UNIQUENESS AND SHAPE OF SIMPLEX GROUND STATES FOR AGGREGATION–DIFFUSION ENERGIES WITH MILD REPULSION

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ABSTRACT. We study global minimizers in $\mathbb{R}^d$ of the free energy $\mathcal{E}_\kappa = \mathcal{W} + \kappa\mathcal{U}$, where $\mathcal{W}$ is a power-law interaction energy with mild repulsion and $\mathcal{U}$ is the porous-medium internal energy with exponent $m > 1$. In a range of exponents that we call the strict simplex regime, results of Lim–McCann and Davies–Lim–McCann show that $\mathcal{W}$ is minimized, uniquely up to rigid motions, by equal point masses at the vertices of a regular unit d-simplex. Diffusion excludes such atomic minimizers for every $\kappa > 0$. We prove that uniqueness nevertheless persists: for every fixed $m > 1$ and all sufficiently small $\kappa > 0$, the free energy has a unique global minimizer up to rigid motions. After a suitable rigid motion, this minimizer is invariant under every symmetry of the simplex, and its support splits into $d + 1$ clusters near the vertices, each of mass exactly $1/(d+1)$; in particular, it is not radially symmetric when $d \geq 2$. The clusters have width of order $\kappa^{1/(d(m-1)+2)}$, which is also the exact order of the quadratic Wasserstein distance from the minimizer to the atomic simplex measure. Rescaled at this scale, the clusters converge in L^1 and L^∞ to explicit Barenblatt-type profiles supported on ellipsoids determined by the Hessian of the simplex potential. For $d \geq 2$ these ellipsoids are spheroids flattened along the directions of the vertices; when the repulsive exponent exceeds two, their aspect ratio equals $(d+1)^{-1/2}$, independently of all other parameters. At the endpoint $(4, 2)$ of this regime in dimensions $d \geq 2$, where the zero-diffusion minimizer is not unique, we show instead that vanishing diffusion selects the uniform spherical shell.

1. INTRODUCTION

For certain radial attractive–repulsive potentials, the interaction energy is minimized, uniquely up to rigid motions, by equal point masses at the vertices of a regular simplex [25, 17]. Adding porous-medium diffusion rules out these atomic minimizers, since point masses have infinite internal energy. We show that rigidity nevertheless survives: for sufficiently small diffusion, the free energy has a unique global minimizer up to rigid motions. Its density forms separated clusters near the simplex vertices and, in dimensions two and higher, is not radially symmetric. Simplex symmetry and exact equality of the cluster masses follow from uniqueness, without being imposed in advance. We also determine the concentration scale and the limiting profiles of the clusters.

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We consider the free energy

$$\mathcal{E}_\kappa(\rho) = \mathcal{W}(\rho) + \kappa\mathcal{U}(\rho), \qquad \kappa > 0, \tag{1.1}$$

on the Borel probability measures $\mathcal{P}(\mathbb{R}^d)$, where

$$\mathcal{W}(\rho) := \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} W_{\alpha,\beta}(x-y)\,d\rho(x)\,d\rho(y),$$

$$W_{\alpha,\beta}(x) = w_{\alpha,\beta}(|x|), \quad w_{\alpha,\beta}(s) = s^\alpha/\alpha - s^\beta/\beta, \qquad \alpha > \beta \geq 2,$$

and

$$\mathcal{U}(\rho) := \begin{cases} \dfrac{1}{m-1}\displaystyle\int_{\mathbb{R}^d} \rho(x)^m\,dx, & \rho \in \mathcal{P}_{ac}(\mathbb{R}^d), \\ +\infty, & \text{otherwise}, \end{cases} \qquad m > 1.$$

We call $\mathcal{W}$ the interaction energy and $\mathcal{U}$ the internal energy. Here $\mathcal{P}_{ac}(\mathbb{R}^d)$ denotes the absolutely continuous probability measures. We also write $W = W_{\alpha,\beta}$, $w = w_{\alpha,\beta}$, and $U(s) = s^m/(m-1)$. Since w is minimized at $s = 1$, the kernel is repulsive at distances below one and attractive at distances above one. The associated aggregation–diffusion equation is

$$\partial_t\rho = \nabla\cdot\big(\rho\nabla(W*\rho)\big) + \kappa\Delta\rho^m. \tag{1.2}$$

Formally, this is the Wasserstein gradient flow of (1.1); see [1, 28]. We study global minimizers of the free energy, also called ground states; their role for the long-time behavior of (1.2) is studied in the companion paper [26].

Minimizers of interaction energies $\mathcal{W}$ have been studied extensively. Existence of global minimizers was established under sharp or almost optimal conditions in [6, 29]; see also [14] for power-law potentials. Balagué, Carrillo, Laurent, and Raoul [2] related the dimension of the support of local minimizers to the strength of the repulsion at the origin, and Carrillo, Delgadino, and Mellet [8] showed, under suitable assumptions, that local minimizers have bounded densities when the repulsion is at least as singular as the Newtonian one. Mild repulsion instead favors discrete minimizers. For a class of kernels with repulsive exponent strictly larger than two, Carrillo, Figalli, and Patacchini [10] proved that local minimizers in the ∞-Wasserstein topology have isolated support points, and that global minimizers have finite support. In one dimension, Kang, Kim, Lim, and Seo [24] studied uniqueness and local minimality for power-law interactions, including how local minimality depends on the Wasserstein topology.

Lim and McCann [25] identified the global minimizer of $\mathcal{W}$ for each fixed $\beta \geq 2$ and sufficiently large α: it assigns equal mass to the vertices of a regular unit d-simplex, up to rigid motions. Their proof uses a sharp bound on the variance of measures with a fixed support diameter. For $\alpha > \beta > 2$, they also showed that simplex configurations with unequal masses can be local minimizers in the ∞-Wasserstein topology. Davies, Lim, and McCann [17] then described the range of parameters for simplex minimizers through a dimension-dependent threshold, above which the equally weighted simplex is the unique global minimizer up to rigid motions.

Other shapes occur when $\beta = 2$. For $d \geq 2$ and $2 < \alpha < 4$, Davies, Lim, and McCann [16] proved that the unique global minimizer up to translation is a spherical shell, that is, a uniform measure on a sphere. In these dimensions, at $(\alpha, \beta) = (4, 2)$, there are

infinitely many centered minimizers: they are precisely the probability measures supported on the sphere of radius $\sqrt{d/(2d+2)}$ with zero first moment and second-moment matrix $I_d/(2d+2)$ [17]. For $d \geq 2$, Frank and Matzke [22] extended the spherical-shell classification to a sharp range of repulsive exponents $\beta \leq 2$ for $2 \leq \alpha \leq 4$, with uniqueness up to translations except at $(\alpha, \beta) = (4, 2)$. These classifications concern the interaction energy without diffusion. They show how strongly the minimizing geometry depends on the exponents, but they do not determine uniqueness once diffusion is added. At the degenerate pair $(4, 2)$, a separate convexity argument gives uniqueness for positive diffusion and selects the uniform shell as diffusion vanishes; see Proposition 5.1.

For energies with diffusion, Carrillo, Delgadino, and Patacchini [9] studied existence and nonexistence of ground states and derived their Euler–Lagrange conditions; see [7] for a survey of aggregation–diffusion equations and their singular limits. Burger and Di Francesco [3] constructed localized stationary profiles for small quadratic diffusion in one dimension. For smooth integrable attractive kernels and quadratic diffusion, Burger, Di Francesco, and Franek [4] characterized the existence of nontrivial steady states and proved their uniqueness up to translation in one dimension, using a strong form of the Krein–Rutman theorem. Burger, Fetecau, and Huang [5] studied compactly supported monotone equilibria in one dimension for general power-law diffusion, including the different free-boundary behavior on either side of the quadratic case. For a class of bounded smooth attractive potentials, Kaib [23] gave existence criteria for compactly supported global minimizers for every $m > 1$ and proved uniqueness of stationary states up to translation in the quadratic case whenever a minimizer exists.

Perturbative constructions also produce separated stationary clusters. Fagioli and Jaafra [20] used a functional implicit-function theorem for a one-dimensional two-species system with quadratic diffusion. They proved existence and uniqueness within a class of multiple even bumps, with the individual bump masses and centers prescribed, the centers satisfying a diffusion-free particle equilibrium condition, and the effective well curvatures assumed positive. Our result concerns all global minimizers in arbitrary dimension for every fixed $m > 1$; the cluster masses and symmetry are determined by minimization.

For purely attractive interactions, Carrillo, Hittmeir, Volzone, and Yao [11] proved radial symmetry of suitably regular stationary states by continuous Steiner symmetrization. Delgadino, Yan, and Yao [18] then proved, under suitable assumptions, uniqueness up to translation of bounded steady states with a fixed mass when $m \geq 2$, and constructed attractive potentials with nonunique steady states when $1 < m < 2$. The present kernels include short-range repulsion, and their ground states have disconnected support and are nonradial when $d \geq 2$. Thus the radial symmetry and interpolation arguments for purely attractive interactions do not apply to these ground states.

The vanishing-diffusion limit has also been studied as a variational approximation. Fetecau, Kovacic, and Topaloglu [21] proved convergence results for weak solutions and energy minimizers in domains with boundaries, under their assumptions on the interaction and the domain. Craig and Topaloglu [15] studied the different limit $m \to \infty$, in which diffusion becomes a density constraint.

In this paper, $m > 1$ is fixed and $\kappa \to 0$, and our principal question is uniqueness at each sufficiently small $\kappa > 0$, not merely the identification of subsequential limits. Compactness and energy comparison identify the atomic limit, but they do not exclude distinct diffuse minimizers converging to the same measure. The strict convexity of the internal energy does not settle this question, because the interaction energy is nonconvex, and competing minimizers may a priori have different cluster masses. We therefore compare minimizers without fixing these masses and prove uniqueness first; simplex symmetry and exact equality of the masses then follow.

We now fix the parameter range. Let $d \geq 1$, and let $\alpha_\Delta(\beta) = \alpha_{\Delta^d}(\beta)$ be the transition threshold of [17, Theorem 1.5]. We call

$$\mathcal{S} := \{(\alpha, \beta) : \beta \geq 2,\ \alpha > \alpha_\Delta(\beta)\}$$

the *strict simplex regime*. Here $\alpha_\Delta(\beta) \geq \beta$, and when $\beta = 2$ the strict condition is $\alpha > 4$ for $d \geq 2$ and $\alpha > 3$ for $d = 1$. In this range, the potential generated by the simplex has isolated minima at its vertices, with positive definite Hessians; see Lemma 3.4. A *rigid motion* is a map $x \mapsto Qx + a$, where $Q \in O(d)$ and $a \in \mathbb{R}^d$; reflections are allowed. We identify a simplex with its vertex set, and "unit" means that each edge has length one. We fix a centered regular unit simplex and its equally weighted measure,

$$\Delta^d = \{x_0, \dots, x_d\}, \qquad \rho_\Delta = \frac{1}{d+1} \sum_{i=0}^{d} \delta_{x_i}.$$

A *symmetry* of Δ^d is a map $G \in O(d)$ that permutes $\{x_0, \dots, x_d\}$.

Our first theorem gives existence, uniqueness, symmetry, localization near the simplex vertices, and exact equality of the cluster masses.

Theorem 1.1. *Suppose $m > 1$ and $(\alpha, \beta) \in \mathcal{S}$, and put $r_\kappa := \kappa^{1/(d(m-1)+2)}$. There exist $\kappa_* > 0$ and $L > 0$ with $Lr_{\kappa_*} \leq 1/2$, depending only on d, m, α, and β, such that for every $0 < \kappa < \kappa_*$ the energy $\mathcal{E}_\kappa$ has a global minimizer, unique up to rigid motions. A representative is the normalized minimizer ρ_κ of Definition 3.9. Moreover, $G_\# \rho_\kappa = \rho_\kappa$ for every symmetry G of Δ^d, so ρ_κ is centered, and*

$$\operatorname{supp} \rho_\kappa \subset \bigcup_{i=0}^{d} B_{Lr_\kappa}(x_i), \qquad \rho_\kappa\big(B_{Lr_\kappa}(x_i)\big) = \frac{1}{d+1}, \quad i = 0, \dots, d.$$

We impose no symmetry a priori and do not prescribe the individual cluster masses. For $d \geq 2$ the minimizer ρ_κ is not radially symmetric, so the rearrangement and symmetrization arguments available for purely attractive kernels [11, 18] are not applicable. To the best of our knowledge, Theorem 1.1 is the first result establishing uniqueness up to rigid motions of global minimizers of an aggregation–diffusion free energy on $\mathbb{R}^d$ with a radial interaction kernel and no external potential, in a setting where these minimizers are not radially symmetric. The simplex symmetry is a consequence of uniqueness; since the symmetries of Δ^d act transitively on its vertices, all cluster masses are equal. This equality holds for every sufficiently small $\kappa > 0$; convergence to the atomic simplex alone would yield equal masses only in the limit.

We also determine the size and shape of the clusters. The scale r_κ in Theorem 1.1 balances the interaction cost r^2 with the diffusion cost $\kappa r^{-d(m-1)}$. Put $u := 1/(d+1)$, $\hat{x}_i := x_i/|x_i|$, and

$$a_\perp := \frac{\alpha-\beta}{2} - \mathbf{1}_{\{\beta=2\}}, \qquad a_\parallel := \frac{(\alpha-\beta)(d+1)}{2} - \mathbf{1}_{\{\beta=2\}}. \tag{1.3}$$

Theorem 1.2. *Suppose $m > 1$ and $(\alpha,\beta) \in \mathcal{S}$, and let κ_*, L be as in Theorem 1.1. For $\kappa \in (0,\kappa_*)$, let ρ_κ be the normalized minimizer of Theorem 1.1, with clusters $\rho_{\kappa,i} := \rho_\kappa \mathbf{1}_{B_{1/2}(x_i)}$. Then $\|\rho_{\kappa,i}\|_{L^\infty} \le L r_\kappa^{-d}$, and each set $\{\rho_{\kappa,i} > 0\}$ is convex with C^2 boundary, with ρ_κ^{m-1} concave on it. Moreover, $r_\kappa^d \rho_{\kappa,i}(x_i + r_\kappa z) \longrightarrow f_i(z)$ as $\kappa \to 0$ in $L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$, where*

$$f_i(z) = \left[\frac{m-1}{m}\big(\lambda_* - z\cdot A_i z\big)\right]_+^{1/(m-1)}, \tag{1.4}$$

$$A_i := \frac{1}{2}D^2(W*\rho_\Delta)(x_i) = \frac{u}{2}\Big(a_\perp\big(I_d - \hat{x}_i\otimes\hat{x}_i\big) + a_\parallel\,\hat{x}_i\otimes\hat{x}_i\Big), \tag{1.5}$$

and $\lambda_* > 0$ is the unique constant satisfying $\int f_i = u$ for every i, given explicitly in (4.5). The rescaled supports converge in Hausdorff distance to the ellipsoids $E_i := \{z \in \mathbb{R}^d : z\cdot A_i z \le \lambda_*\}$. Additionally, the quadratic Wasserstein distance satisfies

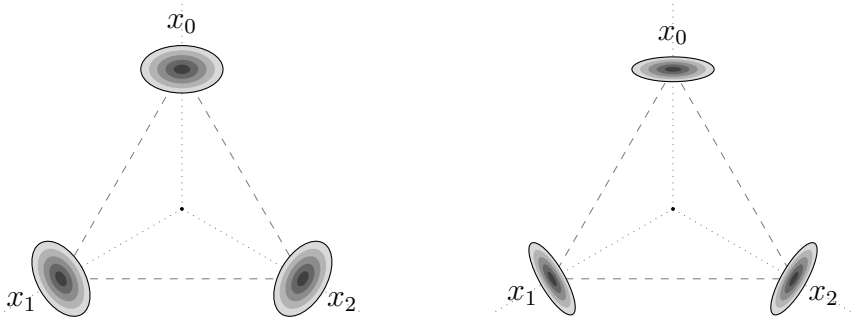
$$\lim_{\kappa\to 0} \frac{d_2(\rho_\kappa,\rho_\Delta)^2}{r_\kappa^2} = \frac{2(d+1)\lambda_*}{d+2+2/(m-1)}\left(\frac{1}{a_\parallel} + \frac{d-1}{a_\perp}\right),$$

where the term involving $a_\perp$ is omitted when $d = 1$.

In the strict simplex regime, $a_\parallel > 0$, and $a_\perp > 0$ when $d \ge 2$; see Lemma 3.4. Thus each limiting profile is a Barenblatt-type profile on the ellipsoid E_i. For $d \ge 2$, E_i is a spheroid with symmetry axis $\hat{x}_i$, flattened along this axis: the ratio of its semi-axis in the direction $\hat{x}_i$ to its other semi-axes is

$$\sqrt{\frac{a_\perp}{a_\parallel}} = \begin{cases} (d+1)^{-1/2}, & \beta > 2, \\ \sqrt{\dfrac{\alpha-4}{(\alpha-2)(d+1)-2}}, & \beta = 2. \end{cases}$$

In particular, these limiting ellipsoids are not balls although the pair potential is radial. The cutoff power in (1.4) is the classical Barenblatt form of porous-medium diffusion [30], while A_i is half the Hessian of the simplex potential $W*\rho_\Delta$ at x_i. Its anisotropic part comes from the other clusters, and this anisotropic confinement makes the clusters non-spherical. When $\beta > 2$, the aspect ratio does not depend on α, β, or m. When $\beta = 2$, it tends to zero as $\alpha \downarrow 4$, where the simplex regime meets the spherical-shell regime of [16]. By Theorem 1.2, r_κ is also the exact order of the quadratic Wasserstein distance to ρ_Δ. Figure 1 illustrates the two cases for $d = 2$.



(a) $\beta > 2$: ratio $1/\sqrt{3} \approx 0.58$ (b) $\beta = 2,\ \alpha = 4.5$: ratio $1/\sqrt{11} \approx 0.30$

FIGURE 1. Limiting cluster shapes of Theorem 1.2 for $d = 2$. The dashed triangle is the unit simplex Δ^2 and the dotted rays are the axes $\hat{x}_i$. Each cluster is drawn as the level sets of its limiting profile f_i, homothetic ellipses centered at the vertex. The cluster widths, of order r_κ, are magnified by a common factor; the shapes and orientations are exact. Each ellipse is flattened along $\hat{x}_i$ with semi-axis ratio $\sqrt{a_\perp/a_\parallel}$: (a) for every $(\alpha, \beta) \in \mathcal{S}$ with $\beta > 2$ and $m > 1$, this ratio is $1/\sqrt{3}$; (b) for $\beta = 2$ it depends on α, here $\alpha = 4.5$, and it tends to 0 as $\alpha \downarrow 4$.

Remark 1.3 (Dynamical stability). Transport and entropy methods for quantitative convergence to equilibrium were developed, in particular, in [12, 13]. The relation between these ground states and the long-time behavior of (1.2) is studied in the companion paper [26], where the algebraic identity of Lemma 3.11 enters a local displacement-convexity argument that gives exponential convergence to a fixed rigid image of ρ_κ for nearby finite-energy data in the ∞-Wasserstein topology, with rates uniform in small κ. The static results proved here do not depend on that analysis. For comparison, Di Francesco and Jaafra [19] established local asymptotic stability for a one-dimensional equation with quadratic diffusion and a purely attractive integrable kernel.

Why the small-diffusion limit is singular. The atomic minimizer ρ_Δ lies outside the finite-energy domain of $\mathcal{U}$ for every $\kappa > 0$, so a smooth perturbation argument cannot be applied directly to $\mathcal{E}_\kappa$ at ρ_Δ. This does not preclude implicit-function constructions in rescaled variables, as in [20]; the difficulty here is to compare arbitrary minimizers while their cluster masses, supports, and symmetries are still unknown. After rescaling, the free boundaries move with the minimizer, and the diffusion weight $U''(f) = mf^{m-2}$ vanishes there when $m > 2$ and is singular when $1 < m < 2$. Rigid motions introduce further degeneracies. We treat these issues by comparing two minimizers directly through their first variations, after an explicit alignment that removes translations and rotations; see Section 3.4.

The proof of Theorem 1.1 starts with a competitor obtained by smoothing the simplex atoms, which gives an $O(r_\kappa^2)$ bound on the energy excess above $\mathcal{W}(\rho_\Delta)$. The global Euler–Lagrange equation has one common Lagrange multiplier even though the support is disconnected; it confines the clusters to the non-degenerate wells of the simplex

potential and determines their width. We then remove the rigid-motion freedom by an alignment condition that involves only the masses and first moments of the clusters.

Two estimates close the comparison of aligned minimizers. First, after the differences of cluster masses have been separated off, the limiting interaction depends only on the first moments, and the simplex geometry makes this quadratic form nonnegative under alignment (Lemma 3.11). Second, the concavity of the rescaled pressure gives a uniform bound on the inverse diffusion weights up to the free boundaries (Lemma 3.12). A weighted Cauchy–Schwarz estimate then bounds the L^1 difference of the rescaled densities by their diffusion contribution, so the interaction errors can be absorbed for small κ, while a positive zeroth-order term controls the differences of the cluster masses. Thus the argument proves uniqueness without assuming equal masses, for every fixed $m > 1$, including the free-boundary degeneracy when $m > 2$.

For Theorem 1.2, we rescale the normalized minimizers, which are Δ^d-symmetric by Theorem 1.1, at the scale r_κ. Translating one cluster at a time gives force-balance equations, which together with the symmetry force the limiting cluster means to vanish. The Euler–Lagrange equation then identifies the profiles.

Section 2 gives the notation and variational tools. Section 3 proves Theorem 1.1, and Section 4 proves Theorem 1.2. Section 5 contains concluding remarks, including the selection result at the degenerate pair $(4, 2)$ and open questions.

2. Preliminaries

2.1. **Notation and elementary bounds.** We write $\mathcal{P}(\mathbb{R}^d)$ for Borel probability measures and $\mathcal{P}_{ac}(\mathbb{R}^d)$ for those that are absolutely continuous with respect to Lebesgue measure. For $p \geq 1$, $\mathcal{P}_p(\mathbb{R}^d)$ denotes the measures with finite p-th moment, and d_p is the p-Wasserstein distance. In contrast, the subscript in $\mathcal{P}_0(\mathbb{R}^d)$ denotes centering:

$$\mathcal{P}_0(\mathbb{R}^d) := \{\rho \in \mathcal{P}_1(\mathbb{R}^d) : \textstyle\int x \, d\rho(x) = 0\}.$$

Narrow convergence means convergence against bounded continuous functions, and $T_\#\rho$ denotes the push-forward. For a finite non-negative measure, $|\rho|$ denotes its total mass. We take $B_r(x)$ to be the open Euclidean ball, put $B_r := B_r(0)$, write $[s]_+ = \max\{s, 0\}$, and use $\operatorname{supp}\rho$ for the closed support. The same symbol denotes an absolutely continuous measure and its density. Unqualified integrals are over $\mathbb{R}^d$. For vectors, $(v \otimes w)_{kl} = v_k w_l$. For matrices, $\langle M, N\rangle := \operatorname{tr}(M^T N)$ and $|M| := \langle M, M\rangle^{1/2}$ denote the Frobenius inner product and norm, and $\|M\| := \sup_{|x|\leq 1} |Mx|$ denotes the operator norm.

Let $\Delta^d = \{x_0, \dots, x_d\}$ be the reference simplex fixed in the introduction, and set

$$u := \frac{1}{d+1}, \qquad \rho_\Delta = u \sum_{i=0}^{d} \delta_{x_i}, \qquad \mathcal{P}_\Delta := \mathcal{P}_0(\mathbb{R}^d) \cap \arg\min \mathcal{W}, \qquad e_{ij} := x_i - x_j.$$

For $(\alpha, \beta) \in \mathcal{S}$, [17, Theorem 1.5] shows that $\mathcal{P}_\Delta = \{Q_\#\rho_\Delta : Q \in O(d)\}$. Up to an orthogonal map, $x_j = (\mathbf{e}_j - \bar{\mathbf{e}})/\sqrt{2}$, where $\mathbf{e}_0, \dots, \mathbf{e}_d$ is the standard basis of $\mathbb{R}^{d+1}$, $\bar{\mathbf{e}} := u \sum_k \mathbf{e}_k$, and the hyperplane $\{y \in \mathbb{R}^{d+1} : \sum_k y_k = 0\}$ is identified with $\mathbb{R}^d$. For v

in this hyperplane, $\sum_j (x_j \cdot v)^2 = |v|^2/2$. This gives

$$\sum_{j=0}^{d} x_j = 0, \qquad |x_i|^2 = \frac{d}{2(d+1)}, \qquad x_i \cdot x_j = -\frac{1}{2(d+1)} \quad (i \neq j), \\ \sum_{j=0}^{d} x_j \otimes x_j = \frac{1}{2} I_d. \tag{2.1}$$

In particular $|e_{ij}| = 1$ for $i \neq j$, and the balls $B_{1/2}(x_i)$ are pairwise disjoint. For a measure ρ supported in $\bigcup_i B_{1/2}(x_i)$, the restrictions $\rho_i := \rho \mathbf{1}_{B_{1/2}(x_i)}$ are called its *clusters*. For a set of measures $\mathcal{A}$, we write $d_\alpha(\rho, \mathcal{A}) = \inf_{\nu \in \mathcal{A}} d_\alpha(\rho, \nu)$. Constants denoted by c, C may change from line to line; unless stated otherwise they depend only on d, m, α, and β, not on a sufficiently small κ or on the choice of global minimizer.

The minimum value of W is $w(1) = 1/\alpha - 1/\beta < 0$, and we put $c_W := -w(1) > 0$. There are constants $c_0, C_0 > 0$ such that

$$c_0 |z|^\alpha - C_0 \leq W(z), \qquad |W(z)| \leq C_0(1 + |z|^\alpha). \tag{2.2}$$

In particular, finite interaction energy implies a finite α-th moment: Fubini first gives a point y_0 with $\int |x - y_0|^\alpha \, d\rho(x) < \infty$. If $b = \int x \, d\rho(x)$, Jensen's inequality then gives

$$\int |x - b|^\alpha \, d\rho(x) \leq \iint |x - y|^\alpha \, d\rho(x) d\rho(y) \leq \frac{2\mathcal{W}(\rho) + C_0}{c_0}. \tag{2.3}$$

Also $W \in C^2(\mathbb{R}^d)$, and its derivatives of order at most two have at most α-power growth. Thus $W * \rho$ is C^2 whenever $\rho \in \mathcal{P}_\alpha(\mathbb{R}^d)$, by differentiation under the integral. These observations will justify both centering and the continuous Euler–Lagrange representative before a support bound is known.

2.2. **The global Euler–Lagrange equation.** A global minimizer has one common Lagrange multiplier, even when its support is disconnected. This will allow us to compare cluster masses. We give the first-variation argument; see also [9, 28].

Proposition 2.1. *Let ρ be a global minimizer of $\mathcal{E}_\kappa$, and set*

$$\Phi := W * \rho, \qquad \ell := \kappa m \mathcal{U}(\rho) + 2\mathcal{W}(\rho).$$

Then

$$\begin{cases} \kappa U'(\rho) + \Phi = \ell, & \rho\text{-almost everywhere}, \\ \kappa U'(\rho) + \Phi \geq \ell, & \text{Lebesgue-almost everywhere}. \end{cases} \tag{2.4}$$

Proof. The identities $\int U'(\rho)\rho = m\mathcal{U}(\rho)$ and $\int \Phi \, d\rho = 2\mathcal{W}(\rho)$ give $\ell = \int (\kappa U'(\rho) + \Phi) \, d\rho$. For any bounded compactly supported probability density ν, minimality along $(1-t)\rho + t\nu$ gives

$$0 \leq \frac{d}{dt}\bigg|_{t=0+} \mathcal{E}_\kappa((1-t)\rho + t\nu) = \int (\kappa U'(\rho) + \Phi)(\nu - \rho). \tag{2.5}$$

The derivative is justified by $\rho \in L^m$, the growth of U', and (2.2). Testing with normalized indicators of bounded measurable sets shows that $\kappa U'(\rho) + \Phi \geq \ell$ almost everywhere. Its integral against ρ equals ℓ, so equality holds ρ-almost everywhere. □

Corollary 2.2 (The continuous density)**.** *With ℓ as above, a global minimizer ρ has the continuous representative*

$$\rho(x) = \left[\frac{m-1}{m\kappa}\big(\ell - W * \rho(x)\big)\right]_+^{1/(m-1)}. \tag{2.6}$$

Proof. On $\{\rho > 0\}$, the equality in (2.4) gives this formula almost everywhere. On $\{\rho = 0\}$, the inequality gives $W * \rho \geq \ell$, so the right-hand side is zero. It is continuous because $W * \rho$ is C^2. □

We use this representative from now on. For a global minimizer ρ_κ we write $\ell_\kappa := \kappa m \mathcal{U}(\rho_\kappa) + 2\mathcal{W}(\rho_\kappa)$ and $\Phi_\kappa := W * \rho_\kappa$, so that

$$\rho_\kappa(x) > 0 \quad \Longleftrightarrow \quad \Phi_\kappa(x) < \ell_\kappa, \qquad \operatorname{supp}\rho_\kappa \subset \{\Phi_\kappa \leq \ell_\kappa\}.$$

2.3. **Compactness up to translations.** For completeness we give the compactness argument for our power-law kernel. It is a special case of the coercive-interaction compactness principle in [9, Section 2].

Lemma 2.3. *If $(\rho_n) \subset \mathcal{P}(\mathbb{R}^d)$ and $\liminf_n \mathcal{W}(\rho_n) < \infty$, then a subsequence converges narrowly to a probability measure after translations.*

Proof. Choose a subsequence with uniformly bounded interaction energy, and translate each measure by its barycenter. The moments in (2.3) are uniformly bounded. Consequently the translated measures assign at most $CR^{-\alpha}$ mass to B_R^c, uniformly along the subsequence. They are tight, and Prokhorov's theorem gives the claimed narrow subsequential convergence to a probability measure. □

3. Proof of Theorem 1.1: Uniqueness, symmetry, and equal masses

3.1. **Existence and zero-diffusion compactness.** This subsection collects three facts about global minimizers as $\kappa \to 0$ used throughout the proof of Theorem 1.1. Lemma 3.1 gives existence and confines all centered minimizers to a fixed ball. Lemma 3.2 compares the minimizers with a smoothed copy of the atomic simplex measure. This gives an energy excess of order r_κ^2, a bound of the same order for the Lagrange multipliers, and convergence of centered minimizers to the set of atomic minimizers $\mathcal{P}_\Delta$. Lemma 3.3 turns this convergence of measures into C^2 convergence of the interaction potentials, which will be used to localize the clusters in the next subsection.

Lemma 3.1 (Existence and uniform support)**.** *For every $\kappa > 0$, the energy $\mathcal{E}_\kappa$ has a global minimizer. There is $R > 0$ such that every centered global minimizer with $0 < \kappa \leq 1$ is supported in B_R.*

Proof. Let (ρ_n) be a minimizing sequence. Since $\mathcal{E}_\kappa \geq \mathcal{W} \geq w(1)/2$ and $\mathcal{U} \geq 0$, both $\mathcal{W}(\rho_n)$ and $\mathcal{U}(\rho_n)$ are bounded uniformly in n. By Lemma 2.3, after translations and passage to a subsequence, ρ_n converges narrowly to some $\rho \in \mathcal{P}(\mathbb{R}^d)$. Both $\mathcal{U}$ and $\mathcal{W}$ are translation invariant, so the translated sequence is still minimizing. Both are also narrowly lower semicontinuous. For $\mathcal{U}$, this holds because $\mathcal{U}$ is the integral functional of the convex superlinear function U with $U(0) = 0$; alternatively, since $\mathcal{U}(\rho_n)$ is bounded, a further subsequence converges weakly in L^m, necessarily to ρ, and the L^m norm is

weakly lower semicontinuous. For $\mathcal{W}$, the measures $\rho_n \otimes \rho_n$ converge narrowly to $\rho \otimes \rho$; we apply this to the bounded continuous truncations $\min\{W - w(1), k\}$ and let $k \to \infty$ by monotone convergence, using that W is continuous and bounded below. Hence ρ is a minimizer. Since $\mathcal{E}_\kappa(\rho) < \infty$, $\rho \in L^m$, and ρ has finite α-th moment by (2.3).

For the support bound, fix a smooth compactly supported probability density ν, and let ρ_κ denote a centered minimizer for $\mathcal{E}_\kappa$. Minimality gives, for $0 < \kappa \le 1$,

$$\mathcal{W}(\rho_\kappa) \le \mathcal{E}_\kappa(\rho_\kappa) \le \mathcal{E}_1(\nu), \qquad \kappa \mathcal{U}(\rho_\kappa) \le \mathcal{E}_1(\nu) - \frac{w(1)}{2}.$$

Thus the Euler–Lagrange multiplier $\ell_\kappa = \kappa m \mathcal{U}(\rho_\kappa) + 2\mathcal{W}(\rho_\kappa)$ is bounded above independently of the minimizer and of $\kappa \le 1$. Jensen's inequality and (2.2) give

$$\Phi_\kappa(x) = W * \rho_\kappa(x) \ge c_0 \int |x - y|^\alpha \, d\rho_\kappa(y) - C_0 \ge c_0 |x|^\alpha - C_0.$$

Choose R so that this lower bound exceeds the multiplier bound for $|x| \ge R$. Formula (2.6) then gives $\operatorname{supp} \rho_\kappa \subset B_R$. □

Set

$$r_\kappa := \kappa^{1/(d(m-1)+2)}.$$

This scale balances the diffusion cost and the quadratic interaction cost:

$$\kappa r_\kappa^{-d(m-1)} = r_\kappa^2. \tag{3.1}$$

Lemma 3.2 (A simplex competitor and compactness)**.** *For $(\alpha, \beta) \in \mathcal{S}$ and every sufficiently small $\kappa > 0$, every global minimizer satisfies*

$$0 \le \mathcal{E}_\kappa(\rho_\kappa) - \mathcal{W}(\rho_\Delta) = \mathcal{W}(\rho_\kappa) - \mathcal{W}(\rho_\Delta) + \kappa \mathcal{U}(\rho_\kappa) \le C r_\kappa^2. \tag{3.2}$$

Moreover, centered minimizers satisfy

$$d_\alpha(\rho_\kappa, \mathcal{P}_\Delta) \longrightarrow 0 \tag{3.3}$$

uniformly over the choice of minimizer. Their multipliers satisfy

$$0 \le \ell_\kappa - \ell_\Delta \le C r_\kappa^2, \qquad \ell_\Delta := 2\mathcal{W}(\rho_\Delta) = (1 - u) w(1). \tag{3.4}$$

Proof. Choose a non-negative $\varphi \in C_c^\infty(B_1)$ with $\int \varphi = 1$, and define the near-simplex measure

$$\nu_\kappa(x) := u \sum_{i=0}^{d} r_\kappa^{-d} \varphi\left(\frac{x - x_i}{r_\kappa}\right).$$

For small κ, we have $r_\kappa \le 1/2$, so the summands have disjoint supports. Write $x = x_i + r_\kappa z$, $y = x_j + r_\kappa z'$ with $z, z' \in B_1$, so that $x - y = e_{ij} + h$ with $|h| \le 2r_\kappa \le 1$. For $i \ne j$, since $|e_{ij}| = 1$, the point e_{ij} minimizes W, with $W(e_{ij}) = w(1)$; in particular $\nabla W(e_{ij}) = 0$, and Taylor's formula gives

$$0 \le W(e_{ij} + h) - W(e_{ij}) \le \tfrac{1}{2}\Big(\max_{\overline{B_2}} |D^2 W|\Big)|h|^2 \le C r_\kappa^2.$$

Integrating against $\nu_\kappa \otimes \nu_\kappa$, we find that the cross-interaction excess of ν_κ from ρ_Δ is at most $C r_\kappa^2$. For $i = j$, $|x - y| \le 2r_\kappa \le 1$, so $|W(x - y)| \le (2r_\kappa)^\alpha/\alpha + (2r_\kappa)^\beta/\beta \le$

$Cr_\kappa^\beta \le Cr_\kappa^2$, using $\alpha > \beta \ge 2$. Thus the self-interactions have absolute value at most Cr_κ^2. Finally, $\kappa\mathcal{U}(\nu_\kappa) \le Cr_\kappa^2$ by (3.1). Hence

$$\mathcal{E}_\kappa(\nu_\kappa) \le \mathcal{W}(\rho_\Delta) + Cr_\kappa^2.$$

Minimality, $\mathcal{U} \ge 0$, and $\mathcal{W} \ge \mathcal{W}(\rho_\Delta)$ then prove (3.2). Since

$$0 \le \ell_\kappa - \ell_\Delta = \kappa m\mathcal{U}(\rho_\kappa) + 2\big(\mathcal{W}(\rho_\kappa) - \mathcal{W}(\rho_\Delta)\big) \le 2m\big(\mathcal{E}_\kappa(\rho_\kappa) - \mathcal{W}(\rho_\Delta)\big),$$

where both terms in the middle are non-negative, (3.2) gives (3.4).

Let $\kappa_n \downarrow 0$ and choose centered global minimizers. Lemma 3.1 places them in a common compact ball, hence a subsequence converges in d_α to a centered probability measure ρ_∞. Continuity of the interaction energy on this ball and (3.2) give $\mathcal{W}(\rho_\infty) = \mathcal{W}(\rho_\Delta)$, so $\rho_\infty \in \mathcal{P}_\Delta$ by [17, Theorem 1.5]. If (3.3) failed uniformly, a sequence at positive distance from $\mathcal{P}_\Delta$ would have such a subsequence, a contradiction. □

Lemma 3.3 (Continuity of the interaction potential)**.** *Let $R > 0$, let $K \subset \mathbb{R}^d$ be compact, and let $V_\Delta := W * \rho_\Delta$. For every $\varepsilon > 0$ there is $\delta > 0$ such that*

$$\|W * \rho - V_\Delta\|_{C^2(K)} < \varepsilon$$

for every probability measure ρ supported in $\overline{B_R}$ with $d_\alpha(\rho, \rho_\Delta) < \delta$.

Proof. We may assume that ρ_Δ is supported in $\overline{B_R}$. Let $R' := R + \max_{x\in K}|x|$. For $j = 0, 1, 2$, the derivatives D^jW are bounded by some M and uniformly continuous on $\overline{B_{R'}}$, with a common modulus of continuity ω. Let π be an optimal coupling of ρ and ρ_Δ for d_α. For $x \in K$ and $t > 0$, split the integral below according to whether $|y-y'| < t$ or $|y-y'| \ge t$. On the first set we use the modulus ω, and on the second we use the bound $2M$ together with Markov's inequality $\pi(|y - y'| \ge t) \le t^{-\alpha} d_\alpha(\rho, \rho_\Delta)^\alpha$:

$$\begin{aligned}\big|D^j(W * \rho)(x) - D^jV_\Delta(x)\big| &\le \int \big|D^jW(x-y) - D^jW(x-y')\big|\, d\pi(y, y') \\ &\le \omega(t) + 2Mt^{-\alpha} d_\alpha(\rho, \rho_\Delta)^\alpha.\end{aligned}$$

Choose t with $\omega(t) < \varepsilon/6$, and then δ with $2Mt^{-\alpha}\delta^\alpha < \varepsilon/6$. □

3.2. **Localization and the cluster scale.** We now use the energy bound (3.2) to determine the size and location of the clusters. The isolated, non-degenerate wells of the simplex potential provide their local confinement.

Lemma 3.4 (Non-degeneracy of the simplex wells)**.** *Let $(\alpha, \beta) \in \mathcal{S}$, let $V_\Delta := W * \rho_\Delta$, and let $a_\perp, a_\parallel$ be as in* (1.3)*. Then*

$$\arg\min_{\mathbb{R}^d} V_\Delta = \{x_0, \dots, x_d\}, \qquad \nabla^2 V_\Delta(x_i) = u\Big(a_\perp\big(I_d - \hat{x}_i \otimes \hat{x}_i\big) + a_\parallel\, \hat{x}_i \otimes \hat{x}_i\Big).$$

Moreover, $a_\parallel > 0$, and $a_\perp > 0$ if $d \ge 2$. In particular, the constant

$$\sigma_\Delta := \min_{0\le i\le d} \lambda_{\min}\big(\nabla^2 V_\Delta(x_i)\big) > 0$$

satisfies $\nabla^2 V_\Delta(x_i) \ge \sigma_\Delta I_d$ for $i = 0, \dots, d$.

Proof. We first identify the minimum set. By [17, Theorem 1.5], ρ_Δ minimizes $\mathcal{W}_{\alpha,\beta}$, hence the Euler–Lagrange inequality gives the inclusion $\{x_0,\dots,x_d\} \subset \arg\min V_\Delta$. To show the reverse inclusion, as $\alpha > \alpha_\Delta(\beta) \geq \beta$, choose $\alpha' \in (\alpha_\Delta(\beta), \alpha)$. By [17, Theorem 1.5], ρ_Δ also minimizes $\mathcal{W}_{\alpha',\beta}$. Since $\alpha > \alpha'$, the pair (α,β) lies in the northeast region $A_{\alpha',\beta}$ of [17]. The northeast comparison principle [17, Theorem 1.2, (1.7)], applied with $\nu = \rho_\Delta$ and (α',β) in place of (α,β), therefore gives

$$\{x_0,\dots,x_d\} = \operatorname{supp}\rho_\Delta = \arg\min_{\mathbb{R}^d}\big(W_{\alpha,\beta} * \rho_\Delta\big) = \arg\min_{\mathbb{R}^d} V_\Delta.$$

For the reader's convenience we recall why the comparison principle yields equality. Write $\overline{w}_{a,b}(r) := (br^a - ar^b)/(a-b)$, which is a positive multiple of $w_{a,b}$ plus a constant, so that $\overline{W}_{a,b} * \rho_\Delta$ and $W_{a,b} * \rho_\Delta$ have the same minimum points. By [17, Lemma 3.1] and the symmetry $\overline{w}_{a,b} = \overline{w}_{b,a}$, for each fixed $r \geq 0$, the function $a \mapsto \overline{w}_{a,\beta}(r)$ is nondecreasing for $a > \beta$, and strictly increasing unless $r \in \{0,1\}$. Hence $\overline{W}_{\alpha',\beta} * \rho_\Delta \leq \overline{W}_{\alpha,\beta} * \rho_\Delta$, with equality at x if and only if $|x - x_j| \in \{0,1\}$ for every j. A point with this property is a vertex: otherwise it would be at distance one from all $d+1$ vertices, and $\mathbb{R}^d$ contains no $d+2$ points at mutual distance one. Since the vertices minimize $\overline{W}_{\alpha',\beta} * \rho_\Delta$ by the Euler–Lagrange equation for ρ_Δ, every non-vertex x satisfies $\overline{W}_{\alpha,\beta} * \rho_\Delta(x) > \overline{W}_{\alpha',\beta} * \rho_\Delta(x) \geq \overline{W}_{\alpha',\beta} * \rho_\Delta(x_0) = \overline{W}_{\alpha,\beta} * \rho_\Delta(x_0)$.

We next compute the Hessian at each vertex. For $i \neq j$,

$$\nabla^2 W(e_{ij}) = (\alpha-\beta) e_{ij} \otimes e_{ij}, \qquad \nabla^2 W(0) = -\mathbf{1}_{\{\beta=2\}} I_d.$$

By (2.1),

$$\sum_{j\neq i} e_{ij}\otimes e_{ij} = (d+1)x_i \otimes x_i + \sum_j x_j \otimes x_j = \frac{1}{2} I_d + \frac{d}{2}\,\hat{x}_i \otimes \hat{x}_i.$$

Consequently

$$\nabla^2 V_\Delta(x_i) = u\Big(\sum_{j\neq i} \nabla^2 W(e_{ij}) + \nabla^2 W(0)\Big) = u\Big((\alpha-\beta)\sum_{j\neq i} e_{ij}\otimes e_{ij} - \mathbf{1}_{\{\beta=2\}} I_d\Big), \quad (3.5)$$

which is the stated formula. If $\beta > 2$, then $a_\parallel > a_\perp = (\alpha-\beta)/2 > 0$. If $\beta = 2$, then $(\alpha,2) \in \mathcal{S}$ means $\alpha > 4$ for $d \geq 2$ and $\alpha > 3$ for $d = 1$; see [17, Theorem 1.5 and Remark 1.3]. Thus $a_\perp = (\alpha-4)/2 > 0$ when $d \geq 2$, and $a_\parallel = ((\alpha-2)(d+1)-2)/2 > 0$ in both cases. When $d = 1$, the term containing $a_\perp$ vanishes. □

The following elementary rigidity statement places an almost regular simplex near the reference simplex.

Lemma 3.5 (Rigidity of almost regular simplices)**.** *There are $\varepsilon_R > 0$ and C_R, depending only on d, with the following property. If $z_0,\dots,z_d \in \mathbb{R}^d$ satisfy $\big||z_i - z_j| - 1\big| \leq \varepsilon \leq \varepsilon_R$ for all $i \neq j$, then there is a rigid motion T with $\max_i |Tz_i - x_i| \leq C_R\varepsilon$.*

Proof. Let X and Y be the $d \times d$ matrices with columns $x_i - x_0$ and $z_i - z_0$, $1 \leq i \leq d$. The polarization identity $2a\cdot b = |a|^2 + |b|^2 - |a-b|^2$ expresses the entries of the Gram matrices X^TX and Y^TY through the edge lengths, which are 1 and $1 + O(\varepsilon)$, respectively. Hence $Y^TY = X^TX + E$ with $|E| \leq C\varepsilon$. Put $M := YX^{-1}$. Then

$$M^TM = X^{-T}(X^TX + E)X^{-1} = I_d + X^{-T}EX^{-1} = I_d + O(\varepsilon).$$

For $\varepsilon \le \varepsilon_R$ small, M^TM is positive definite, so M is invertible and has the polar decomposition $M = QP$ with $Q \in O(d)$ and $P = (M^TM)^{1/2} = I_d + O(\varepsilon)$. Consequently $|M - Q| = |Q(P - I_d)| \le C\varepsilon$ and $|Y - QX| \le |M - Q|\,|X| \le C\varepsilon$, that is, $|(z_i - z_0) - Q(x_i - x_0)| \le C\varepsilon$ for every i. The rigid motion $T(x) := Q^T(x - z_0) + x_0$ satisfies $Tz_i - x_i = Q^T\big((z_i - z_0) - Q(x_i - x_0)\big)$, which proves the claim. □

We now show that every centered minimizer close to the simplex splits, after a rotation, into $d+1$ clusters of width $O(r_\kappa)$ around the vertices, with densities of order r_κ^{-d} and masses within $O(r_\kappa)$ of u.

Lemma 3.6 (The scale of the clusters)**.** *There exist $\eta_0 \in (0, 1/8)$, $\delta_{\mathrm{sc}} > 0$, $C > 1$, and $\kappa_{\mathrm{sc}} > 0$ with the following property. Let $0 < \kappa < \kappa_{\mathrm{sc}}$, and let $\rho_\kappa \in \mathcal{P}_0(\mathbb{R}^d) \cap \arg\min \mathcal{E}_\kappa$ satisfy $d_\alpha(\rho_\kappa, \rho_\Delta) < \delta_{\mathrm{sc}}$. Then $\operatorname{supp}\rho_\kappa \subset \bigcup_i B_{\eta_0/2}(x_i)$, and there is $Q \in O(d)$ such that the clusters $\rho_{\kappa,i}$ of $Q_\#\rho_\kappa$, with masses $M_{\kappa,i} := |\rho_{\kappa,i}|$, satisfy*

$$\frac{u}{2} \le M_{\kappa,i} \le \frac{3u}{2}, \qquad \operatorname{supp}\rho_{\kappa,i} \subset B_{Cr_\kappa}(x_i), \qquad \|\rho_{\kappa,i}\|_{L^\infty} \le Cr_\kappa^{-d}, \tag{3.6}$$

and

$$\sum_{i=0}^{d} |M_{\kappa,i} - u|^2 \le Cr_\kappa^2. \tag{3.7}$$

Proof. We localize the support in uniformly convex wells, use the mass constraint to determine their heights and radii, and then use the interaction excess to locate the wells relative to the reference simplex.

Step 1: Localization in the wells. Choose $\eta_0 \in (0, 1/8)$ so small that $D^2V_\Delta \ge (3\sigma_\Delta/4)I_d$ on $\overline{B_{2\eta_0}(x_i)}$ for every i. Lemma 3.1 places every centered minimizer in a common ball B_R, and we may assume $R \ge 1$, so that $K := \overline{B_R}$ contains these closed balls. By Lemma 3.4, there is $g > 0$ such that $V_\Delta - \ell_\Delta \ge g$ on the compact set $K \setminus \bigcup_i B_{\eta_0/2}(x_i)$, where $\ell_\Delta = V_\Delta(x_i)$ is the minimum value of V_Δ. By Lemma 3.3, Φ_κ is close to V_Δ in $C^2(K)$ when $d_\alpha(\rho_\kappa, \rho_\Delta) < \delta_{\mathrm{sc}}$ with δ_{sc} small, and $\ell_\kappa \to \ell_\Delta$ uniformly over minimizers by (3.4). First choose δ_{sc}, and then κ_{sc}, so that

$$\Phi_\kappa - \ell_\kappa \ge \frac{g}{2} \quad \text{on } K \setminus \bigcup_i B_{\eta_0/2}(x_i), \qquad \|D^2\Phi_\kappa - D^2V_\Delta\| \le \frac{\sigma_\Delta}{4} \quad \text{on } K.$$

Since $\operatorname{supp}\rho_\kappa \subset K$, the first bound and (2.6) give $\operatorname{supp}\rho_\kappa \subset \bigcup_i B_{\eta_0/2}(x_i)$. The second bound gives, with $c_* := \sigma_\Delta/2$ and some $C_* > c_*$ independent of the minimizer,

$$c_*I_d \le \nabla^2\Phi_\kappa \le C_*I_d \quad \text{on } B_{2\eta_0}(x_i), \qquad i = 0, \dots, d. \tag{3.8}$$

By decreasing δ_{sc} further, the masses of the clusters of ρ_κ lie between $u/2$ and $3u/2$. To see this, let π be an optimal coupling of ρ_κ and ρ_Δ for d_α, and write $B_i := B_{\eta_0/2}(x_i)$. Since ρ_κ is concentrated on $\bigcup_j B_j$, we have

$$M_{\kappa,i} - u = \pi\big(B_i \times \{x_j : j \ne i\}\big) - \pi\Big(\bigcup_{j\ne i} B_j \times \{x_i\}\Big).$$

Both sets on the right consist of pairs at distance at least $1 - \eta_0/2 \ge 1/2$, so Markov's inequality gives $|M_{\kappa,i} - u| \le 2^\alpha d_\alpha(\rho_\kappa, \rho_\Delta)^\alpha$. It suffices that $2^\alpha\delta_{\mathrm{sc}}^\alpha \le u/2$.

Step 2: Heights and radii of the clusters. The C^1-closeness to V_Δ, together with (3.8), gives a unique critical point $z_{\kappa,i} \in B_{\eta_0/2}(x_i)$, the minimum of Φ_κ in $B_{2\eta_0}(x_i)$. Indeed, since $\nabla V_\Delta(x_i) = 0$ and $D^2 V_\Delta \geq (3\sigma_\Delta/4) I_d$ on $B_{2\eta_0}(x_i)$, every x with $|x - x_i| = \eta_0/2$ satisfies

$$(x - x_i) \cdot \nabla \Phi_\kappa(x) \geq \frac{3\sigma_\Delta}{4} \frac{\eta_0^2}{4} - \frac{\eta_0}{2} \|\nabla \Phi_\kappa - \nabla V_\Delta\|_{L^\infty(K)} > 0$$

if the C^1 distance is below $3\sigma_\Delta \eta_0/16$. Thus the outward radial derivative of the strictly convex function Φ_κ is positive on $\partial B_{\eta_0/2}(x_i)$, its minimum over the closed ball $\overline{B_{2\eta_0}(x_i)}$ lies in $B_{\eta_0/2}(x_i)$, and strict convexity gives uniqueness of the critical point. Put

$$h_{\kappa,i} := \ell_\kappa - \Phi_\kappa(z_{\kappa,i}).$$

By (2.6),

$$\rho_\kappa(x) = \left[\frac{m-1}{m\kappa} \big(\ell_\kappa - \Phi_\kappa(x) \big) \right]_+^{1/(m-1)}. \tag{3.9}$$

Since the i-th cluster has positive mass, $h_{\kappa,i} > 0$. For $x \in B_{2\eta_0}(x_i)$, (3.8) implies

$$\frac{c_*}{2} |x - z_{\kappa,i}|^2 \leq \Phi_\kappa(x) - \Phi_\kappa(z_{\kappa,i}) \leq \frac{C_*}{2} |x - z_{\kappa,i}|^2.$$

First, $h_{\kappa,i} \to 0$ uniformly over the minimizers in question: Otherwise there are $h_0 > 0$ and minimizers with $\kappa \downarrow 0$ and $h_{\kappa,i} \geq h_0$. The upper quadratic bound gives $\ell_\kappa - \Phi_\kappa \geq h_0/2$ on $B_{(h_0/C_*)^{1/2}}(z_{\kappa,i})$, which lies in $B_{2\eta_0}(x_i)$ if h_0 is small. By (3.9), the mass of this ball is at least $c\,(h_0/C_*)^{d/2} \big(h_0/\kappa\big)^{1/(m-1)} \to \infty$, contradicting $M_{\kappa,i} \leq 3u/2$.

By the two quadratic bounds, on $B_{2\eta_0}(x_i)$ we have

$$h_{\kappa,i} - \frac{C_*}{2} |x - z_{\kappa,i}|^2 \leq \ell_\kappa - \Phi_\kappa(x) \leq h_{\kappa,i} - \frac{c_*}{2} |x - z_{\kappa,i}|^2.$$

Hence $\ell_\kappa - \Phi_\kappa \geq h_{\kappa,i}/2$ on $B_{(h_{\kappa,i}/C_*)^{1/2}}(z_{\kappa,i})$, while $[\ell_\kappa - \Phi_\kappa]_+ \leq h_{\kappa,i}$ on $B_{2\eta_0}(x_i)$ and $\{\ell_\kappa > \Phi_\kappa\} \cap B_{2\eta_0}(x_i) \subset B_{(2h_{\kappa,i}/c_*)^{1/2}}(z_{\kappa,i})$. Since $h_{\kappa,i} \to 0$, both balls lie in $B_{2\eta_0}(x_i)$ for small κ. Since $\operatorname{supp} \rho_\kappa \subset \bigcup_j B_{\eta_0/2}(x_j)$, the mass of the i-th cluster is $M_{\kappa,i} = \rho_\kappa(B_{2\eta_0}(x_i))$. Integrating (3.9) over the two balls therefore gives

$$c\kappa^{-1/(m-1)} h_{\kappa,i}^{\frac{d}{2} + \frac{1}{m-1}} \leq M_{\kappa,i} \leq C\kappa^{-1/(m-1)} h_{\kappa,i}^{\frac{d}{2} + \frac{1}{m-1}}, \tag{3.10}$$

with constants depending only on c_*, C_*, d, and m. Since the cluster masses lie between $u/2$ and $3u/2$, (3.10) gives

$$c r_\kappa^2 \leq h_{\kappa,i} \leq C r_\kappa^2. \tag{3.11}$$

Equations (3.9)–(3.11) now imply that the i-th cluster of ρ_κ is supported in $B_{Cr_\kappa}(z_{\kappa,i})$ and is bounded by $\big[\frac{m-1}{m\kappa} h_{\kappa,i}\big]^{1/(m-1)} \leq C r_\kappa^{-d}$, since $r_\kappa^2/\kappa = r_\kappa^{-d(m-1)}$ by (3.1).

Step 3: Masses and positions of the clusters. The radius estimate is currently centered at $z_{\kappa,i}$, not at the reference vertex x_i. We now extract the information needed to place these centers. Let $\rho_{\kappa,i}$ denote the clusters of ρ_κ, with masses $M_{\kappa,i}$, and put

$$I_{\kappa,ij} := \iint W(x - y)\, d\rho_{\kappa,i}(x)\, d\rho_{\kappa,j}(y).$$

The preceding support estimate gives $|I_{\kappa,ii}| \le Cr_\kappa^\beta \le Cr_\kappa^2$, since $\beta \ge 2$ and $r_\kappa \le 1$. For $i \ne j$, define the cross excess

$$X_{\kappa,ij} := I_{\kappa,ij} - w(1)M_{\kappa,i}M_{\kappa,j} \ge 0,$$

which is non-negative because $w(1) = \min W$. Since $\rho_\kappa = \sum_i \rho_{\kappa,i}$ and W is even, $\mathcal{W}(\rho_\kappa) = \frac{1}{2}\sum_i I_{\kappa,ii} + \sum_{i<j} I_{\kappa,ij}$. Using $\sum_i M_{\kappa,i} = 1$, we have $\sum_{i<j} M_{\kappa,i}M_{\kappa,j} = \frac{1}{2}\big(1 - \sum_i M_{\kappa,i}^2\big)$ and $\sum_i M_{\kappa,i}^2 - u = \sum_i (M_{\kappa,i} - u)^2$. With $\mathcal{W}(\rho_\Delta) = \frac{w(1)}{2}(1-u)$, this gives

$$\mathcal{W}(\rho_\kappa) - \mathcal{W}(\rho_\Delta) = \frac{c_W}{2}\sum_i (M_{\kappa,i} - u)^2 + \sum_{i<j} X_{\kappa,ij} + \frac{1}{2}\sum_i I_{\kappa,ii}$$

where $c_W = -w(1) > 0$. Combining this identity with (3.2), we get (3.7) and

$$0 \le X_{\kappa,ij} \le Cr_\kappa^2. \tag{3.12}$$

It remains to find $Q \in O(d)$ with $\max_i |Qz_{\kappa,i} - x_i| \le Cr_\kappa$. Indeed, since $\operatorname{supp}\rho_{\kappa,i} \subset B_{Cr_\kappa}(z_{\kappa,i})$, such a Q gives $\operatorname{supp}(Q_\#\rho_{\kappa,i}) \subset B_{2Cr_\kappa}(x_i) \subset B_{1/2}(x_i)$ for small κ, so $Q_\#\rho_{\kappa,i}$ is the i-th cluster of $Q_\#\rho_\kappa$, with the same mass, and (3.6) and (3.7) hold for $Q_\#\rho_\kappa$.

Since w has a non-degenerate minimum at $s = 1$, there is $c > 0$ such that, whenever s is close to one, $w(s) - w(1) \ge c(s-1)^2$. For $x \in \operatorname{supp}(\rho_{\kappa,i})$ and $y \in \operatorname{supp}(\rho_{\kappa,j})$, the preceding support estimate gives $||x-y| - |z_{\kappa,i} - z_{\kappa,j}|| \le Cr_\kappa$. Hence

$$W(x-y) - w(1) \ge c\big(|z_{\kappa,i} - z_{\kappa,j}| - 1\big)^2 - Cr_\kappa^2.$$

After integration by $\rho_{\kappa,i} \otimes \rho_{\kappa,j}$, (3.12) and the mass bound $\frac{1}{2}u \le M_{\kappa,i} \le \frac{3}{2}u$ give

$$\big||z_{\kappa,i} - z_{\kappa,j}| - 1\big| \le Cr_\kappa, \qquad i \ne j.$$

For small κ, Lemma 3.5, applied with $\varepsilon = Cr_\kappa$, provides a rigid motion $T_\kappa(x) = Q_\kappa x + a_\kappa$ such that $\max_i |T_\kappa(z_{\kappa,i}) - x_i| \le Cr_\kappa$. Since ρ_κ is centered and $\operatorname{supp}\rho_{\kappa,i} \subset B_{Cr_\kappa}(z_{\kappa,i})$,

$$0 = \sum_i \int x\, d\rho_{\kappa,i}(x) = \sum_i M_{\kappa,i} z_{\kappa,i} + O(r_\kappa).$$

Since $\sum_i M_{\kappa,i} = 1$, this gives

$$\sum_i M_{\kappa,i} T_\kappa(z_{\kappa,i}) = Q_\kappa \sum_i M_{\kappa,i} z_{\kappa,i} + a_\kappa = a_\kappa + O(r_\kappa).$$

On the other hand, by the estimate for $T_\kappa(z_{\kappa,i})$, (3.7), and $\sum_i x_i = 0$,

$$\sum_i M_{\kappa,i} T_\kappa(z_{\kappa,i}) = \sum_i M_{\kappa,i} x_i + O(r_\kappa) = \sum_i (M_{\kappa,i} - u)x_i + O(r_\kappa) = O(r_\kappa).$$

Hence $|a_\kappa| \le Cr_\kappa$, and therefore $\max_i |Q_\kappa z_{\kappa,i} - x_i| \le Cr_\kappa$. □

3.3. **Alignment and normalized minimizers.** The scale estimates leave the rigid-motion freedom unresolved. We fix it by the first-order conditions for the best rigid fit of the clusters to the labelled vertices.

Definition 3.7 (Alignment)**.** Let $\rho_0, \dots, \rho_d$ be finite non-negative measures with finite second moments. The labelled family (ρ_i), or the measure $\rho = \sum_i \rho_i$ with these clusters, is *aligned with* Δ^d if

$$\sum_{i=0}^{d} \int (x - x_i)\, d\rho_i(x) = 0, \qquad \sum_{i=0}^{d} \int (x - x_i) \cdot S x_i \, d\rho_i(x) = 0 \tag{3.13}$$

for every skew-symmetric matrix S.

The conditions (3.13) say that the identity is a critical point of

$$J(T) := \sum_{i=0}^{d} \int |Tx - x_i|^2 \, d\rho_i(x)$$

on the group of rigid motions. Indeed, for a skew-symmetric S and $b \in \mathbb{R}^d$, the maps $R_t(x) := e^{tS}x + tb$ form a C^1 curve of rigid motions with $R_0 = \mathrm{id}$ and velocity $x \mapsto Sx + b$ at $t = 0$, because $(e^{tS})^T e^{tS} = e^{-tS} e^{tS} = I_d$. Conversely, if $t \mapsto Q_t x + a_t$ is any C^1 curve of rigid motions with $Q_0 = I_d$ and $a_0 = 0$, differentiating $Q_t^T Q_t = I_d$ at $t = 0$ shows that $\dot{Q}_0$ is skew-symmetric, so its velocity $x \mapsto \dot{Q}_0 x + \dot{a}_0$ is again of this form. Since the first variation of J along a curve depends only on its velocity at $t = 0$, it suffices to consider the curves R_t. Using $(x - x_i) \cdot S(x - x_i) = 0$, differentiation at $t = 0$ gives

$$\frac{d}{dt}\Big|_{t=0} J(R_t) = 2\, b \cdot \sum_i \int (x - x_i)\, d\rho_i(x) + 2 \sum_i \int (x - x_i) \cdot S x_i \, d\rho_i(x).$$

This vanishes for all (S, b) if and only if (3.13) holds. Note that the conditions involve only the masses $M_i := |\rho_i|$ and the first moments $\mathbf{m}_i := \int x \, d\rho_i$, and since $v \cdot Sw = \langle S, v \otimes w \rangle$, the second condition says exactly that $\sum_i (\mathbf{m}_i - M_i x_i) \otimes x_i$ is symmetric.

Lemma 3.8 (Fixing translation and orientation)**.** *Let $\rho = \sum_i \rho_i$ be a probability measure with finite second moment, with labelled clusters ρ_i, masses M_i, and first moments $\mathbf{m}_i$, and put*

$$\bar{x} := \sum_i M_i x_i, \qquad \bar{\mathbf{m}} := \sum_i \mathbf{m}_i, \qquad K := \sum_i \mathbf{m}_i \otimes (x_i - \bar{x}).$$

(i) *A rigid motion $x \mapsto Q'x + a'$ aligns the clusters if and only if $a' = \bar{x} - Q'\bar{\mathbf{m}}$ and $Q'K$ is symmetric. If K is invertible, then $Q := (K^T K)^{1/2} K^{-1}$ is orthogonal, QK is symmetric and positive definite, and $T(x) := Qx + a$ with $a := \bar{x} - Q\bar{\mathbf{m}}$ aligns the clusters. Moreover, T is the unique global minimizer of J over all rigid motions, and if $\|K - \frac{u}{2} I_d\| \le \frac{u}{8}$, then every aligning rigid motion $x \mapsto Q'x + a'$ with $\|Q' - I_d\| \le \frac{1}{8}$ coincides with T.*

(ii) *For every $C > 0$ there are $r_0, C' > 0$ such that, if $0 < r \le r_0$, $\operatorname{supp} \rho_i \subset B_{Cr}(x_i)$, and $|M_i - u| \le Cr$ for all i, then K is invertible and $\|Q - I_d\| + |a| \le C'r$.*

(iii) *If G is a symmetry of Δ^d with $Gx_i = x_{\pi(i)}$ and (ρ_i) is aligned, then the relabelled family $(\widetilde{\rho}_j)$, $\widetilde{\rho}_{\pi(i)} := G_{\#}\rho_i$, is aligned.*

Proof. (i) For a rigid motion $T'(x) = Q'x + a'$, expand the square and use $\sum_i M_i = 1$, $|Q'x| = |x|$, and $(Q'\mathbf{m}_i) \cdot (x_i - \bar{x}) = \operatorname{tr}\big(Q'\,\mathbf{m}_i \otimes (x_i - \bar{x})\big)$. Completing the square in a' gives

$$J(T') = c_0 - 2\operatorname{tr}(Q'K) + \big|a' - \bar{x} + Q'\bar{\mathbf{m}}\big|^2, \tag{3.14}$$

where $c_0 := \sum_i \int |x|^2 \, d\rho_i + \sum_i M_i|x_i|^2 - |\bar{\mathbf{m}}|^2 - |\bar{x}|^2$ does not depend on T'.

The clusters $T'_{\#}\rho_i$ are aligned if and only if the identity is a critical point of $R \mapsto \sum_i \int |Rx - x_i|^2 \, d(T'_{\#}\rho_i) = J(R \circ T')$. Along $R_t(x) = e^{tS}x + tb$, the motion $R_t \circ T'$ has linear part $e^{tS}Q'$ and translation $e^{tS}a' + tb$. Put $\delta := a' - \bar{x} + Q'\bar{\mathbf{m}}$. By (3.14),

$$\frac{d}{dt}\Big|_{t=0} J(R_t \circ T') = -2\operatorname{tr}(SQ'K) + 2\,\delta \cdot \big(S(a' + Q'\bar{\mathbf{m}}) + b\big).$$

Taking $S = 0$ and b arbitrary shows that alignment forces $\delta = 0$. When $\delta = 0$, the derivative is $-2\operatorname{tr}(SQ'K) = 2\langle S, Q'K\rangle$, which vanishes for every skew-symmetric S if and only if $Q'K$ is symmetric. This proves the characterization.

If K is invertible, then $P := (K^TK)^{1/2}$ is symmetric and positive definite, $Q^TQ = K^{-T}P^2K^{-1} = I_d$, and $QK = P$. The characterization shows that T aligns the clusters. To see that T minimizes J, note by (3.14) that it suffices to maximize $\operatorname{tr}(Q'K)$ over $Q' \in O(d)$. Write $O := Q'Q^T \in O(d)$, so that $\operatorname{tr}(Q'K) = \operatorname{tr}(OP)$, and let (e_j) be an orthonormal eigenbasis of P with eigenvalues $\lambda_j > 0$. Then

$$\operatorname{tr}(OP) = \sum_j \lambda_j \, e_j \cdot Oe_j \le \sum_j \lambda_j = \operatorname{tr}(QK),$$

with equality only if $Oe_j = e_j$ for all j, that is, $Q' = Q$. Thus T uniquely minimizes J.

Finally, let $x \mapsto Q'x + a'$ align the clusters, with $\|Q' - I_d\| \le \frac{1}{8}$, and suppose $\|K - \frac{u}{2}I_d\| \le \frac{u}{8}$. Then $\|K\| \le \frac{5u}{8}$ and $\|Q'K - \frac{u}{2}I_d\| \le \|Q' - I_d\|\,\|K\| + \|K - \frac{u}{2}I_d\| < \frac{u}{4}$. So the symmetric matrix $Q'K$ is positive definite. Hence $K = Q'^T(Q'K) = Q^TP$ are two polar decompositions of K, and uniqueness of the polar decomposition gives $Q' = Q$. Then $a' = a$ by the characterization.

(ii) Under these assumptions, $|\mathbf{m}_i - M_ix_i| \le Cr$, $\bar{x} = \sum_i (M_i - u)x_i = O(r)$, and $\bar{\mathbf{m}} = \sum_i (\mathbf{m}_i - M_ix_i) + \bar{x} = O(r)$. The identity $\sum_{j=0}^d x_j \otimes x_j = \frac{1}{2}I_d$ in (2.1) then gives

$$K = \sum_i (\mathbf{m}_i - M_ix_i) \otimes x_i + \sum_i M_ix_i \otimes x_i - \bar{\mathbf{m}} \otimes \bar{x} = \frac{u}{2}I_d + O(r).$$

The map $K \mapsto (K^TK)^{1/2}K^{-1}$ is smooth near $\frac{u}{2}I_d$ and equals I_d there. Hence $\|Q - I_d\| \le C'r$, and then $|a| \le |\bar{x}| + |\bar{\mathbf{m}}| \le C'r$.

(iii) The measures $G_{\#}\rho_i$ have finite second moments, and

$$\sum_i \int (y - x_{\pi(i)}) \, d\widetilde{\rho}_{\pi(i)}(y) = G \sum_i \int (x - x_i) \, d\rho_i(x) = 0.$$

For a skew-symmetric S, the rotational condition for the relabelled family becomes $\sum_i \int (x - x_i) \cdot (G^TSG)x_i \, d\rho_i(x) = 0$, which holds because G^TSG is again skew-symmetric. □

Alignment alone does not determine the rigid motion: by Lemma 3.8(i), every $Q' \in O(d)$ with $Q'K$ symmetric gives an aligning motion, and only $Q' = Q$ makes $Q'K$ positive definite. This is why the uniqueness statement in Lemma 3.8(i) requires Q' to be close to I_d.

Definition 3.9 (Normalized minimizers)**.** Let C be the constant of Lemma 3.6, let C' be given by Lemma 3.8(ii) for this C, and put $L := C + 2C' + C^{1/2}$. For $\kappa > 0$ with $Lr_\kappa < 1/2$, let $\mathcal{N}_\kappa$ be the set of global minimizers ρ of $\mathcal{E}_\kappa$ such that $\operatorname{supp}\rho \subset \bigcup_i B_{Lr_\kappa}(x_i)$, the clusters of ρ are aligned with Δ^d, and

$$\big|\,|\rho_i| - u\,\big| \le Lr_\kappa, \qquad \|\rho_i\|_{L^\infty} \le Lr_\kappa^{-d}, \qquad i = 0, \dots, d. \tag{3.15}$$

Lemma 3.10 (Normalization)**.** *There is $\kappa_3 > 0$ such that, for $0 < \kappa < \kappa_3$, every global minimizer of $\mathcal{E}_\kappa$ is the image of an element of $\mathcal{N}_\kappa$ under a rigid motion; in particular, $\mathcal{N}_\kappa \neq \emptyset$. Moreover, $G_\#\rho \in \mathcal{N}_\kappa$ for every $\rho \in \mathcal{N}_\kappa$ and every symmetry G of Δ^d.*

Proof. Choose small $\kappa_3 \in (0, \kappa_{\mathrm{sc}}]$ so that, for $\kappa \in (0, \kappa_3)$, every centered global minimizer satisfies $d_\alpha(\rho, \mathcal{P}_\Delta) < \delta_{\mathrm{sc}}$ by Lemma 3.2, $r_\kappa \le r_0$ in Lemma 3.8(ii), and $Lr_\kappa < 1/2$. Let ρ be a centered global minimizer with $0 < \kappa < \kappa_3$. Since $\mathcal{P}_\Delta$ is the $O(d)$-orbit of ρ_Δ, an orthogonal map then brings ρ within d_α-distance δ_{sc} of ρ_Δ. Lemma 3.6 provides a further orthogonal map after which (3.6) and (3.7) hold; in particular, the clusters are compactly supported and $|M_{\kappa,i} - u| \le C^{1/2} r_\kappa$. Lemma 3.8(ii) then gives a rigid motion $T(x) = Qx + a$ with $\|Q - I_d\| + |a| \le C' r_\kappa$ that aligns the clusters. It maps $B_{Cr_\kappa}(x_i)$ into $B_{(C+2C')r_\kappa}(x_i)$, and it preserves masses and L^∞ bounds. Hence $T_\#\rho \in \mathcal{N}_\kappa$.

Now let $\rho \in \mathcal{N}_\kappa$, and let G be a symmetry of Δ^d. Then $G_\#\rho$ is a global minimizer and the map G permutes the balls $B_{Lr_\kappa}(x_i)$ and the clusters, so (3.15) holds for $G_\#\rho$, which is aligned by Lemma 3.8(iii). Thus $G_\#\rho \in \mathcal{N}_\kappa$. □

Alignment is not the same as centering when cluster masses are unequal: its first condition says $\int x\, d\rho = \sum_i |\rho_i| x_i$. Because of this, the arguments below use the support and scale estimates in (3.15), not membership in $\mathcal{P}_0(\mathbb{R}^d)$. Once equal masses are proved, normalized minimizers are centered.

3.4. **Uniqueness of normalized minimizers.** For a measure ρ with clusters ρ_i and for $r > 0$, we call

$$f_i(z) := r^d \rho_i(x_i + rz)$$

its rescaled clusters. We also define the rescaled kernels

$$K^r_{ii}(z, z') := \frac{W(r(z - z'))}{r^2}, \quad K^r_{ij}(z, z') := \frac{W(e_{ij} + r(z - z')) - w(1)}{r^2} \quad (i \neq j). \tag{3.16}$$

Taylor's formula, $W(0) = 0$, $\nabla W(0) = \nabla W(e_{ij}) = 0$, and continuity of $D^2 W$ show that these kernels converge in C^2 on every bounded set as $r \downarrow 0$ to

$$K^0_{ii}(z, z') = -\frac{1}{2}\mathbf{1}_{\{\beta=2\}}|z - z'|^2, \quad K^0_{ij}(z, z') = \frac{\alpha - \beta}{2}\big(e_{ij} \cdot (z - z')\big)^2 \quad (i \neq j). \tag{3.17}$$

If a perturbation (δ_i) has zero mass in each cluster, then its limiting interaction, computed with the kernels (3.17), depends only on the first moments $p_i := \int z\, \delta_i(z)\, dz$: it equals the quadratic form $\mathcal{B}(p)$ introduced below, as the proof of Lemma 3.13 shows. The next lemma shows $\mathcal{B}(p) \ge 0$ whenever p satisfies the alignment conditions (3.18).

Lemma 3.11 (Nonnegativity on aligned first moments)**.** *For $p = (p_0, \dots, p_d) \in (\mathbb{R}^d)^{d+1}$ define $\mathcal{B}(p) := \mathbf{1}_{\{\beta=2\}} \sum_i |p_i|^2 - 2(\alpha-\beta) \sum_{i<j} (e_{ij} \cdot p_i)(e_{ij} \cdot p_j)$ and $M_p := \sum_i p_i \otimes x_i$. If*

$$\sum_i p_i = 0 \qquad \text{and} \qquad \sum_i p_i \cdot S x_i = 0 \quad \text{for every skew-symmetric } S, \tag{3.18}$$

then M_p is symmetric and

$$\mathcal{B}(p) = \mathbf{1}_{\{\beta=2\}} \sum_i |p_i|^2 + (\alpha-\beta)\Big((\operatorname{tr} M_p)^2 + |M_p|^2 \Big) \geq 0, \tag{3.19}$$

with equality only for $p = 0$.

Proof. Since $p_i \cdot S x_i = \langle S, p_i \otimes x_i \rangle$, the second condition in (3.18) says that M_p is orthogonal to all skew-symmetric matrices, that is, M_p is symmetric. Put $s_{ij} := x_i \cdot p_j$. The first condition gives $\sum_j s_{ij} = 0$ for every i. Since $e_{ij} \cdot p_i = s_{ii} - s_{ji}$ and $e_{ij} \cdot p_j = s_{ij} - s_{jj}$, and since the summand below is symmetric in i and j,

$$2 \sum_{i<j} (e_{ij} \cdot p_i)(e_{ij} \cdot p_j) = \sum_{i \neq j} \big(s_{ii} s_{ij} - s_{ii} s_{jj} - s_{ji} s_{ij} + s_{ji} s_{jj} \big).$$

Using $\sum_{j \neq i} s_{ij} = -s_{ii}$ in the first and last terms, we find

$$2 \sum_{i<j} (e_{ij} \cdot p_i)(e_{ij} \cdot p_j) = -\Big(\sum_i s_{ii} \Big)^2 - \sum_{i,j} s_{ij} s_{ji} = -(\operatorname{tr} M_p)^2 - \operatorname{tr}(M_p^2).$$

As M_p is symmetric, $\operatorname{tr}(M_p^2) = |M_p|^2$, which proves (3.19). If $\mathcal{B}(p) = 0$, then $M_p = 0$ because $\alpha > \beta$, so $\sum_i p_i \otimes (1, x_i) = 0$ in $\mathbb{R}^d \otimes \mathbb{R}^{d+1}$. The vectors $(1, x_i) \in \mathbb{R}^{d+1}$ are linearly independent, since the vertices are affinely independent, and therefore $p = 0$. □

Lemma 3.12 (Convex wells and inverse diffusion weights)**.** *There are $\kappa_2 \in (0, \kappa_3]$ and $C_w > 0$ such that, for $0 < \kappa < \kappa_2$ and every $\rho \in \mathcal{N}_\kappa$,*

$$\nabla^2 (W * \rho) \geq c_* I_d \quad \text{on } B_{2\eta_0}(x_i), \qquad i = 0, \dots, d, \tag{3.20}$$

where η_0 is as in Lemma 3.6 and $c_* = \sigma_\Delta / 2$ is the constant in (3.8). The rescaled clusters of ρ with $r = r_\kappa$ also satisfy

$$\int_{\{f_i > 0\}} f_i^{2-m} \, dz \leq C_w, \qquad i = 0, \dots, d. \tag{3.21}$$

Proof. Let $\rho \in \mathcal{N}_\kappa$, $r := r_\kappa$, $\Phi := W * \rho$, and $\ell := \kappa m \mathcal{U}(\rho) + 2\mathcal{W}(\rho)$. We take κ_2 so small that $L r_\kappa \leq \min\{\eta_0, u/2\}$ for $\kappa < \kappa_2$; in particular $\operatorname{supp} \rho \subset B_1$, and every cluster has mass at least $u/2$. To obtain an upper bound for $d_\alpha(\rho, \rho_\Delta)$, we may move each cluster to its vertex, and then move the excess masses along edges of length one. This gives

$$d_\alpha(\rho, \rho_\Delta)^\alpha \leq (Lr)^\alpha + \sum_i \big| |\rho_i| - u \big| (1 + Lr)^\alpha \leq (Lr)^\alpha + \sum_i (Lr)(1 + Lr)^\alpha \leq Cr.$$

Recall from Step 1 of the proof of Lemma 3.6 that $D^2V_\Delta \geq (3\sigma_\Delta/4)I_d$ on $\overline{B_{2\eta_0}(x_i)}$. Lemma 3.3, applied with $R = 1$ and $K := \bigcup_i \overline{B_{2\eta_0}(x_i)}$, therefore gives (3.20) with the same $c_* = \sigma_\Delta/2$ for small enough κ_2.

Set $D_r := B_{2\eta_0/r}$. For $z \in D_r$, we have $f_i(z) = r^d\rho(x_i + rz)$, so (2.6) gives

$$f_i(z) = \Big[\frac{m-1}{m}\,\frac{r^{d(m-1)}}{\kappa}\big(\ell - \Phi(x_i + rz)\big)\Big]_+^{1/(m-1)} = \Big[\frac{m-1}{m}P_i(z)\Big]_+^{1/(m-1)}, \qquad (3.22)$$

where $P_i(z) := (\ell - \Phi(x_i + rz))/r^2$ and $r^{d(m-1)+2} = \kappa$ from (3.1). Since $D_z^2[\Phi(x_i + rz)] = r^2D^2\Phi(x_i + rz)$, (3.20) gives $D^2P_i \leq -c_*I_d$ on D_r. All level and superlevel sets below are taken inside D_r. The rescaled clusters satisfy $\operatorname{supp} f_i \subset \overline{B_L}$, $f_i \leq L$, and $\int f_i \geq u/2$. Since P_i is nonpositive on $\overline{D_r} \setminus B_L$, and positive somewhere in $\overline{B_L}$ because $\int f_i \geq u/2$, its maximum over $\overline{D_r}$ is positive and attained in $\overline{B_L}$. Hence $h_i := \max_{\overline{D_r}} P_i$ satisfies

$$\frac{u}{2} \leq \int f_i \leq |B_L|\Big(\frac{m-1}{m}h_i\Big)^{1/(m-1)},$$

so that $h_i \geq c_h$ for some $c_h > 0$, independent of κ.

If $1 < m \leq 2$, then $f_i^{2-m} \leq L^{2-m}$, and (3.21) is immediate. Let $m > 2$, and put $\theta := (m-2)/(m-1) \in (0,1)$, so that $f_i^{2-m} = ((m-1)/m)^{-\theta}P_i^{-\theta}$ on $\{f_i > 0\}$. Fix a maximum point z^* of P_i and $0 < t \leq c_h/2$. By concavity, the superlevel set $\{P_i \geq t\}$ is convex. It is contained in $\overline{B_L}$, because $f_i > 0$ there, and its boundary is the level set $\{P_i = t\}$. Concavity also gives $P_i(z^*) \leq P_i(z) + \nabla P_i(z)\cdot(z^* - z)$, hence

$$|\nabla P_i| \geq \frac{h_i - t}{2L} \geq \frac{c_h}{4L} \quad \text{on } \{P_i = t\}.$$

The perimeter of a convex set does not exceed that of a convex set containing it, so $\mathcal{H}^{d-1}(\{P_i = t\}) \leq \mathcal{H}^{d-1}(\partial B_L)$; for $d = 1$, $\mathcal{H}^0$ is the counting measure. The coarea formula $\int g\,dx = \int_{-\infty}^{\infty}(\int_{\{f=t\}} \frac{g}{|\nabla f|}\,d\mathcal{H}^{d-1})dt$ with $g = P_i^{-\theta}$ and $f = P_i$ yields

$$\begin{aligned}\int_{D_r\cap\{0<P_i<c_h/2\}} P_i^{-\theta}\,dz &= \int_0^{c_h/2} t^{-\theta}\int_{D_r\cap\{P_i=t\}} \frac{d\mathcal{H}^{d-1}}{|\nabla P_i|}\,dt \\ &\leq \frac{4L}{c_h}\,\mathcal{H}^{d-1}(\partial B_L)\int_0^{c_h/2} t^{-\theta}\,dt < \infty,\end{aligned}$$

while $\int_{D_r\cap\{P_i\geq c_h/2\}} P_i^{-\theta}\,dz \leq (c_h/2)^{-\theta}|B_L|$. This proves (3.21). □

The bound (3.21) says that the inverse of the diffusion weight $U''(f_i) = mf_i^{m-2}$ is integrable on the positivity set of each cluster, uniformly in κ. The proof of the following lemma needs this when $m > 2$, where U'' degenerates at the free boundary.

Lemma 3.13 (Uniqueness of normalized minimizers)**.** *There exists $\kappa_1 \in (0, \kappa_2]$ such that, for every $0 < \kappa < \kappa_1$, the set $\mathcal{N}_\kappa$ has exactly one element.*

Proof. Let $0 < \kappa < \kappa_2$, $r := r_\kappa$, and $\rho, \mu \in \mathcal{N}_\kappa$, with rescaled clusters $f_i(z) = r^d\rho_i(x_i + rz)$ and $g_i(z) = r^d\mu_i(x_i + rz)$, which are supported in $\overline{B_L}$. Set

$$\delta_i := f_i - g_i, \qquad b_i := \int \delta_i, \qquad p_i := \int z\,\delta_i(z)\,dz.$$

Write $b = (b_i)$ and $p = (p_i)$. On $\Omega_i := \{f_i + g_i > 0\}$ define the mean diffusion coefficient

$$q_i := \frac{U'(f_i) - U'(g_i)}{f_i - g_i} = \frac{m}{m-1}\,\frac{f_i^{m-1} - g_i^{m-1}}{f_i - g_i},$$

with $q_i := m f_i^{m-2}$ where $f_i = g_i$. Note that $q_i > 0$ on Ω_i. Define

$$D := \sum_i \int_{\Omega_i} q_i \delta_i^2 \, dz, \qquad H := \sum_i \|\delta_i\|_{L^1}.$$

D is finite since $\max(f_i, g_i) \le L$. Our goal is to show $D = 0$.

To begin, q_i is positively homogeneous of degree $m-2$ in (f_i, g_i): with $s := f_i + g_i$ and $\theta := f_i/s$, we have $q_i = s^{m-2}\varphi(\theta)$ for a positive continuous function φ on $[0,1]$. Hence $q_i \ge c_m (f_i + g_i)^{m-2}$ on Ω_i with $c_m = \min_{[0,1]} \varphi > 0$. This implies $\int_{\Omega_i} q_i^{-1} \le C$: If $1 < m \le 2$, then $(f_i+g_i)^{2-m} \le (2L)^{2-m}$. If $m > 2$, then $(f_i+g_i)^{2-m} \le \max(f_i, g_i)^{2-m} \le f_i^{2-m}\,\mathbf{1}_{\{f_i>0\}} + g_i^{2-m}\,\mathbf{1}_{\{g_i>0\}}$, and we use (3.21). Then the Cauchy–Schwarz inequality $\|\delta_i\|_{L^1}^2 \le \int_{\Omega_i} q_i \delta_i^2 \int_{\Omega_i} q_i^{-1}$ yields

$$H^2 \le C_1 D. \tag{3.23}$$

We now establish the inequality (3.25). Both ρ and μ are bounded, compactly supported, and absolutely continuous, so $U'(\rho)$, $U'(\mu)$, $W * \rho$, and $W * \mu$ are bounded on the common support and all integrals below are finite. (2.5) gives $\int (\kappa U'(\rho) + W * \rho)\, d(\mu - \rho) \ge 0$, and the same holds with ρ and μ exchanged. Adding the two inequalities gives

$$0 \ge \kappa \int \big(U'(\rho) - U'(\mu)\big)(\rho - \mu)\, dx + \iint W(x-y)\, d(\rho-\mu)(x)\, d(\rho-\mu)(y). \tag{3.24}$$

Both measures are supported in $\bigcup_i B_{Lr}(x_i)$. In each ball, the change of variables $x = x_i + rz$, $\rho = r^{-d} f_i$, $\mu = r^{-d} g_i$, $dx = r^d\, dz$, and $U'(s) = \frac{m}{m-1} s^{m-1}$ turn the first term into

$$\kappa r^{-d(m-1)} \sum_i \int_{\Omega_i} \frac{m}{m-1} \big(f_i^{m-1} - g_i^{m-1}\big)(f_i - g_i)\, dz = \kappa r^{-d(m-1)} D = r^2 D,$$

by (3.1). In the second term, for $x = x_i + rz$ and $y = x_j + rz'$ we have $x - y = e_{ij} + r(z - z')$, so by (3.16), $W(x-y) = w(1) + r^2 K_{ij}^r(z, z')$ for $i \ne j$ and $W(x-y) = r^2 K_{ii}^r(z, z')$ for $i = j$. The zeroth-order part of the cross interactions is therefore $w(1) \sum_{i \ne j} b_i b_j = w(1)\big((\sum_i b_i)^2 - |b|^2\big) = c_W |b|^2$, since $\sum_i b_i = 0$. Hence (3.24) becomes

$$0 \ge c_W |b|^2 + r^2 (D + I), \qquad I := \sum_i \iint K_{ii}^r \delta_i \delta_i + 2 \sum_{i<j} \iint K_{ij}^r \delta_i \delta_j, \tag{3.25}$$

where each kernel is evaluated at (z, z'), and the two density factors at z and z'.

Let I^0 denote I with every kernel replaced by its limit in (3.17). We have

$$\iint |z - z'|^2 \delta_i(z) \delta_i(z')\, dz\, dz' = 2 b_i \int |z|^2 \delta_i\, dz - 2|p_i|^2,$$

$$\iint \big(e \cdot (z - z')\big)^2 \delta_i(z) \delta_j(z')\, dz\, dz' = b_j \int (e \cdot z)^2 \delta_i\, dz + b_i \int (e \cdot z)^2 \delta_j\, dz - 2 (e \cdot p_i)(e \cdot p_j),$$

for any unit vector e. Inserting these identities into I^0 yields $I^0 = \mathcal{B}(p) + R$, where

$$R = -\mathbf{1}_{\{\beta=2\}} \sum_i b_i \int |z|^2 \delta_i \, dz + (\alpha - \beta) \sum_{i<j} \Big(b_j \int (e_{ij} \cdot z)^2 \delta_i \, dz + b_i \int (e_{ij} \cdot z)^2 \delta_j \, dz \Big).$$

Since $\{z : \delta_i(z) \neq 0\} \subset \overline{B_L}$, $|R| \le C|b|H$. Moreover we have $|I - I^0| \le \varepsilon(r) H^2$, where

$$\varepsilon(r) := \max_{i,j} \sup_{\overline{B_L} \times \overline{B_L}} |K_{ij}^r - K_{ij}^0| \longrightarrow 0 \quad \text{as } r \downarrow 0.$$

Now in rescaled variables, the alignment conditions of ρ read

$$\sum_i \int z \, f_i(z) \, dz = 0, \qquad \sum_i \Big(\int z \, f_i(z) \, dz \Big) \cdot S x_i = 0 \quad (S^T = -S),$$

and the same identities hold for g_i. Subtracting them shows that p satisfies (3.18), and hence $\mathcal{B}(p) \ge 0$ by Lemma 3.11. By (3.23), we get the lower estimate

$$\begin{aligned} D + I &\ge D - C|b|H - \varepsilon(r) H^2 \\ &\ge \big(1 - C_1 \varepsilon(r)\big) D - C|b| \sqrt{C_1 D} \ge \Big(\frac{1}{2} - C_1 \varepsilon(r) \Big) D - C_2 |b|^2. \end{aligned}$$

Inserting this into (3.25) gives

$$0 \ge \big(c_W - C_2 r^2 \big) |b|^2 + r^2 \Big(\frac{1}{2} - C_1 \varepsilon(r) \Big) D.$$

Choose $\kappa_1 \in (0, \kappa_2]$ such that $C_2 r_\kappa^2 \le c_W/2$ and $C_1 \varepsilon(r_\kappa) \le 1/4$ for $\kappa < \kappa_1$. Then both coefficients are positive, so $D = 0$. Since $q_i > 0$ on Ω_i, this forces $\delta_i = 0$ for every i, and hence $\rho = \mu$. Finally, Lemma 3.10 shows that $\mathcal{N}_\kappa$ is nonempty. □

3.5. **Proof of Theorem 1.1.** We first normalize arbitrary minimizers, then prove uniqueness, and finally use symmetry to identify the equal cluster masses.

Proof of Theorem 1.1. Let $\kappa_* := \kappa_1$ from Lemma 3.13, and let $0 < \kappa < \kappa_*$. By Lemma 3.1, $\mathcal{E}_\kappa$ has a global minimizer, and by Lemma 3.10 it is the image of an element of $\mathcal{N}_\kappa$ under a rigid motion. By Lemma 3.13, $\mathcal{N}_\kappa$ consists of exactly one measure, which we denote by ρ_κ. Hence every global minimizer is the image of ρ_κ under a rigid motion. Let G be a symmetry of Δ^d. By Lemma 3.10, $G_\# \rho_\kappa \in \mathcal{N}_\kappa$, hence $G_\# \rho_\kappa = \rho_\kappa$. For $i \neq j$, let G_{ij} be the reflection in the hyperplane orthogonal to $x_i - x_j$. By (2.1), $|x_i| = |x_j|$ and $x_k \cdot (x_i - x_j) = 0$ for $k \notin \{i, j\}$, so G_{ij} exchanges x_i and x_j and fixes the other vertices; thus it is a symmetry of Δ^d. The barycenter b of ρ_κ satisfies $G_{ij} b = b$, that is, $b \perp x_i - x_j$, for all $i \neq j$. These vectors span $\mathbb{R}^d$, so $b = 0$. Since $\kappa_* \le \kappa_3$ and $L r_\kappa < 1/2$ for $\kappa < \kappa_3$, we have $L r_{\kappa_*} \le 1/2$; as r_κ is increasing in κ, the balls $B_{L r_\kappa}(x_i)$ are pairwise disjoint for $0 < \kappa < \kappa_*$. By Definition 3.9, $\operatorname{supp} \rho_\kappa \subset \bigcup_i B_{L r_\kappa}(x_i)$. Since G_{ij} maps $B_{L r_\kappa}(x_i)$ onto $B_{L r_\kappa}(x_j)$ and preserves ρ_κ, the two balls carry the same mass. The masses of the $d+1$ disjoint balls sum to one, so each equals $1/(d+1)$. □

4. Proof of Theorem 1.2: Asymptotic shape of the clusters

Throughout this section, $0 < \kappa < \kappa_*$ and ρ_κ is the unique element of $\mathcal{N}_\kappa$ from the proof of Theorem 1.1. We write $r = r_\kappa$, $\rho_{\kappa,i}$ for its clusters, $f_{\kappa,i}(z) := r^d \rho_{\kappa,i}(x_i + rz)$ for its rescaled clusters, ℓ_κ for its multiplier, and $\Phi_\kappa := W * \rho_\kappa$. By Theorem 1.1, $|\rho_{\kappa,i}| = u$, and $G_\# \rho_\kappa = \rho_\kappa$ for every symmetry G of Δ^d.

Lemma 4.1 (The limiting cluster profile)**.** *For each i, $f_{\kappa,i} \to f_i$ in $L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ as $\kappa \to 0$, where f_i and A_i are given by* (1.4) *and* (1.5)*, and $\lambda_* > 0$ is the unique constant satisfying $\int f_i = u$ for every i. Moreover,* $\operatorname{supp} f_{\kappa,i} \to E_i$ *in Hausdorff distance.*

Proof. Splitting $\Phi_\kappa(x_i + rz)$ into the contributions of the equal-mass clusters and using (3.16) (the d clusters $j \neq i$ each contribute $uw(1)$ at zeroth order) gives

$$\Phi_\kappa(x_i + rz) = (1-u)w(1) + r^2 \Psi_{\kappa,i}(z), \qquad \Psi_{\kappa,i}(z) := \sum_j \int K^r_{ij}(z, z') f_{\kappa,j}(z')\, dz'.$$

Recall $\ell_\Delta = (1-u)w(1)$, and put $\lambda_\kappa := (\ell_\kappa - \ell_\Delta)/r^2$. By (3.4), $|\lambda_\kappa| \le C$. By (3.22),

$$f_{\kappa,i}(z) = \left[\frac{m-1}{m} \big(\lambda_\kappa - \Psi_{\kappa,i}(z) \big) \right]_+^{1/(m-1)}, \qquad |z| < \frac{2\eta_0}{r}. \tag{4.1}$$

$(f_{\kappa,i})_i$ are bounded by L and supported in $\overline{B_L}$, and the convergence of the kernels gives local uniform C^2 bounds for $\Psi_{\kappa,i}$, so $f_{\kappa,i}^{m-1}$ are uniformly Lipschitz on $\overline{B_{L+1}}$. Let $\kappa_n \downarrow 0$. After passing to a subsequence, $\lambda_{\kappa_n} \to \bar\lambda$, and $f_{\kappa_n,i}^{m-1}$ converges uniformly on $\overline{B_{L+1}}$ by Arzelà–Ascoli, so $f_{\kappa_n,i}$ also converges uniformly, and the common support bound gives convergence in $L^1(\mathbb{R}^d)$ and $L^\infty(\mathbb{R}^d)$. Write the limits as f_i. Then $\int f_i = u$, and

$$\Psi_{\kappa_n,i} \longrightarrow \Psi_i(z) := \sum_j \int K^0_{ij}(z, z') f_j(z')\, dz' \quad \text{in } C^2 \text{ on every bounded set.}$$

Passing to the limit in (4.1) yields

$$f_i(z) = \left[\frac{m-1}{m} \big(\bar\lambda - \Psi_i(z) \big) \right]_+^{1/(m-1)} \qquad \text{for all } z \in \mathbb{R}^d. \tag{4.2}$$

At this stage, the limits may depend on the chosen subsequence. We will show that $\bar\lambda - \Psi_i(z) = \lambda_* - z \cdot A_i z$, independently of this choice.

Let $a_i := u^{-1} \int z f_i(z)\, dz$. We will show $a_i = 0$. If G is a symmetry with $Gx_i = x_l$, then G maps $B_{1/2}(x_i)$ onto $B_{1/2}(x_l)$, and $G_\# \rho_\kappa = \rho_\kappa$ gives $f_{\kappa,l}(Gz) = f_{\kappa,i}(z)$; hence $a_l = G a_i$. For $j, k \neq i$, the reflection in the hyperplane orthogonal to $x_j - x_k$ fixes x_i, so it fixes a_i, hence $a_i \cdot (x_j - x_k) = 0$. Since the vectors $x_j - x_k$ with $j, k \neq i$ span $x_i^\perp$, $a_i = t_i x_i$ for some $t_i \in \mathbb{R}$, and $a_l = G a_i$ shows that $t_i = t$ does not depend on i.

Translate just the i-th cluster of ρ_κ by a small vector v, leaving the other clusters fixed, and let ρ^v denote the resulting measure. Their supports remain disjoint. Since the internal energy and the self-interaction of the translated cluster are unchanged,

$$\mathcal{E}_\kappa(\rho^v) - \mathcal{E}_\kappa(\rho_\kappa) = \sum_{j \neq i} \iint \big(W(x + v - y) - W(x - y) \big)\, d\rho_{\kappa,i}(x)\, d\rho_{\kappa,j}(y).$$

Minimality at $v = 0$ in all directions gives, by differentiation in v, the vector identity

$$\sum_{j\neq i} \iint \nabla W(x-y)\, d\rho_{\kappa,i}(x)\, d\rho_{\kappa,j}(y) = 0. \tag{4.3}$$

Since $\nabla W(e_{ij}) = 0$ and $D^2W(e_{ij}) = (\alpha-\beta)e_{ij}\otimes e_{ij}$, Taylor's formula gives

$$\frac{\nabla W(e_{ij} + r(z-z'))}{r} \longrightarrow (\alpha-\beta)(e_{ij}\otimes e_{ij})(z-z')$$

uniformly for $z, z' \in \overline{B_L}$. We rescale (4.3), divide by r, and pass to the limit along the subsequence. Using the L^1 convergence of the rescaled clusters, the limit is

$$0 = (\alpha-\beta)\sum_{j\neq i}(e_{ij}\otimes e_{ij}) \iint (z-z')f_i(z)f_j(z')\, dz\, dz' = (\alpha-\beta)u^2 \sum_{j\neq i}(e_{ij}\otimes e_{ij})(a_i - a_j).$$

Hence $\sum_{j\neq i}(e_{ij}\otimes e_{ij})(a_i-a_j) = 0$. With $a_i = tx_i$, $(e_{ij}\otimes e_{ij})(a_i-a_j) = t\, e_{ij}|e_{ij}|^2 = t\, e_{ij}$, hence $t\sum_{j\neq i} e_{ij} = t(d+1)x_i = 0$. Hence $t = 0$, and all limiting cluster means a_i vanish.

Since each limiting cluster has mass u and zero first moment, direct computation gives $\nabla\Psi_i(0) = 0$ and $\nabla^2\Psi_i(z) = u\big((\alpha-\beta)\sum_{j\neq i}(e_{ij}\otimes e_{ij}) - \mathbf{1}_{\{\beta=2\}}I_d\big)$. Lemma 3.4 with (3.5) gives $\nabla^2\Psi_i(z) = \nabla^2 V_\Delta(x_i) = 2A_i$. As Ψ_i is quadratic, $\Psi_i(z) = \Psi_i(0) + z\cdot A_i z$. Hence (4.2) is (1.4) with λ_* replaced by $\lambda_i := \bar\lambda - \Psi_i(0)$. Since A_i is positive definite, the positive mass forces $\lambda_i > 0$. The change of variables $z = \sqrt{\lambda_i}\, A_i^{-1/2} y$ gives

$$\int f_i = \Big(\frac{m-1}{m}\Big)^{\frac{1}{m-1}} \omega_{d,m} (\det A_i)^{-1/2} \lambda_i^{\frac{d(m-1)+2}{2(m-1)}}, \quad \omega_{d,m} := \int_{B_1} (1-|y|^2)^{\frac{1}{m-1}}\, dy, \tag{4.4}$$

which increases strictly from zero to infinity with λ_i. By (1.5), $\det A_i = (u/2)^d a_\parallel a_\perp^{d-1}$ does not depend on i (for $d = 1$ the factor $a_\perp$ is absent). Hence the mass condition $\int f_i = u$ determines a common value $\lambda_i = \lambda_*$, and this determines f_i by (1.4). Since the limit does not depend on the subsequence, the whole family converges as $\kappa \to 0$.

By the same argument, $\lambda_\kappa - \Psi_{\kappa,i} \to \lambda_* - z\cdot A_i z$ uniformly on $\overline{B_{L+1}}$, and $\operatorname{supp} f_{\kappa,i}$ is the closure of the set $\{z \in \overline{B_L} : \lambda_\kappa - \Psi_{\kappa,i}(z) > 0\}$. Let $E_i^+ = \{z \in \overline{B_{L+1}} : \operatorname{dist}(z, E_i) \le \varepsilon\}$ and $E_i^- = \{z \in E_i : \operatorname{dist}(z, E_i^c) \ge \varepsilon\}$ given $\varepsilon > 0$. The limit $\lambda_* - z\cdot A_i z$ is negative and bounded away from zero on $\overline{B_{L+1}} \setminus E_i^+$, while positive and bounded away from zero on E_i^-. Hence the uniform convergence gives Hausdorff convergence of $\operatorname{supp} f_{\kappa,i}$ to E_i. □

Remark 4.2 (Explicit constants). Since $\omega_{d,m} = \pi^{d/2}\Gamma\big(\frac{m}{m-1}\big)/\Gamma\big(\frac{m}{m-1} + \frac{d}{2}\big)$, (4.4) gives

$$\lambda_* = \left[\frac{u\,(u/2)^{d/2}\, a_\parallel^{1/2}\, a_\perp^{(d-1)/2}}{\big(\frac{m-1}{m}\big)^{1/(m-1)}\, \omega_{d,m}}\right]^{\frac{2(m-1)}{d(m-1)+2}}, \tag{4.5}$$

where the factor $a_\perp$ is absent for $d = 1$. For the Wasserstein asymptotics below, we also record that (1.5) gives

$$\operatorname{tr}(A_i^{-1}) = \frac{2}{u}\left(\frac{1}{a_\parallel} + \frac{d-1}{a_\perp}\right) \qquad (d \ge 2),$$

while $\operatorname{tr}(A_i^{-1}) = 2/(ua_\parallel)$ when $d = 1$.

Proof of Theorem 1.2. Fix $0 < \kappa < \kappa_*$ and write $r := r_\kappa$. Since $\rho_\kappa \in \mathcal{N}_\kappa$, (3.15) gives $\|\rho_{\kappa,i}\|_{L^\infty} \le Lr^{-d}$ for every i. Let $O_{\kappa,i} := \{\rho_{\kappa,i} > 0\}$. Since $\kappa_* \le \kappa_2$, Lemma 3.12 gives $D^2\Phi_\kappa \ge c_* I_d$ on $B_{2\eta_0}(x_i)$, and the choice of κ_2 ensures $Lr \le \eta_0$. Thus $\operatorname{supp}\rho_{\kappa,i} \subset B_{Lr}(x_i) \subset B_{\eta_0}(x_i)$. By (2.6) and the separation of the clusters,

$$O_{\kappa,i} = \{x \in B_{2\eta_0}(x_i) : \Phi_\kappa(x) < \ell_\kappa\}.$$

Hence $O_{\kappa,i}$ is a nonempty convex open set contained in $B_{\eta_0}(x_i)$, and since Φ_κ is convex, $\partial O_{\kappa,i} = \{x \in B_{2\eta_0}(x_i) : \Phi_\kappa(x) = \ell_\kappa\}$. Moreover $\nabla\Phi_\kappa \neq 0$ on $\partial O_{\kappa,i}$: by strict convexity, a critical point would minimize Φ_κ on $B_{2\eta_0}(x_i)$, contradicting $\Phi_\kappa < \ell_\kappa$ on $O_{\kappa,i}$. Since $\Phi_\kappa \in C^2$, the implicit function theorem shows that $\partial O_{\kappa,i}$ is C^2, and on $O_{\kappa,i}$, $\rho_\kappa^{m-1} = \frac{m-1}{m\kappa}(\ell_\kappa - \Phi_\kappa)$, which is concave. Now Lemma 4.1 gives the convergence of the rescaled densities in $L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ and the Hausdorff convergence of their supports. The common normalization constant λ_* is given by (4.5).

It remains to prove the Wasserstein asymptotics. Since $Lr < 1/2$ and the vertices have mutual distance one, every point in the i-th cluster is closer to x_i than to any other vertex. By Theorem 1.1, each cluster has mass u, so the transport plan sending the entire i-th cluster to x_i is optimal for d_2 and has second marginal ρ_Δ. Hence

$$d_2(\rho_\kappa, \rho_\Delta)^2 = \sum_{i=0}^{d} \int |x - x_i|^2 \, d\rho_{\kappa,i}(x) = r^2 \sum_{i=0}^{d} \int |z|^2 f_{\kappa,i}(z)\, dz.$$

The L^1 convergence in Lemma 4.1 and the common support bound $\operatorname{supp} f_{\kappa,i} \subset \overline{B_L}$ give

$$\lim_{\kappa\to 0} \frac{d_2(\rho_\kappa, \rho_\Delta)^2}{r_\kappa^2} = \sum_{i=0}^{d} \int |z|^2 f_i(z)\, dz.$$

Put $s = \frac{1}{m-1}$. The change of variables $z = \sqrt{\lambda_*}\, A_i^{-1/2} y$, together with $u = \int f_i$, yields

$$\frac{\int |z|^2 f_i(z)\, dz}{u} = \lambda_* \frac{\displaystyle\int_{B_1} y \cdot A_i^{-1} y \,(1 - |y|^2)^s \, dy}{\displaystyle\int_{B_1} (1 - |y|^2)^s \, dy}.$$

By radial symmetry of the weight,

$$\int_{B_1} y \cdot A_i^{-1} y \,(1 - |y|^2)^s \, dy = \frac{\operatorname{tr}(A_i^{-1})}{d} \int_{B_1} |y|^2 (1 - |y|^2)^s \, dy.$$

The Beta-function identity $\dfrac{\int_{B_1} |y|^2 (1 - |y|^2)^s \, dy}{\int_{B_1} (1 - |y|^2)^s \, dy} = \dfrac{d}{d + 2s + 2}$ thus gives

$$\int |z|^2 f_i(z)\, dz = \frac{u\lambda_* \operatorname{tr}(A_i^{-1})}{d + 2 + 2/(m-1)}.$$

Summing over i, using $(d+1)u = 1$, and substituting $\operatorname{tr}(A_i^{-1}) = \frac{2}{u}\left(\frac{1}{a_\parallel} + \frac{d-1}{a_\perp}\right)$, with the second term omitted when $d = 1$, proves the asserted limit. $\square$

5. Concluding remarks

Small porous-medium diffusion replaces the atomic simplex ground state by diffuse clusters while preserving its uniqueness up to rigid motions; because uniqueness is proved before symmetry is invoked, the exact equality of the cluster masses is a consequence rather than an assumption. The boundary of the strict simplex regime behaves differently. For $d \geq 2$ we have $\alpha_\Delta(2) = 4$ [17], so $(\alpha, \beta) = (4, 2) \notin \mathcal{S}$. At this pair ρ_Δ is still a minimizer of $\mathcal{W}$ [17], but small diffusion selects a different geometry.

Proposition 5.1 (Selection at the degenerate pair $(4, 2)$)**.** *Let $d \geq 2$, $m > 1$, $(\alpha, \beta) = (4, 2)$, and $R = \sqrt{d/(2d+2)}$. For every $\kappa > 0$, $\mathcal{E}_\kappa$ has exactly one global minimizer ρ_κ in $\mathcal{P}_0(\mathbb{R}^d)$; it is radially symmetric, and every global minimizer of $\mathcal{E}_\kappa$ is a translate of ρ_κ. As $\kappa \downarrow 0$, ρ_κ converges narrowly to the normalized surface measure σ_R on ∂B_R.*

Proof. Write $\mathcal{W}_{4,2}$ for the interaction energy at this pair. Measures of finite energy have finite fourth moments by (2.3). For such $\rho \in \mathcal{P}_0(\mathbb{R}^d)$, put $C_\rho := \int x \otimes x \, d\rho(x)$ and $s_\rho := \operatorname{tr} C_\rho$. Expanding $|x-y|^4 = (|x|^2 + |y|^2 - 2x \cdot y)^2$ and using $\int x \, d\rho(x) = 0$, we get

$$\mathcal{W}_{4,2}(\rho) = \frac{1}{4} \int |x|^4 \, d\rho(x) + \frac{1}{4} s_\rho^2 + \frac{1}{2} |C_\rho|^2 - \frac{1}{2} s_\rho.$$

Along linear interpolations in $\mathcal{P}_0(\mathbb{R}^d)$, the quantities $\int |x|^4 \, d\rho$, s_ρ, and C_ρ are affine, so the right-hand side is convex; this convexity argument goes back to Lopes [27] and was used in [17, Lemma 2.2]. Since U is strictly convex, $\mathcal{E}_\kappa$ is strictly convex along linear interpolations of centered densities of finite energy.

The proof of Lemma 3.1 applies at this pair, so $\mathcal{E}_\kappa$ has a global minimizer, which we may translate into $\mathcal{P}_0(\mathbb{R}^d)$. Strict convexity gives uniqueness in $\mathcal{P}_0(\mathbb{R}^d)$; hence every global minimizer, translated by its barycenter, equals ρ_κ. For $Q \in O(d)$, $Q_\# \rho_\kappa$ is again a global minimizer in $\mathcal{P}_0(\mathbb{R}^d)$, so $Q_\# \rho_\kappa = \rho_\kappa$. The same proof gives a fixed ball containing $\operatorname{supp} \rho_\kappa$ for $0 < \kappa \leq 1$. Hence every sequence $\kappa_n \downarrow 0$ has a subsequence along which ρ_{κ_n} converges narrowly to an orthogonally invariant $\rho_0 \in \mathcal{P}_0(\mathbb{R}^d)$, with $\mathcal{W}_{4,2}(\rho_{\kappa_n}) \to \mathcal{W}_{4,2}(\rho_0)$ because W is continuous and the supports are uniformly bounded. For every smooth compactly supported probability density ν,

$$\mathcal{W}_{4,2}(\rho_{\kappa_n}) \leq \mathcal{E}_{\kappa_n}(\rho_{\kappa_n}) \leq \mathcal{E}_{\kappa_n}(\nu) \longrightarrow \mathcal{W}_{4,2}(\nu).$$

Taking for ν mollifications of σ_R gives $\mathcal{W}_{4,2}(\rho_0) \leq \mathcal{W}_{4,2}(\sigma_R) = \min \mathcal{W}_{4,2}$, where the equality holds by [17, Theorem 1.1]. Thus ρ_0 is a centered minimizer of $\mathcal{W}_{4,2}$, and by the same theorem it is supported on ∂B_R. Being orthogonally invariant, it equals σ_R. Since the limit does not depend on the subsequence, the whole family converges. □

Proposition 5.1 shows that our estimates cannot be uniform as $\alpha \downarrow 4$ when $\beta = 2$: the tangential eigenvalue $ua_\perp = u(\alpha - 4)/2$ of the simplex wells degenerates, and the selected geometry changes from separated clusters to a uniform shell. The estimates are likewise not uniform as $\alpha \to \infty$ or $m \to \infty$; these limits lead to the isodiametric problem of [25] and the density-constrained problem of [15].

For other radial kernels $W(x) = w(|x|)$ whose zero-diffusion minimizer is the equally weighted simplex, the localization and normalization steps carry over once the vertices are isolated, non-degenerate minima of the simplex potential. The uniqueness step

uses in addition that $w'(1) = 0$, $w''(1) > 0$, and $D^2W(0) \leq 0$; the limiting interaction then has the form of Lemma 3.11, with the same positivity on aligned first moments.

Several questions remain open: whether uniqueness up to rigid motions persists for all $\kappa > 0$; how the clusters merge into the shell in the joint limit $\kappa \downarrow 0$, $\alpha \downarrow 4$ with $\beta = 2$; whether, for linear diffusion, the clusters rescaled at the scale $\kappa^{1/2}$ converge to Gaussian profiles proportional to $e^{-z \cdot A_i z}$, the $m \downarrow 1$ limits of (1.4); and whether, for $\alpha > \beta > 2$, the unequal-mass simplex configurations that are local minimizers of $\mathcal{W}$ [25] give rise to steady states or local minimizers of $\mathcal{E}_\kappa$ with unequal cluster masses.

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