minimizes $\mathcal{E}_{W_{\alpha,\beta}}$, but the graph of the threshold function α_{Δ^2} must lie entirely in this region.

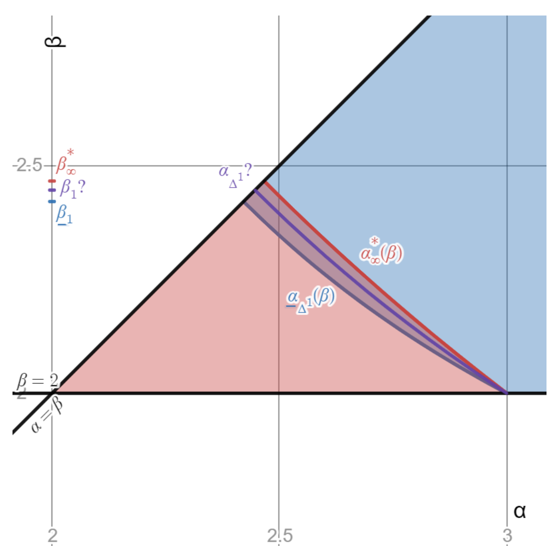


FIGURE 4. The analogous graph for the $n = 1$ case. All coloured regions and graphs have the same meaning as their counterparts in Figure 3, although the scale of this graph differs from its higher dimensional counterparts, due the fact that $4^* = 3$ when $n = 1$.

Notably, even this weaker lower bound tends to the upper bound α^*_∞ as $n \to \infty$.

Proposition 4.14 (Bounds converge in the high dimensional limit)**.** *For all $\beta \geq 2$, we have* $\lim_{n\to\infty} \underline{\alpha}_{\Delta^n}(\beta) = \alpha^*_\infty(\beta) \qquad (n \neq 1)$.

Proof. For $\beta \geq 2$, observe that the unimodal functions $f_n(\beta)$ of Lemma 4.11 converge to the unimodal limit $f^*_\infty(\beta)$ of Remark 4.3:

$$\lim_{n\to\infty} f_n(\beta) = \lim_{n\to\infty} \frac{n - \left(\frac{2n}{n+1}\right)^{\beta/2} - n\left(\frac{n-1}{n+1}\right)^{\beta/2}}{\beta} = -\frac{2^{\beta/2}}{\beta} = f^*_\infty(\beta) \qquad (n \neq 1).$$

Since $\underline{\alpha}_{\Delta^n}(\beta)$ and $\alpha^*_\infty(\beta)$ are defined as the largest α satisfying $f_n(\alpha) = f_n(\beta)$ and $f^*_\infty(\alpha) = f^*_\infty(\beta)$ respectively, it follows that $\underline{\alpha}_{\Delta^n}(\beta) \to \alpha^*_\infty(\beta)$ as $n \to \infty$. $\square$

Remark 4.15 (Monotonicity)**.** *Numerical experiments displayed in Figure 5 suggest $(4-t)(t-2)\underline{\alpha}_{\Delta^n}(t)$ is a non-decreasing function of $n \geq 2$ on $t > 0$; for $t \geq 2$ its large n limit is established in the previous proposition. To confirm the observed monotonicity rigorously, it would suffice to show that unimodality of $f_{n+1} - f_n$ on $(0, \infty)$ for all $n \geq 2$. This is because, for $n \geq 2$, $f_n(t)$ has zeroes only at $t = 2$ and $t = 4$, and hence, assuming unimodality, these are the only two zeroes of $f_{n+1} - f_n$. Since $\lim_{t\to\infty}(f_{n+1}(t) - f_n(t)) = -\infty$, this implies positivity of $(4-t)(t-2)(f_{n+1}(t) - f_n(t))$ away from $t \in \{2, 4\}$.*

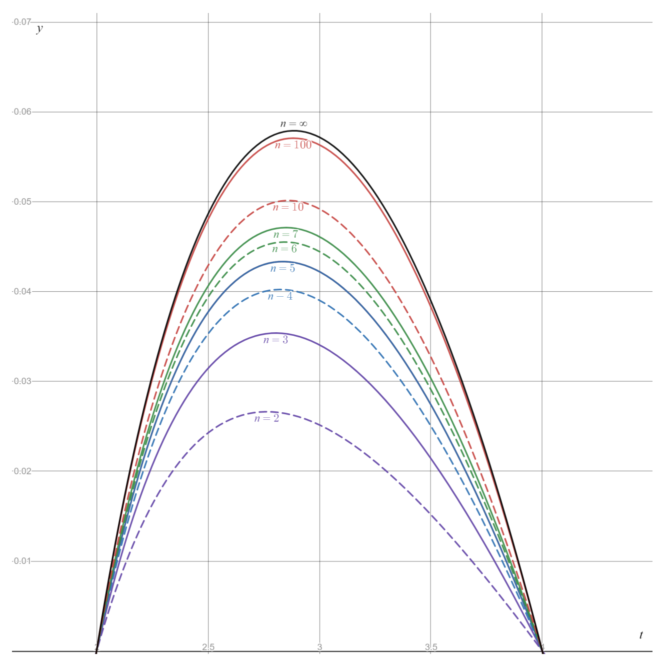


FIGURE 5. Graphs of $f_n(t)$ for selected values of n. Our numerical experiments indicate that, for all $t \in [2, 4]$, $f_n(t)$ increases monotonically to $f^*_\infty(t) := 1 - \frac{2^{t/2}}{t}$.

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