GROUND STATES AND PHASE TRANSITIONS FOR AN AGGREGATION MODEL WITH FAST DIFFUSION ON SPHERE

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Abstract. We consider a free energy on the sphere that contains an entropy associated to nonlinear fast diffusion, and a nonlocal interaction energy. The two components of the free energy compete with each other, as one favours spreading and the other promotes concentration, respectively. The model is a generalization of the Onsager free energy with dipolar potential, used to study polymer orientation. We study the global energy minimizers of the energy functional, and in particular the various phase transitions that occur with respect to the strength of the nonlocal attractive interactions. In the considered regime, diffusion reduces as the density increases, for which reason the global energy minimizers can contain Dirac mass concentrations. We identify various ranges of the fast diffusion exponent and of the interaction strength, which give qualitatively different equilibria and ground states. The theoretical results are supported by numerical illustrations.

1. Introduction

In this paper we investigate the minimizers of the free energy functional

$$E[\mu] = \frac{1}{m-1}\int_{\mathbb{S}^d} \rho(x)^m \mathrm{d}S(x) + \frac{\kappa}{4}\iint\limits_{\mathbb{S}^d\times\mathbb{S}^d} \|x-y\|^2 \mathrm{d}\mu(x)\mathrm{d}\mu(y) \tag{1.1}$$

defined on the space $\mathcal{P}(\mathbb{S}^d)$ of probability measures on the unit sphere $\mathbb{S}^d$, where the integration is with respect to the standard Lebesgue measure $\mathrm{d}S$ of the sphere, and $\rho\,\mathrm{d}S$ represents the absolutely continuous part of the measure μ (the notion of absolute continuity is with respect to the measure $\mathrm{d}S$). Also, $0 < m < 1$ is the diffusion exponent, $\kappa > 0$ represents the interaction strength, and $\|\cdot\|$ denotes the Euclidean norm in $\mathbb{R}^{d+1}$.

The energy functional (1.1) consists of two terms: the first is the entropy and the second is a nonlocal interaction energy, with an interaction potential $W : \mathbb{S}^d \times \mathbb{S}^d \to \mathbb{R}$ given by $W(x, y) = \frac{1}{2}\|x-y\|^2$. The two terms in (1.1) have competing effects, as the first favours spreading, while the second promotes aggregation. In its most general form, the energy (1.1) can be set up on arbitrary Riemannian manifolds M, with general interaction potentials $W : M \times M \to \mathbb{R}$. There is an extensive literature on this class of aggregation-diffusion energies and associated equations, due to their wide range of applications in sciences and engineering; it is beyond our scope to give a comprehensive review of this literature, we simply refer here to [2, 13, 32] for some recent reviews on the topic. For example, nonlinear diffusion was considered in the Keller-Segel model for chemotaxis [12], in swarming models [10, 11, 44], granular media [21], machine learning [42], and opinion formation [24].

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Particularly relevant to the current work, the free energy (1.1) for the special case $m = 1$ (in this case the entropic term is given by $\int_{\mathbb{S}^d} \rho(x)\log\rho(x)\mathrm{d}S(x)$), known as the Onsager free energy [41], has been used to study isotropic-nematic phase transitions in rod-like polymers [22, 25]. In this application, ρ represents the probability distribution function for the orientation of a polymer interpreted as a rigid rod of unit vector $x \in \mathbb{S}^2$. The quadratic interaction potential in (1.1) (in fact, its equivalent expression $-\kappa\langle x, y\rangle$) is called the dipolar potential. As shown in [25, 29, 23], there exists a critical value of the interaction strength κ at which the isotropic state (provided by the uniform distribution) loses stability to a nematic equilibrium density. Similar phase transitions are investigated in the present paper, but with nonlinear diffusion replacing the linear diffusion. The current work complements the recent research on phase transitions with nonlinear diffusion in the porous media regime ($m > 1$) done in [28].

The range $0 < m < 1$ of the diffusion exponent corresponds to the fast diffusion regime; this is in contrast with the range $m > 1$ for the slow diffusion (porous media) regime. The terminology comes from the evolution equation (gradient flow) associated to the entropic term in (1.1). Indeed, in a suitable Wasserstein space, the gradient flow of the entropy component (the interaction term in (1.1) is ignored here) leads to the nonlinear diffusion equation $\rho_t = \Delta\rho^m$ [1]. The nonlinear diffusion $\Delta\rho^m$ can be written as $\nabla\cdot(m\rho^{m-1}\nabla\rho)$, and the coefficient $m\rho^{m-1}$ in front of $\nabla\rho$ is the (density-dependent) diffusion coefficient. As $0 < m < 1$, the diffusion coefficient becomes larger as ρ gets smaller. Conversely, as ρ increases, the diffusion coefficient becomes smaller, which suppresses the diffusion rate. Hence, regions of low density correspond to faster diffusion, while in regions of high density the diffusion is slower. As an extreme example, if ρ contains a singular part at some point (i.e., $\rho = \infty$ at that point), then $\rho^{m-1} = 0$, and the diffusion vanishes there. For example, fast diffusion behaviour can be observed in dilute plasmas or rarefied gases, where particles in low-density regions move more freely and spread rapidly [4, 38].

This behaviour of the diffusion coefficient in fast diffusion is opposite to that in the slow diffusion (porous media) regime, where $m > 1$. The two types of diffusion (fast and slow) are very different, and the fast diffusion is by far the one that is less studied and understood. In the Euclidean setting, aggregation–diffusion dynamics in the fast diffusion regime was studied in [16, 17], where the so-called partial mass concentration phenomenon was introduced. This phenomenon occurs as the aggregation interactions lead to high densities, while diffusion is too weak in order to prevent the blow-up. Mass concentration occurs only in the fast diffusion regime, and does not appear for slow or linear diffusion.

An alternative viewpoint on fast versus slow diffusion comes from the variational perspective. Indeed, write the entropy term in the energy as $\frac{1}{m-1}\int \rho(x)^{m-1}\mathrm{d}\rho(x)$, where the integration is with respect to the measure $\mathrm{d}\rho = \rho\,\mathrm{d}S$. In the slow diffusion regime ($m > 1$), as ρ concentrates, ρ^{m-1} diverges to infinity, which makes the entropy itself infinite. Hence, energy minimizers in this regime cannot have mass concentrations. However, for fast diffusion ($0 < m < 1$), ρ^{m-1} tends to zero as ρ increases, and the entropy remains finite even when ρ develops a singular part. Due to this fundamental difference between the two regimes, in the present research we allow singular measures as admissible energy minimizers, whereas in previous work on the slow diffusion case only absolutely continuous measures were considered [28].

Steady states and energy minimization for aggregation models with fast diffusion in Euclidean space have been studied recently in several papers. In [15], energy minimizers are analyzed using a reverse HLS (Hardy–Littlewood–Sobolev) inequality that relates the fast-diffusion entropy and the interaction energy. In [20], the existence of a global minimizer is proved by a variational method, and radial symmetry is obtained via a rearrangement inequality. The partial mass concentration in the steady states of aggregation equations with fast diffusion is explored in [16] and [17]. The minimization problem for aggregation-diffusion energies has also been studied on Cartan–Hadamard manifolds [18, 19, 26, 27] - for example, the fast diffusion range is considered in [19]. On Cartan–Hadamard manifolds, the faster volume growth of geodesic balls effectively strengthens the diffusion, so the conditions ensuring the existence of an energy minimizer differ from the flat case. Specifically, such conditions depend on the behaviour of the manifold's curvature at infinity. We also note that the fast diffusion equation (with no aggregation terms) has been extensively studied in the literature, with particular interest on the well-posedness and long time behaviour of its solutions [5, 6, 7, 35, 45, 46], including works on manifolds [8, 34, 39].

In our study we consider the free energy set up on the unit sphere, with fast diffusion entropy and interactions modelled by a quadratic potential. As noted above, one of the main motivations for the present work is to extend the Onsager free energy [41] to nonlinear diffusion in the fast regime, and investigate the phase transitions (in terms of the interaction strength κ) of its ground states. In our analysis we have identified three different subranges of $0 < m < 1$ (specifically, i) $1 - \frac{2}{d} < m < 1$, ii) $1 - \frac{2}{d-1} < m < 1 - \frac{2}{d}$, and iii) $0 < m < 1 - \frac{2}{d-1}$), where the global minimizers are qualitatively different, and the phase transitions are different too. For example, although the entropy remains finite for all $0 < m < 1$, even when ρ has a singular part, the global energy minimizer of (1.1) contains a singular part only for $0 < m < 1 - \frac{2}{d}$ (ranges ii) and iii) – see Theorem 4.1), and any such singular part must be a single Dirac delta concentration. This result is consistent with the fast diffusion theory on the Euclidean space. For the fast diffusion equation on the Euclidean space, it is known that the Dirac delta mass is stable for $0 < m < 1 - \frac{2}{d}$ and unstable for $1 - \frac{2}{d} < m < 1$; see [9] and Remarks 2.1 and 2.2. Since concentration is a local phenomenon, this consistency of the ranges of m with the Euclidean case is natural.

To contrast the three types of diffusion (fast, linear and slow), in Table 1 we show all types of ground states that can occur, as the interaction strength κ increases. For all the three types of diffusion, the uniform distribution is the global energy minimizer as κ starts increasing from 0. But then, depending on the range of the diffusion exponent m, one can experience various transitions of the ground states. In particular, we note transitions to (fully-supported) measure-valued ground states in cases ii) and iii) of fast diffusion, while for slow diffusion we see transitions to minimizers that are strictly supported on the sphere. In all cases, as κ increases to infinity, the grounds states concentrate around a point on the sphere, but their shape and structure can be very different, depending on the type of diffusion and the specific value of m.

We also mention that there has been an increased interest recently on aggregation-diffusion models on sphere and other manifolds, due to applications of these models to machine learning [36, 40]. We note in particular the application to large language models,

Diffusion	Range of m	Ground-state transition as κ increases
Fast (case iii)	$0 < m < 1 - \frac{2}{d-1}$	$\rho_{\text{uni}} \to$ f.s. density + a Dirac delta
Fast (case ii)	$1 - \frac{2}{d-1} < m < 1 - \frac{2}{d}$	$\rho_{\text{uni}} \to$ f.s. density $\to$ f.s. density + a Dirac delta
Fast (case i)	$1 - \frac{2}{d} < m < 1$	$\rho_{\text{uni}} \to$ f.s. density
Linear [25, 29]	$m = 1$	$\rho_{\text{uni}} \to$ f.s. density
Slow [28]	$1 < m < 2$	$\rho_{\text{uni}} \to$ f.s. density $\to$ s.s. density
Slow [28]	$m > 2$ (for $d = 2$)	$\rho_{\text{uni}} \to$ s.s. density

Table 1. The various transitions in the ground states that can occur by increasing the interaction strength κ, for three types of diffusion: fast ($0 < m < 1$), linear ($m = 1$) and slow ($m > 1$). We used the abbreviations: *f.s.* for *fully supported*, and *s.s.* for *strictly supported*. A major distinction between the fast and the slow diffusion regimes is that in some ranges of the fast diffusion exponent we see transitions of the ground state to a measure-valued (but fully supported) minimizer, while for slow diffusion we have transitions to ground states that are strictly supported on the sphere.

specifically to transformers [31]. Various recent works have been motivated by such application, where a common theme is phase transitions from the uniform distribution, similar to the focus of this paper [3, 30, 42, 43].

The rest of the paper is organized as follows. In Section 2 we establish the variational framework by setting up the admissible class of minimizers, and derive the possible critical points from the Euler-Lagrange equations. In Section 3 we find the critical values of κ at which equilibria undergo phase transitions, and we characterize these equilibria for various ranges of κ and m (Proposition 3.1). Finally, in Section 4 we compare the energies associated with the found critical points, and determine which ones yield the global minimizer (Theorem 4.1).

2. Admissible class and critical points of the energy

In this section we present the admissible set of energy minimizers and derive various expressions for the equilibrium points. For any two points on the unit sphere $x, y \in \mathbb{S}^d$, $\|x - y\|^2$ can be expressed as

$$\|x - y\|^2 = \|x\|^2 + \|y\|^2 - 2\langle x, y\rangle = 2 - 2\langle x, y\rangle,$$

which can be used to rewrite the energy (1.1) as

$$E[\mu] = \frac{1}{m-1}\int_{\mathbb{S}^d} \rho(x)^m \mathrm{d}S(x) - \frac{\kappa}{2}\iint\limits_{\mathbb{S}^d\times\mathbb{S}^d} \langle x, y\rangle \,\mathrm{d}\mu(x)\mathrm{d}\mu(y) + \frac{\kappa}{2}. \tag{2.2}$$

Here, $\langle\cdot,\cdot\rangle$ denotes the inner product in $\mathbb{R}^{d+1}$.

The centre of mass $c_\mu \in \mathbb{R}^{d+1}$ of a measure $\mu \in \mathcal{P}(\mathbb{S}^d)$ is defined as

$$c_\mu = \int_{\mathbb{S}^d} x \,\mathrm{d}\mu(x).$$

It holds that

$$\begin{aligned} \|c_\mu\|^2 &= \left\langle \int_{\mathbb{S}^d} x\,\mathrm{d}\mu(x), \int_{\mathbb{S}^d} y\,\mathrm{d}\mu(y)\right\rangle \\ &= \iint\limits_{\mathbb{S}^d\times\mathbb{S}^d} \langle x, y\rangle \,\mathrm{d}\mu(x)\mathrm{d}\mu(y), \end{aligned}$$

and hence, the energy functional can be written as

$$E[\mu] = \frac{1}{m-1}\int_{\mathbb{S}^d} \rho(x)^m \mathrm{d}S(x) - \frac{\kappa}{2}\|c_\mu\|^2 + \frac{\kappa}{2}. \tag{2.3}$$

2.1. **Admissible class.** We first need to set up the set of admissible energy minimizers. Note that there are infinitely many critical points of the energy functional. For instance, any symmetric distribution of Dirac delta measures (e.g., a regular n-gon on the great circle or a regular d-simplex on $\mathbb{S}^d$) are equilibrium states of the energy. The following lemma excludes a large class of such equilibria from being candidates for energy minimizers.

Lemma 2.1. *Let $\mu \in \mathcal{P}(\mathbb{S}^d)$ be a critical point of the energy $E[\mu]$. If the singular part of μ with respect to $\mathrm{d}S$ is not concentrated at one point, then μ cannot be a global energy minimizer.*

Proof. A generic probability measure μ on $\mathbb{S}^d$ can be written as

$$\mu = \alpha\mu_s + (1-\alpha)\rho\,\mathrm{d}S, \tag{2.4}$$

where $0 \leqslant \alpha \leqslant 1$, and $\alpha\mu_s$ and $(1-\alpha)\rho\,\mathrm{d}S$ are the singular and the absolutely continuous parts of μ, respectively. Here, we assumed that both μ_s and $\rho\,\mathrm{d}S$ are in $\mathcal{P}(\mathbb{S}^d)$. Note that the regular part of μ here is $(1-\alpha)\rho\mathrm{d}S$, and the extra factor of $1-\alpha$ has to be considered when computing $E[\mu]$ (cf., (1.1) or (2.3)). We will show that provided the singular component of μ is not concentrated at one point, then a change of μ_s can decrease the energy $E[\mu]$. See Appendix A for the rest of the proof. □

By Lemma 2.1, we can assume that the singular part of a ground state μ is a single Dirac delta mass $\alpha\delta_{x_0}$ concentrated at a fixed point $x_0 \in \mathbb{S}^d$. In the next lemma we show that a delta concentration with no regular part ($\alpha = 1$) cannot be a global minimizer either.

Lemma 2.2. *The Dirac delta concentration δ_{x_0} is not a global energy minimizer.*

Proof. As δ_{x_0} has no regular part and its centre of mass is at x_0 with $\|x_0\| = 1$, by (2.3) we have $E[\delta_{x_0}] = 0$. Consider the following perturbation of δ_{x_0}:

$$\mu^t = (1-t)\delta_{x_0} + \frac{t}{|\mathbb{S}^d|}\mathrm{d}S,$$

where $0 \leqslant t < 1$. One can easily check that $\int_{\mathbb{S}^d} \mathrm{d}\mu^t = 1$, and that $c_{\mu^t} = (1-t)x_0$. Then, by (2.3) the corresponding energy can be expressed as

$$\begin{aligned} E[\mu^t] &= \frac{t^m}{(m-1)|\mathbb{S}^d|^{m-1}} - \frac{\kappa}{2}(1-t)^2 + \frac{\kappa}{2} \\ &= -\left(\frac{1}{(1-m)|\mathbb{S}^d|^{m-1}}\right)t^m + \kappa\left(t - \frac{t^2}{2}\right). \end{aligned}$$

As $0 < m < 1$, we have $E[\mu^t] < E[\mu^0] = E[\delta_{x_0}]$ for small $t > 0$. In fact, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}E[\mu^t]\bigg|_{t=0+} = -\infty.$$

We infer that δ_{x_0} is not a global energy minimizer. □

Next, we will investigate the absolutely continuous part of μ. We denote by $\mathcal{P}_{ac}(\mathbb{S}^d) \subset \mathcal{P}(\mathbb{S}^d)$ the space of probability measures that are absolutely continuous with respect to $\mathrm{d}S$. By an abuse of notation we will often refer to an absolutely continuous measure $\rho\mathrm{d}S$ directly by its density ρ.

Lemma 2.3 (Radial symmetry of global minimizers)**.** *Let $\mu = \alpha\delta_{x_0} + (1-\alpha)\rho\mathrm{d}S$ be a global energy minimizer, where $0 \leqslant \alpha < 1$ and $\rho \in \mathcal{P}_{ac}(\mathbb{S}^d)$. Then,*
a) The density ρ is radially symmetric with respect to some $z \in \mathbb{S}^d$, i.e., for any two points $y_1, y_2 \in \mathbb{S}^d$ satisfying $\langle z, y_1\rangle = \langle z, y_2\rangle$, we have $\rho(y_1) = \rho(y_2)$.
b) Furthermore, if $0 < \alpha < 1$, then $z = x_0$. That is, ρ is symmetric with respect to x_0, and $c_\rho = \|c_\rho\|x_0$.

Proof. *a*) Take a rotation $R : \mathbb{S}^d \to \mathbb{S}^d$ that preserves the centre of mass c_ρ of ρ. Note that the centre of $\rho' := R_{\#}\rho$ is also c_ρ (i.e., $c_{\rho'} = c_\rho$). Define

$$\mu' = \alpha\delta_{x_0} + (1-\alpha)\rho'\mathrm{d}S.$$

Then,

$$c_{\mu'} = \alpha x_0 + (1-\alpha)c_{\rho'} = \alpha x_0 + (1-\alpha)c_\rho = c_\mu,$$

and by (2.3), this yields

$$\begin{aligned} E[\mu'] &= \frac{1}{m-1}\int_{\mathbb{S}^d} \rho'(x)^m \mathrm{d}S(x) - \frac{\kappa}{2}\|c_{\mu'}\|^2 + \frac{\kappa}{2} \\ &= \frac{1}{m-1}\int_{\mathbb{S}^d} \rho(x)^m \mathrm{d}S(x) - \frac{\kappa}{2}\|c_\mu\|^2 + \frac{\kappa}{2} \\ &= E[\mu], \end{aligned}$$

where for the second equality we used that ρ' is a rotation of ρ, and that $c_{\mu'} = c_\mu$.

Consider a convex combination of ρ and ρ':

$$\rho_\lambda = (1-\lambda)\rho + \lambda\rho', \qquad 0 < \lambda < 1.$$

As the function $x \mapsto \frac{x^m}{m-1}$ is convex for any $0 < m < 1$, we get

$$\frac{1}{m-1}\int_{\mathbb{S}^d} \rho_\lambda(x)^m \mathrm{d}S(x) \leqslant \int_{\mathbb{S}^d}\left((1-\lambda)\left(\frac{1}{m-1}\rho(x)^m\right) + \lambda\left(\frac{1}{m-1}\rho'(x)^m\right)\right)\mathrm{d}S(x)$$
$$= (1-\lambda)\left(\frac{1}{m-1}\int_{\mathbb{S}^d}\rho(x)^m\mathrm{d}S(x)\right) + \lambda\left(\frac{1}{m-1}\int_{\mathbb{S}^d}\rho'(x)^m\mathrm{d}S(x)\right),$$

where equality holds only for $\rho = \rho'$. Together with the fact that $c_{\mu_\lambda} = (1-\lambda)c_\mu + \lambda c_{\mu'} = c_\mu$, we get from (2.3) that

$$E[\mu_\lambda] \leqslant (1-\lambda)E[\mu] + \lambda E[\mu'] = E[\mu],$$

with equality holding only for $\rho = \rho'$. Since $E[\mu]$ is the global minimum, then $E[\mu_\lambda] = E[\mu]$ and hence, $\rho = \rho'$ for any rotation R that preserves c_ρ. Let $z \in \mathbb{S}^d$ satisfy $c_\rho = \|c_\rho\| z$. Then, $\rho = R_\# \rho$ for any rotation R that preserves z. It implies that ρ is symmetric with respect to z (or equivalently symmetric with respect to $-z$).

b) Now assume that $0 < \alpha < 1$, i.e., μ has both a Dirac delta and a regular component. Using the notation from part a), we have $c_\rho = \|c_\rho\| z$. If $\|c_\rho\| = 0$ then z can be any vector and we can set $z = x_0$. If $\|c_\rho\| > 0$, then express the energy as

$$E[\mu] = \frac{1}{m-1}\int_{\mathbb{S}^d}(1-\alpha)^m \rho(x)^m \mathrm{d}S(x) - \frac{\kappa}{2}\left\|\alpha x_0 + (1-\alpha)\|c_\rho\| z\right\|^2 + \frac{\kappa}{2}.$$

Now note that this energy is minimized when $x_0 = z$, as both $1-\alpha$ and $\alpha\|c_\alpha\|$ are positive. In particular, ρ is symmetric with respect to x_0. This concludes the proof. $\square$

Based on Lemmas 2.1-2.3, we consider the following admissible set $\mathcal{P}_{\mathrm{sym}}(\mathbb{S}^d) \subset \mathcal{P}(\mathbb{S}^d)$ for the energy minimizers:

$$\mathcal{P}_{\mathrm{sym}}(\mathbb{S}^d) = \left\{\alpha\delta_{x_0} + (1-\alpha)\rho\mathrm{d}S(x) : \ 0 \leqslant \alpha < 1,\ \rho \in \mathcal{P}_{ac}(\mathbb{S}^d),\ c_\rho = \|c_\rho\| x_0\right\}, \tag{2.5}$$

where x_0 is a fixed point on $\mathbb{S}^d$. Note that when $\alpha = 0$, $\mu = \rho\mathrm{d}S$ and we can assume that ρ is symmetric with respect to x_0 without loss of generality. Indeed, by Lemmas 2.1-2.3, it holds that

$$\min_{\mu\in\mathcal{P}_{\mathrm{sym}}(\mathbb{S}^d)} E[\mu] = \min_{\mu\in\mathcal{P}(\mathbb{S}^d)} E[\mu].$$

2.2. **Critical points of the energy.** We now investigate the equilibria that are in the set $\mathcal{P}_{\mathrm{sym}}(\mathbb{S}^d)$ of admissible minimizers. We will distinguish between equilibria that are absolutely continuous with respect to $\mathrm{d}S$, and equilibria that contain a singular part. The interaction strength $\kappa > 0$ is arbitrary, but fixed. In this section we do not yet indicate, however, the dependence of the equilibria on κ; hence, the equilibria computed here depend on κ, unless otherwise noted.

a. Absolutely continuous equilibria. Consider first an equilibrium $\mu = \rho\mathrm{d}S$ which has no singular component. In this case, write the energy (2.3) as a function of ρ:

$$E[\rho] = \frac{1}{m-1}\int_{\mathbb{S}^d}\rho(x)^m\mathrm{d}S(x) - \frac{\kappa}{2}\|c_\rho\|^2 + \frac{\kappa}{2}. \tag{2.6}$$

The functional derivative of $E[\rho]$ can be computed by taking variations of the form

$$\rho^\epsilon = \rho + \epsilon\delta\rho,$$

where $\int_{\mathbb{S}^d} \delta\rho(x)\mathrm{d}S(x) = 0$, so that ρ^ϵ are probability densities. Then, by (2.6), we compute

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}E[\rho^\epsilon] = \frac{m}{m-1}\int_{\mathbb{S}^d} \rho^\epsilon(x)^{m-1}\delta\rho(x)\mathrm{d}S(x) - \kappa\left\langle c_{\rho^\epsilon}, \int_{\mathbb{S}^d} x\delta\rho(x)\mathrm{d}S(x)\right\rangle,$$

and upon evaluating at $\epsilon = 0$, we find

$$\frac{\delta E}{\delta\rho} = \left(\frac{m}{m-1}\right)\rho(x)^{m-1} - \kappa\langle c_\rho, x\rangle.$$

At an equilibrium, the first variation of the energy vanishes. Note that here we only consider perturbations that preserve the unit mass. In turn, this introduces a Lagrange multiplier, and we infer that a density $\rho \in \mathcal{P}_{ac}(\mathbb{S}^d)$ is a critical point of the energy if $\frac{\delta E}{\delta\rho}$ is equal to a constant in the support of ρ. There is an additional caveat that in general, the support of an equilibrium density can have multiple disjoint components, in which case the value of the constant can take different values in different components [14, 37]. It is not the case here however, as the support of an equilibrium ρ must be the entire sphere $\mathbb{S}^d$ – see justification below.

By the observations above, we arrive at the following Euler-Lagrange equation:

$$\left(\frac{m}{m-1}\right)\rho(x)^{m-1} - \kappa\langle c_\rho, x\rangle = \lambda, \qquad x \in \operatorname{supp}(\rho), \tag{2.7}$$

for some constant λ. The equilibria satisfying (2.7) are fully supported on the entire sphere. Indeed, since the exponent of ρ in (2.7) is negative, if the support was strictly contained in $\mathbb{S}^d$, then λ would be infinite. This also explains why we ruled out the case that $\operatorname{supp}(\rho)$ can have disconnected components in $\mathbb{S}^d$: by the same argument, if (2.7) held on a certain component of $\operatorname{supp}(\rho)$, then the constant would be infinite. Also from (2.7) and $0 < m < 1$, we infer that

$$\lambda + \kappa\langle c_\rho, x\rangle \leqslant 0, \qquad \forall x \in \mathbb{S}^d.$$

Recall that $c_\rho = \|c_\rho\|x_0$, with $x_0 \in \mathbb{S}^d$ fixed. Define $\theta_x = \arccos\langle x_0, x\rangle \in [0, \pi]$, to write the equilibria from (2.7) as

$$\rho(x) = \left(\frac{m}{1-m}\right)^{\frac{1}{1-m}} (-\lambda - \kappa\|c_\rho\|\cos\theta_x)^{\frac{1}{m-1}}, \qquad \forall\, x \in \mathbb{S}^d. \tag{2.8}$$

Also, since $-\lambda - \kappa\|c_\rho\|\cos\theta_x \geqslant 0$, for all $\theta_x \in [0, \pi]$, we have $\lambda \leqslant -\kappa\|c_\rho\|$. If the inequality is strict, i.e., $\lambda < -\kappa\|c_\rho\|$, then $-\lambda - \kappa\|c_\rho\|\cos\theta_x > 0$ for all $x \in \mathbb{S}^d$, and hence $\rho \in L^\infty(\mathbb{S}^d)$. However, $\lambda = -\kappa\|c_\rho\|$ is a limiting case, where ρ becomes infinite at $\theta = 0$; see part b, in particular Remark 2.1.

To find λ and $\|c_\rho\|$, and hence determine the equilibrium (2.8), we ask that ρ has mass 1 and centre of mass at c_ρ. Using hyperspherical coordinates, we arrive at the following system of equations:

$$\begin{aligned} 1 &= dw_d \int_0^\pi \left(\frac{m}{1-m}\right)^{\frac{1}{1-m}} (-\lambda - \kappa\|c_\rho\|\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta\,\mathrm{d}\theta, \\ \|c_\rho\| &= dw_d \int_0^\pi \left(\frac{m}{1-m}\right)^{\frac{1}{1-m}} (-\lambda - \kappa\|c_\rho\|\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta\cos\theta\,\mathrm{d}\theta, \end{aligned} \tag{2.9}$$

where w_d denotes the volume of the d-dimensional unit ball. In the integration above we used $|\mathbb{S}^{d-1}| = dw_d$, where $|\mathbb{S}^{d-1}|$ denotes the area of the $(d-1)$-dimensional unit sphere. System (2.9) needs to be solved for λ and $\|c_\rho\|$, for a given κ.

b. Equilibria that have a singular component. By (2.5), we consider probability measures of the form

$$\mu_\alpha = \alpha\delta_{x_0} + (1-\alpha)\rho\,\mathrm{d}S, \tag{2.10}$$

where $\alpha \in (0,1)$ and x_0 is the normalized centre of mass of the density $\rho \in \mathcal{P}_{ac}(\mathbb{S}^d)$:

$$x_0 = \frac{c_\rho}{\|c_\rho\|} = \frac{\int_{\mathbb{S}^d} x\rho(x)\mathrm{d}S}{\left\|\int_{\mathbb{S}^d} x\rho(x)\mathrm{d}S\right\|}. \tag{2.11}$$

Similar to how (2.3) was derived, we can write

$$E[\mu_\alpha] = \frac{1}{m-1}\int_{\mathbb{S}^d}(1-\alpha)^m\rho(x)^m\mathrm{d}S(x) - \frac{\kappa}{2}\|c_{\mu_\alpha}\|^2 + \frac{\kappa}{2}, \tag{2.12}$$

where the centre of mass of μ_α is given by

$$c_{\mu_\alpha} = \int_{\mathbb{S}^d} x\mathrm{d}\mu_\alpha(x) = \alpha x_0 + (1-\alpha)c_\rho. \tag{2.13}$$

Also, using (2.11), we can further write

$$\begin{aligned} E[\mu_\alpha] =& \frac{1}{m-1}\int_{\mathbb{S}^d}(1-\alpha)^m\rho(x)^m\mathrm{d}S(x) \\ &- \frac{\kappa}{2}\left(\alpha^2 + 2\alpha(1-\alpha)\|c_\rho\| + (1-\alpha)^2\|c_\rho\|^2\right) + \frac{\kappa}{2}. \end{aligned} \tag{2.14}$$

In computing the Euler-Lagrange equations for the energy $E[\mu_\alpha]$, we consider variations in both the parameter α and density ρ. First, by setting $\frac{\partial}{\partial\alpha}E[\mu_\alpha] = 0$, we find

$$\frac{m(1-\alpha)^{m-1}}{1-m}\int_{\mathbb{S}^d}\rho(x)^m\mathrm{d}S(x) - \kappa\left(\alpha + (1-2\alpha)\|c_\rho\| + (\alpha-1)\|c_\rho\|^2\right) = 0.$$

After factorizing the expression in the round brackets in the l.h.s. above, we arrive at the following Euler-Lagrange equation (by perturbing with respect to α only):

$$\frac{m(1-\alpha)^{m-1}}{1-m}\int_{\mathbb{S}^d}\rho(x)^m\mathrm{d}S(x) - \kappa\left(1-\|c_\rho\|\right)\left(\alpha + (1-\alpha)\|c_\rho\|\right) = 0. \tag{2.15}$$

Now consider perturbations with respect to ρ. The functional derivative of the energy (2.12) with respect to ρ can be computed by taking variations μ_α^ϵ of μ_α of the form

$$\mu_\alpha^\epsilon = \alpha\delta_{x_0} + (1-\alpha)\rho^\epsilon\,\mathrm{d}S,$$

where $\rho^\epsilon = \rho + \epsilon\delta\rho$, with $\int_{\mathbb{S}^d} \delta\rho(x)\mathrm{d}S(x) = 0$. Calculate, using (2.12) and (2.13):

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\epsilon}E[\mu_\alpha^\epsilon] &= \frac{\mathrm{d}}{\mathrm{d}\epsilon}\Bigg(\frac{1}{m-1}\int_{\mathbb{S}^d}(1-\alpha)^m\rho^\epsilon(x)^m\mathrm{d}S(x) \\ &\quad - \frac{\kappa}{2}\langle\alpha x_0 + (1-\alpha)c_{\rho^\epsilon}, \alpha x_0 + (1-\alpha)c_{\rho^\epsilon}\rangle + \frac{\kappa}{2}\Bigg) \\ &= \frac{m}{m-1}\int_{\mathbb{S}^d}(1-\alpha)^m\rho^\epsilon(x)^{m-1}\delta\rho(x)\mathrm{d}S(x) \\ &\quad - \kappa\Big\langle \alpha x_0 + (1-\alpha)c_{\rho^\epsilon}, (1-\alpha)\int_{\mathbb{S}^d} x\delta\rho(x)\mathrm{d}S(x)\Big\rangle.\end{aligned}$$

By evaluating the above at $\epsilon = 0$ we then find

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\epsilon}E[\mu_\alpha^\epsilon]\Big|_{\epsilon=0} &= \frac{m}{m-1}\int_{\mathbb{S}^d}(1-\alpha)^m\rho(x)^{m-1}\delta\rho(x)\mathrm{d}S(x) \\ &\quad - \kappa(1-\alpha)\int_{\mathbb{S}^d}\langle\alpha x_0 + (1-\alpha)c_\rho, x\rangle\,\delta\rho(x)\mathrm{d}S(x) \\ &= \frac{m}{m-1}\int_{\mathbb{S}^d}(1-\alpha)^m\rho(x)^{m-1}\delta\rho(x)\mathrm{d}S(x) \\ &\quad - \kappa(1-\alpha)\int_{\mathbb{S}^d}\left(\frac{\alpha}{\|c_\rho\|} + 1 - \alpha\right)\langle c_\rho, x\rangle\,\delta\rho(x)\mathrm{d}S(x).\end{aligned}$$

From this calculation we find that the functional derivative of the energy with respect to ρ is given by

$$\frac{\delta E}{\delta\rho} = \frac{m}{m-1}(1-\alpha)^m\rho(x)^{m-1} - \kappa(1-\alpha)\langle c_\rho, x\rangle\left(\frac{\alpha}{\|c_\rho\|} + 1 - \alpha\right).$$

Note again that perturbations $\delta\rho$ have zero mass, which introduces a Lagrange multiplier. We then arrive at the following Euler–Lagrange equation (by perturbating with respect to ρ):

$$\frac{m}{m-1}(1-\alpha)^m\rho(x)^{m-1} - \kappa(1-\alpha)\langle c_\rho, x\rangle\left(\frac{\alpha}{\|c_\rho\|} + 1 - \alpha\right) = \lambda, \qquad x \in \mathrm{supp}(\rho), \tag{2.16}$$

for some constant λ.

The support of ρ is the entire sphere; if we assume otherwise, λ would be infinite. From (2.16), by writing in hyperspherical coordinates, we have

$$\rho(x) = \left(\frac{m(1-\alpha)^m}{1-m}\right)^{\frac{1}{1-m}}\big(-\lambda - \kappa(1-\alpha)\cos\theta_x\left(\alpha + (1-\alpha)\|c_\rho\|\right)\big)^{\frac{1}{m-1}}, \qquad \forall x \in \mathbb{S}^d. \tag{2.17}$$

Note that for $\alpha = 0$, (2.17) reduces to (2.8).

An equilibrium μ_α in the form (2.10) must satisfy both (2.15) and (2.16). Multiply (2.16) by $\frac{\rho(x)}{\alpha-1}$ and integrate over $x \in \mathbb{S}^d$ to get

$$\frac{m(1-\alpha)^{m-1}}{1-m}\int_{\mathbb{S}^d}\rho(x)^m\mathrm{d}S(x) + \kappa\|c_\rho\|\left(\alpha + (1-\alpha)\|c_\rho\|\right) = \frac{\lambda}{\alpha-1}. \tag{2.18}$$

Now subtract (2.18) from (2.15) to find the following relationship between $\lambda, \|c_\rho\|$ and α:

$$-\frac{\lambda}{1-\alpha} = \kappa(\alpha + (1-\alpha)\|c_\rho\|). \tag{2.19}$$

We remark here that $\alpha = 0$ corresponds to the limiting case $\lambda = -\kappa\|c_\rho\|$ pointed out in part a.

Finally, by using (2.19), we write (2.17) as

$$\rho(x) = \left(\frac{m(1-\alpha)^m}{1-m}\right)^{\frac{1}{1-m}} (-\lambda)^{\frac{1}{m-1}} \big(1 - \cos\theta_x\big)^{\frac{1}{m-1}}, \qquad \forall x \in \mathbb{S}^d. \tag{2.20}$$

Also, we find the compatibility conditions for the mass and centre of mass:

$$\begin{aligned} 1 &= dw_d \int_0^\pi \left(\frac{m(1-\alpha)^m}{1-m}\right)^{\frac{1}{1-m}} (-\lambda)^{\frac{1}{m-1}} \big(1-\cos\theta\big)^{\frac{1}{m-1}} \sin^{d-1}\theta \,\mathrm{d}\theta, \\ \|c_\rho\| &= dw_d \int_0^\pi \left(\frac{m(1-\alpha)^m}{1-m}\right)^{\frac{1}{1-m}} (-\lambda)^{\frac{1}{m-1}} \big(1-\cos\theta\big)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \,\mathrm{d}\theta. \end{aligned} \tag{2.21}$$

The constants $\lambda, \|c_\rho\|$ and α are then found by solving (2.19) and (2.21).

First note that by dividing the two equations in (2.21), we find

$$\|c_\rho\| = \frac{\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \mathrm{d}\theta}{\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta}, \tag{2.22}$$

so the centre of mass of ρ does not depend on κ. Furthermore, by the first equation in (2.21), we have

$$(-\lambda)^{\frac{1}{m-1}} = \frac{1}{dw_d} \left(\frac{m(1-\alpha)^m}{1-m}\right)^{\frac{1}{m-1}} \frac{1}{\int_0^\pi \big(1-\cos\theta\big)^{\frac{1}{m-1}} \sin^{d-1}\theta \,\mathrm{d}\theta}, \tag{2.23}$$

which upon substitution in (2.20) yields

$$\rho(x) = \frac{\big(1-\cos\theta_x\big)^{\frac{1}{m-1}}}{dw_d \int_0^\pi \big(1-\cos\theta\big)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta}, \qquad \forall x \in \mathbb{S}^d. \tag{2.24}$$

Hence, we conclude that the density ρ of the regular component of an equilibrium in the form (2.10) is *fixed*, in the sense that it does not depend on κ. The only variable that needs to be determined is α, which can be done by solving (2.19) and (2.23) for α and λ, with $\|c_\rho\|$ given by (2.22).

Remark 2.1. *The density ρ from* (2.24) *is not in $L^\infty(\mathbb{S}^d)$, as it blows up at $\theta_x = 0$. We need however that $\rho \in L^1(\mathbb{S}^d)$ (ρ is unit mass in fact). By hyperspherical coordinates (see first equation in* (2.21)*), this reduces to checking whether $(1-\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta$ has an integrable singularity at $\theta = 0$. As $1 - \cos\theta$ behaves as $\theta^2/2$ near $\theta = 0$, we need to check the integrability of $\theta^{\frac{2}{m-1}+d-1}$. We find that ρ is integrable when $0 < m < 1 - \frac{2}{d}$, and not integrable for $1 - \frac{2}{d} < m < 1$. Also note that for $d = 1$ and $d = 2$, ρ is not integrable for any $0 < m < 1$. We infer from these observations that equilibria in the form* (2.10) *(i.e., with a* *singular component) do not occur for $d = 1$ and $d = 2$, and only occur when $0 < m < 1 - \frac{2}{d}$ for $d \geqslant 3$.*

Remark 2.2. *The critical value $m = 1 - \frac{2}{d}$ also appears in distinguishing different behaviours of solutions to the nonlinear diffusion equation $\rho_t = \Delta\rho^m$ in the Euclidean space $\mathbb{R}^d$. For $0 < m < 1 - \frac{2}{d}$, it was shown that the Dirac delta remains stable in a certain sense, for all times* [9]. *In informal terms, diffusion does not spread out very localized initial densities when $0 < m < 1 - \frac{2}{d}$; we also note that this result applies only in dimensions $d \geqslant 3$. On the other hand, also shown in* [9], *diffusion does spread out a Dirac delta when $1 - \frac{2}{d} < m < 1$. Even though we work here on the sphere, as opposed to the flat Euclidean space, these consideration are very local in space, and the effects or curvature do not seem important. Hence, as noted in Remark 2.1, equilibria of* (1.1) *that contain a Dirac delta can only occur for $0 < m < 1 - \frac{2}{d}$ and $d \geqslant 3$, which is consistent with the case when the Dirac delta is "stable" for the nonlinear diffusion evolution equation.*

2.3. **Uniform distribution.** The uniform distribution on the sphere, given by

$$\rho_{\text{uni}}(x) = \frac{1}{|\mathbb{S}^d|}, \qquad \forall x \in \mathbb{S}^d,$$

where $|\mathbb{S}^d|$ denotes the area of $\mathbb{S}^d$, is a solution of (2.7) for all $\kappa > 0$. Indeed, in this case, $c_{\rho_{\text{uni}}} = 0$, and the constant λ is given by

$$\lambda_{\text{uni}} = \left(\frac{m}{m-1}\right)\frac{1}{|\mathbb{S}^d|^{m-1}}.$$

In applications to polymer orientation, this equilibrium corresponds to the isotropic state.

The full nonlinear stability of the uniform distribution can be established, in terms of the strength κ of the attractive interactions. The result is the following.

Proposition 2.1 (Stability of the uniform distribution)**.** *The uniform distribution ρ_{uni} is a stable critical point of the energy functional E if and only if $\kappa \leqslant \kappa_1$, where*

$$\kappa_1 := \frac{m(d+1)}{|\mathbb{S}^d|^{m-1}}. \tag{2.25}$$

Proof. We consider two types of perturbations of the uniform distribution: i) absolutely continuous perturbations, and ii) perturbations that contain a singular part.

Case i) Absolutely continuous perturbations. First consider perturbations $\{\rho^\epsilon\} \subset \mathcal{P}_{ac}(\mathbb{S}^d)$ of the uniform distribution, that are absolutely continuous:

$$\rho^0 = \rho_{\text{uni}}, \qquad \int_{\mathbb{S}^d} \rho^\epsilon(x)\mathrm{d}S(x) = 1, \quad \text{for all } \epsilon. \tag{2.26}$$

The energy of ρ^ϵ is given by (use (2.2)):

$$E[\rho^\epsilon] = \frac{1}{m-1}\int_{\mathbb{S}^d} \rho^\epsilon(x)^m \mathrm{d}S(x) - \frac{\kappa}{2}\iint\limits_{\mathbb{S}^d\times\mathbb{S}^d} \langle x, y\rangle \rho^\epsilon(x)\rho^\epsilon(y)\mathrm{d}S(x)\mathrm{d}S(y) + \frac{\kappa}{2}.$$

The uniform distribution is a local minimizer with respect to absolutely continuous perturbations provided

$$\frac{\mathrm{d}^2}{\mathrm{d}\epsilon^2} E[\rho^\epsilon]\Big|_{\epsilon=0} \geqslant 0, \tag{2.27}$$

for all perturbations ρ^ϵ that satisfy (2.26).

The stability calculations in this case are identical to those carried out in [28] for slow diffusion, and we will only summarize them here. Denote

$$\delta\rho^\epsilon = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\rho^\epsilon, \qquad \text{and} \qquad \delta^2\rho^\epsilon = \frac{\mathrm{d}^2}{\mathrm{d}\epsilon^2}\rho^\epsilon.$$

Using the unit mass condition in (2.26), we note that

$$\int_{\mathbb{S}^d} \delta\rho^\epsilon(x)\mathrm{d}S(x) = 0, \qquad \text{and} \qquad \int_{\mathbb{S}^d} \delta^2\rho^\epsilon(x)\mathrm{d}S(x) = 0, \qquad \text{for all } \epsilon.$$

By direct calculations, one finds

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}E[\rho^\epsilon] = \frac{1}{m-1}\int_{\mathbb{S}^d} m\rho^\epsilon(x)^{m-1}\delta\rho^\epsilon(x)\mathrm{d}S(x) - \kappa \iint\limits_{\mathbb{S}^d\times\mathbb{S}^d} \langle x,y\rangle\, \rho^\epsilon(x)\delta\rho^\epsilon(y)\mathrm{d}S(x)\mathrm{d}S(y), \tag{2.28}$$

and

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}\epsilon^2}E[\rho^\epsilon] &= m\int_{\mathbb{S}^d} \rho^\epsilon(x)^{m-2}\left(\delta\rho^\epsilon(x)\right)^2\mathrm{d}S(x) + \frac{m}{m-1}\int_{\mathbb{S}^d}\rho^\epsilon(x)^{m-1}\delta^2\rho^\epsilon(x)\mathrm{d}S(x) \\ &\quad - \kappa \iint\limits_{\mathbb{S}^d\times\mathbb{S}^d} \langle x,y\rangle(\delta\rho^\epsilon(x)\delta\rho^\epsilon(y) + \rho^\epsilon(x)\delta^2\rho^\epsilon(y))\mathrm{d}S(x)\mathrm{d}S(y).\end{aligned} \tag{2.29}$$

Evaluate (2.28) and (2.29) at $\epsilon = 0$. Using that $\rho^0 = \rho_{\text{uni}}$ is constant, that $\delta\rho^\epsilon(x)$ integrates to 0, and also that the centre of mass of ρ^0 is at the origin, we find $\frac{\mathrm{d}}{\mathrm{d}\epsilon}E[\rho^\epsilon]_{|\epsilon=0} = 0$ – as expected, since ρ_{uni} is a critical point of the energy. Similarly, using that $\rho^0 = \rho_{\text{uni}}$ is constant, that $\delta^2\rho^\epsilon(x)$ integrates to 0, and that the centre of mass of ρ^0 is at the origin, we find that two of the terms in the r.h.s. of (2.29) vanish:

$$\int_{\mathbb{S}^d}\rho^0(x)^{m-1}\delta^2\rho^0(x)\mathrm{d}S(x) = \frac{1}{|\mathbb{S}^d|^{m-1}}\int_{\mathbb{S}^d}\delta^2\rho^0(x)\mathrm{d}S(x) = 0.$$

and

$$\begin{aligned}\iint\limits_{\mathbb{S}^d\times\mathbb{S}^d}\langle x,y\rangle\rho^0(x)\delta^2\rho^0(y)\mathrm{d}S(x)\mathrm{d}S(y) &= \left\langle \int_{\mathbb{S}^d} x\rho^0(x)\mathrm{d}S(x), \int_{\mathbb{S}^d} y\,\delta^2\rho^0(x)\mathrm{d}S(y)\right\rangle \\ &= 0.\end{aligned}$$

Therefore, by dropping the superscript 0 and by denoting $\delta\rho = \delta\rho^\epsilon_{|\epsilon=0}$, we find from (2.29):

$$\frac{\mathrm{d}^2}{\mathrm{d}\epsilon^2}E[\rho^\epsilon]_{|\epsilon=0} = \frac{m}{|\mathbb{S}^d|^{m-2}}\int_{\mathbb{S}^d}\left(\delta\rho(x)\right)^2\mathrm{d}S(x) - \kappa\left\|\int_{\mathbb{S}^d} x\delta\rho(x)\mathrm{d}S(x)\right\|^2.$$

For (2.27) to hold, the r.h.s. above has to be non-negative, i.e.,

$$\kappa \leqslant \frac{m}{|\mathbb{S}^d|^{m-2}}\cdot\frac{\int_{\mathbb{S}^d}\left(\delta\rho(x)\right)^2\mathrm{d}S(x)}{\left|\int_{\mathbb{S}^d} x\delta\rho(x)\mathrm{d}S(x)\right|^2},$$

for all perturbations $\delta\rho$ that have zero mass.

Define $\mathcal{A} = \{\psi \in L^2(\mathbb{S}^d) : \int_{\mathbb{S}^d} \psi(x)\mathrm{d}S(x) = 0\}$ and the following functional on $\mathcal{A}$:

$$\mathcal{F}[\psi] = \frac{\int_{\mathbb{S}^d} (\psi(x))^2 \,\mathrm{d}S(x)}{\left|\int_{\mathbb{S}^d} x\psi(x)\mathrm{d}S(x)\right|^2}. \tag{2.30}$$

The uniform distribution is a local minimum (and hence, stable) with respect to absolutely continuous perturbations, provided

$$\kappa \leqslant \frac{m}{|\mathbb{S}^d|^{m-2}} \cdot \inf_{\psi\in\mathcal{A}} \mathcal{F}[\psi], \tag{2.31}$$

and unstable otherwise.

The following lemma is proved in [28], and we simply list it here.

Lemma 2.4 (Lemma 3.1, [28])**.** *Let $\mathcal{F} : \mathcal{A} \to \mathbb{R}$ be given by* (2.30)*. Then,*

$$\inf_{\psi\in\mathcal{A}} \mathcal{F}[\psi] = \frac{d+1}{|\mathbb{S}^d|}.$$

By Lemma 2.4, (2.31) holds only for $\kappa \leqslant \kappa_1$, and this shows the claimed stability with respect to absolutely continuous perturbations.

Case ii) Singular perturbations. Consider a singular perturbation $\{\mu^\epsilon\}_{\epsilon>0} \subset \mathcal{P}(\mathbb{S}^d)$ of the form

$$\mu^\epsilon = \alpha^\epsilon \nu + (1-\alpha^\epsilon)\rho_{\mathrm{uni}}\mathrm{d}S,$$

where $\nu = \nu_s + \tilde{\rho}\mathrm{d}S \in \mathcal{P}(\mathbb{S}^d)$, with ν_s and $\tilde{\rho}\mathrm{d}S$ being the singular and the absolutely continuous parts of ν, respectively. Also, $\{\alpha^\epsilon\}_{\epsilon>0}$ satisfy

$$\alpha^0 = 0, \qquad \text{and} \qquad \delta\alpha := \frac{\mathrm{d}}{\mathrm{d}\epsilon}\alpha^\epsilon\Big|_{\epsilon=0+} > 0.$$

Note that these are one-sided perturbations with respect to α, as $\alpha = 0$ is a boundary value of the interval $(0, 1)$.

Then, by (2.3) we have

$$E[\mu^\epsilon] = \frac{1}{m-1}\int_{\mathbb{S}^d} (\alpha^\epsilon\tilde{\rho}(x) + (1-\alpha^\epsilon)\rho_{\mathrm{uni}}(x))^m \,\mathrm{d}S - \frac{\kappa}{2}(\alpha^\epsilon\|c_\nu\|)^2 + \frac{\kappa}{2},$$

and its derivative at $\epsilon = 0+$ is

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}E[\mu^\epsilon]\Big|_{\epsilon=0+} = \frac{m}{1-m}\delta\alpha\int_{\mathbb{S}^d} \rho_{\mathrm{uni}}^{m-1}(x)\left(\rho_{\mathrm{uni}}(x) - \tilde{\rho}(x)\right)\mathrm{d}S.$$

Since ρ_{uni} is constant, we can simplify the above as

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}E[\mu^\epsilon]\Big|_{\epsilon=0+} = \frac{m(\delta\alpha)\rho_{\mathrm{uni}}^{m-1}}{1-m}\int_{\mathbb{S}^d} (\rho_{\mathrm{uni}}(x) - \tilde{\rho}(x))\,\mathrm{d}S = \frac{m(\delta\alpha)\rho_{\mathrm{uni}}^{m-1}\int_{\mathbb{S}^d}\mathrm{d}\nu_s}{1-m},$$

where we used $\rho_{\mathrm{uni}}, \nu \in \mathcal{P}(\mathbb{S}^d)$.

As we considered singular perturbations ν, we have $\int_{\mathbb{S}^d}\mathrm{d}\nu_s > 0$. Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}E[\mu^\epsilon]\Big|_{\epsilon=0+} > 0, \tag{2.32}$$

and we conclude that the energy of the uniform distribution increases with the formation of a singular measure.

More generally, if we consider perturbations of the form

$$\mu^\epsilon = \alpha^\epsilon \nu + (1-\alpha^\epsilon)\rho^\epsilon \mathrm{d}S,$$

where

$$\alpha^0 = 0, \quad \rho^0 = \rho_{\text{uni}}, \quad \delta\alpha := \frac{\mathrm{d}}{\mathrm{d}\epsilon}\alpha^\epsilon\Big|_{\epsilon=0+} > 0, \quad \text{and} \quad \int_{\mathbb{S}^d} \rho^\epsilon(x)\mathrm{d}S(x) = 1,$$

then the considerations follow the previous calculations. Indeed, by taking a derivative of $E[\mu^\epsilon]$ with respect to ϵ, and evaluate at $\epsilon = 0+$, we find again (2.32), as the contributions from the variations ρ^ϵ lead to 0.

We conclude that the energy increases by perturbing ρ_{uni} with a singular measure. Note that this fact applies to all values of κ. Hence, the stability of ρ_{uni} for different ranges of κ is as found using absolutely continuous perturbations. □

We will find in the next section that for $\kappa < \kappa_1$, the uniform distribution is the only critical point of the energy (and hence, a global minimizer), and at $\kappa = \kappa_1$ a bifurcation occurs.

3. Critical values of κ and phase transitions

In this section, we will identify various critical values of κ at which equilibria experience phase transitions, for several ranges of m within $0 < m < 1$.

3.1. **Bifurcation from the uniform distribution.** We first study the bifurcation that occurs at $\kappa = \kappa_1$ (cf., Proposition 2.1). We consider the fully supported equilibrium (2.8), with λ and $\|c_\rho\|$ that solve (2.9), where in this case, $-\lambda \geqslant \kappa\|c_\rho\|$.

For a simpler notation, we denote

$$s = \|c_\rho\|, \qquad \lambda = -\kappa s \eta. \tag{3.33}$$

To guarantee the condition on λ, we assume $\eta \geqslant 1$. The compatibility conditions (2.9) for mass and centre of mass become

$$1 = d w_d \left(\frac{m}{(1-m)\kappa s}\right)^{\frac{1}{1-m}} \int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \,\mathrm{d}\theta,$$

$$s = d w_d \left(\frac{m}{(1-m)\kappa s}\right)^{\frac{1}{1-m}} \int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \,\mathrm{d}\theta.$$

From the above, we find s and κ in terms of η as

$$s = \frac{\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \mathrm{d}\theta}{\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta}, \tag{3.34a}$$

$$\kappa^{-1} = \frac{1-m}{m}(d w_d)^{m-1} \left(\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \mathrm{d}\theta\right) \left(\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta\right)^{m-2}. \tag{3.34b}$$

We define the following function in the range $\eta \geqslant 1$:

(3.35)
$$H(\eta) = \frac{1-m}{m}(dw_d)^{m-1}\left(\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta\right)\left(\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta\right)^{m-2}.$$

Equation (3.34b) can then be written as

(3.36)
$$H(\eta) = \kappa^{-1}.$$

Finding a fully supported equilibrium in the form (2.8) reduces to finding solutions to equation (3.36). Indeed, with κ fixed, once a solution η of (3.36) is found (note that such solutions need to be in the range $1 \leqslant \eta < \infty$), then s can be determined from (3.34a), λ is computed from (3.33), and the equilibrium ρ in the form (2.8) is fully determined. For this reason, the behaviour of the function $H(\eta)$ for $1 \leqslant \eta < \infty$, is essential for investigating the existence (and uniqueness) of fully supported equilibria (2.8). In the next lemma we establish some remarkable monotonicity properties of this function.

Lemma 3.1. *The function $H(\eta)$ defined in* (3.35) *for $\eta \geqslant 1$, is strictly increasing for $1-\frac{2}{d-1} < m < 1$, strictly decreasing for $0 < m < 1-\frac{2}{d-1}$, and constant when $m = 1-\frac{2}{d-1}$.*

Proof. The proof is quite lengthy and nontrivial. It involves investigating the sign of $H'(\eta)$ using associated Legendre functions of the first kind and the Chebyshev inequality; see Appendix B. □

Remark 3.1. *Note that $d = 1$ and $d = 2$ in Lemma 3.1 are special, in the sense that for these cases, $H(\eta)$ is strictly decreasing for all $0 < m < 1$.*

Lemma 3.2. *The following holds:*

(3.37)
$$\left(\lim_{\eta\to\infty} H(\eta)\right)^{-1} = \kappa_1,$$

where κ_1 is the critical κ identified in Proposition 2.1.

Proof. The proof follows a direct calculation – see Appendix C. □

Remark 3.2. *In the limit $\eta \to \infty$ (along with $s \to 0$ and $\lambda \to \lambda_{uni}$), the equilibria approach the uniform distribution ρ_{uni}. As discussed below (Remark 3.3, Proposition 3.1), there is a bifurcation at $\kappa = \kappa_1$, where a fully supported equilibrium ρ_κ gets born from the uniform distribution ρ_{uni}. In this sense, equation* (3.37) *indicates κ_1 as a critical value, as depending on the monotonicity of H, equation* (3.36) *has solutions $\eta \in (1,\infty)$ when $\kappa < \kappa_1$ or $\kappa > \kappa_1$.*

The function $H(\eta)$ is plotted in Figure 1; for plot (a) we used $m = 0.5$, $d = 2$, for (b) we have $m = 0.25$, $d = 3$, and for plot (c) we used $m = 0.3$, $d = 5$. For both cases (a) and (b), $H(\eta)$ is increasing, but the cases are different in the behaviour $\eta \searrow 1$ – see discussion below. Case (c) corresponds to $H(\eta)$ being decreasing; see Lemma 3.1.

Limit $\eta \searrow 1$. We investigate the convergence of the integrals that appear in the function H – note the singularity of $(1-\cos\theta)^{\frac{1}{m-1}}$ at $\theta = 0$. Near $\theta = 0$, $(1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta$, as well as $(1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta$, behave as $\theta^{\frac{2}{m-1}+d-1}$. The integrals are convergent provided $\frac{2}{m-1}+d-1 > -1$, which is equivalent to $m < 1-\frac{2}{d}$; see also Remark 2.1.

Based on Lemma 3.1 and the limit $\eta \searrow 1$, we distinguish three cases:

$$\text{i) } 1-\tfrac{2}{d} < m < 1, \quad \text{ii) } 1-\tfrac{2}{d-1} < m < 1-\tfrac{2}{d}, \quad \text{and iii) } 0 < m < 1-\tfrac{2}{d-1}.$$

Note that in dimensions $d = 1$ and $d = 2$, only case i) applies (for $d = 1$, the lower bound $1 - 2/d$ should be interpreted as 0; see also Remark 3.1), while in dimension $d = 3$, only cases i) and ii) apply.

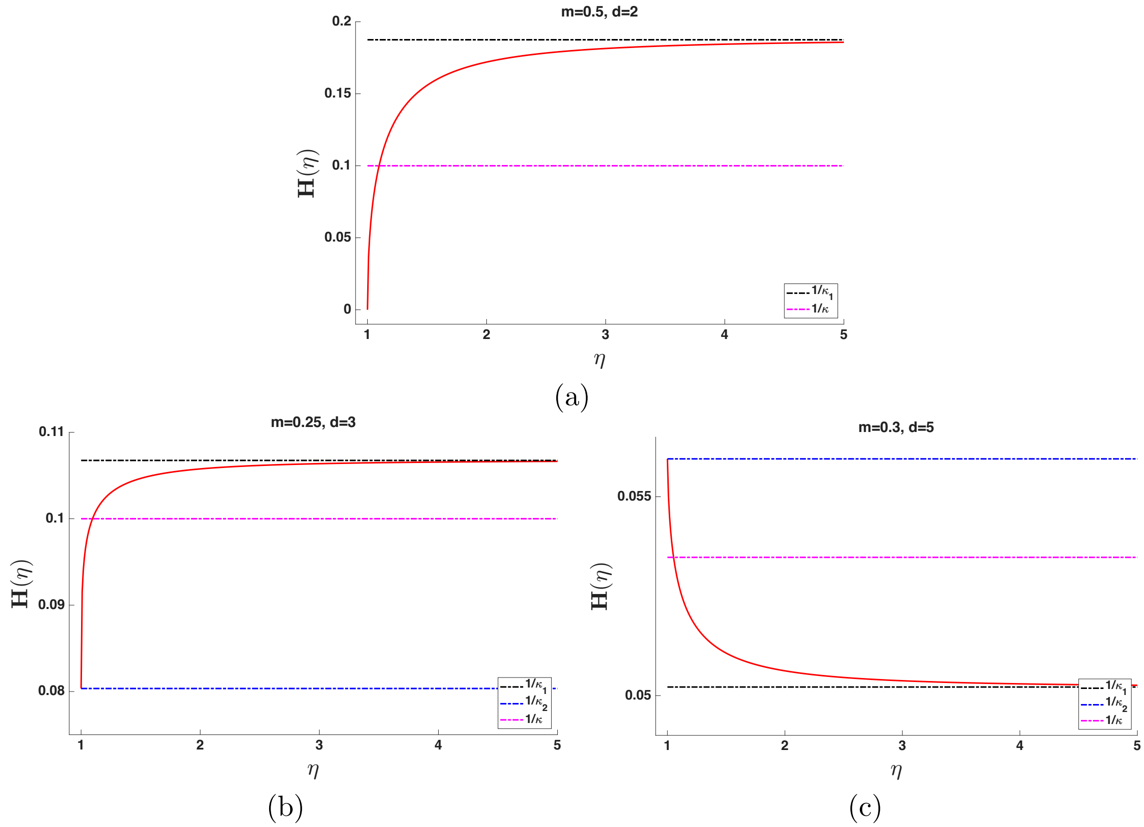


FIGURE 1. Plot of function H defined in (3.35). (a) $1 - 2/d < m < 1$. For this range of m, $H(1) = 0$. For any $\kappa > \kappa_1$, there exists a unique $\eta_\kappa > 1$ such that $\kappa^{-1} = H(\eta_\kappa)$ – see equation (3.34b). (b) $1 - 2/(d-1) < m < 1 - 2/d$. In this case, $H(1) = 1/\kappa_2$, with $\kappa_2 > \kappa_1$. For any $\kappa_1 < \kappa < \kappa_2$, there exists a unique $\eta_\kappa > 1$ that solves $\kappa^{-1} = H(\eta_\kappa)$. (c) $0 < m < 1 - 2/(d-1)$. In this case, $H(1) = 1/\kappa_2$, with $\kappa_2 < \kappa_1$. For any $\kappa_2 < \kappa < \kappa_1$, there exists a unique $\eta_\kappa > 1$ that solves $\kappa^{-1} = H(\eta_\kappa)$. For plot (a) we used $m = 0.5$ and $d = 2$, for plot (b), $m = 0.25$ and $d = 3$, and for plot (c), $m = 0.3$ and $d = 3$.

Case i) $1 - \frac{2}{d} < m < 1$. Write

$$H(\eta) = \frac{1-m}{m}(dw_d)^{m-1} \frac{\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \mathrm{d}\theta}{\left(\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta\right)^{2-m}}.$$

Due to the non-integrability of the integrands, the limit $\eta \searrow 1$ is of the type ∞/∞. Write the above as

$$H(\eta) = \frac{1-m}{m}(dw_d)^{m-1} \frac{\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \mathrm{d}\theta}{\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta} \times \frac{1}{\left(\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta\right)^{1-m}}.$$

The quotient of the two integrals in the r.h.s. is bounded in absolute value by 1, as

$$\left|\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \mathrm{d}\theta\right| \leqslant \int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta,$$

and also,

$$\lim_{\eta\searrow 1} \frac{1}{\left(\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta\right)^{1-m}} = 0,$$

due to the non-integrability of the integrand in the limit.

Hence, in case i) we have

$$\lim_{\eta\searrow 1} H(\eta) = 0.$$

Figure 1(a) corresponds to this case (for dimension $d = 2$, all $0 < m < 1$ fall in this regime in fact). Together with Lemmas 3.1 and 3.2, we infer that for any $\kappa > \kappa_1$, there is a unique $\eta_\kappa > 1$ that solves $\kappa^{-1} = H(\eta_\kappa)$ – see equation (3.34b). This value of η_κ determines uniquely the corresponding s_κ from (3.34a), and then set $\lambda_\kappa = -\kappa s_\kappa \eta_\kappa$. Together they determine a unique (fully supported) equilibrium in the form (2.8). For the range of m in case i), there is no second critical value of κ.

Case ii) $1 - \frac{2}{d-1} < m < 1 - \frac{2}{d}$. In this case, the integrals that appear in $H(\eta)$ are convergent in the limit $\eta \searrow 1$, and hence,

$$\lim_{\eta\searrow 1} H(\eta) = H(1) > 0.$$

Denote by

$$\kappa_2 := \frac{1}{H(1)}. \tag{3.38}$$

Since $H(\eta)$ is increasing on $\eta \in (1, \infty)$, we have $\kappa_2 > \kappa_1$ (see Lemma 3.2). We also infer that for $1 - \frac{2}{d-1} < m < 1 - \frac{2}{d}$ fixed, where $d \geqslant 3$, for any κ in the range $\kappa \in (\kappa_1, \kappa_2)$, there exists a unique $\eta_\kappa > 1$ that solves (3.34b) – see Figure 1(b) for an illustration that corresponds to this case. This value of η_κ determines s_κ by (3.34a) and then λ_κ, uniquely. This determines uniquely a fully supported equilibrium ρ_κ in the form (2.8).

Case iii) $0 < m < 1 - \frac{2}{d-1}$. Similar to case ii), the integrals in (3.35) are convergent. Define again κ_2 by (3.38); however, for this range of m, $H(\eta)$ is decreasing, so $\kappa_2 < \kappa_1$. In this case, for $0 < m < 1 - \frac{2}{d-1}$ fixed, with $d \geqslant 3$, for any $\kappa \in (\kappa_2, \kappa_1)$, there exists a unique $\eta_\kappa > 1$ that solves (3.34b) – see Figure 1(c). Then, by (3.34a) one determines s_κ, and finally set $\lambda_\kappa = -\kappa s_\kappa \eta_\kappa$. Hence, a unique equilibrium ρ_κ in the form (2.8) is determined.

Remark 3.3. *For any $0 < m < 1$, a fully supported equilibrium ρ_κ gets born at $\kappa = \kappa_1$, from the uniform distribution ρ_{uni}. For $1 - 2/d < m < 1$ (case i), this equilibrium exists for all $\kappa > \kappa_1$, and no further bifurcation occurs. However, when $0 < m < 1 - 2/d$ (cases ii)* *and iii)), a transition occurs at* $\kappa = \kappa_2$*, where an equilibrium of the form* (2.10) *(a measure with a singular component) gets born from* ρ_κ*.*

Remark 3.4. *The explicit expression of* κ_2 *can be obtained as*

$$\kappa_2 = \frac{m\left(\frac{1}{m-1}+d\right)}{2^{1+(d-1)(m-1)}|\mathbb{S}^d|^{m-1}}\left(\frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{1}{m-1}+d\right)}{\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d+1}{2}\right)}\right)^{m-1}.$$

The derivation is provided in Appendix D. Note that $0 < m < 1-\frac{2}{d}$ *here, so* $\frac{1}{m-1}+d > \frac{d}{2} > 0$*. As* $m \nearrow 1-\frac{2}{d}$*,* $\kappa_2 \to +\infty$ *since* $\frac{1}{m-1}+\frac{d}{2} \searrow 0+$*, and this yields* $\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right) \to \infty$ *while* $m-1<0$*. This limiting behaviour is consistent with the fact that there is no second critical value* κ_2 *when* $1-\frac{2}{d} \leqslant m < 1$*.*

3.2. **Second critical value** $\kappa = \kappa_2$**.** We only consider here cases ii) and iii) from Section 3.1 and investigate the ranges $\kappa > \kappa_2$ and $\kappa < \kappa_2$, respectively (see (3.38)).

At $\kappa = \kappa_2$ we have $\eta_{\kappa_2} = 1$ and $-\lambda_{\kappa_2} = \kappa_2 s_{\kappa_2}$, with s_{κ_2} given by (see (3.34a))

$$s_{\kappa_2} = \frac{\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta}{\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta}. \tag{3.39}$$

Correspondingly, the equilibrium in the form (2.8) is given by

$$\rho_{\kappa_2}(x) = \left(\frac{m}{1-m}\right)^{\frac{1}{1-m}}(-\lambda_{\kappa_2})^{\frac{1}{m-1}}(1-\cos\theta_x)^{\frac{1}{m-1}}, \qquad \forall x \in \mathbb{S}^d. \tag{3.40}$$

Using the first equation in (2.9), we find

$$(-\lambda_{\kappa_2})^{\frac{1}{m-1}} = \frac{1}{dw_d}\left(\frac{m}{1-m}\right)^{\frac{1}{m-1}}\frac{1}{\int_0^\pi \left(1-\cos\theta\right)^{\frac{1}{m-1}}\sin^{d-1}\theta \,\mathrm{d}\theta}, \tag{3.41}$$

which used in (3.40) yields

$$\rho_{\kappa_2}(x) = \frac{\left(1-\cos\theta_x\right)^{\frac{1}{m-1}}}{dw_d\int_0^\pi \left(1-\cos\theta\right)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta}, \qquad \forall x \in \mathbb{S}^d.$$

Remarkably, this is the density (see (2.24)) of the regular component of the measure-valued equilibrium in the form (2.10); also compare (3.39) with (2.22) and note that (3.41) corresponds to (2.23) for $\alpha = 0$. We infer that at $\kappa = \kappa_2$, an equilibrium μ_α of the form (2.10) gets born from the fully supported equilibrium ρ_{κ_2}.

We investigate now the measure-valued equilibria in the form (2.10), for a fixed $\kappa > \kappa_2$ (case ii) or $\kappa < \kappa_2$ (case iii). Recall from Section 2 that the density ρ given by (2.24) does not depend on κ. To avoid confusing notation, we redenote the density from (2.24) by $\bar\rho$:

$$\bar\rho(x) = \frac{\left(1-\cos\theta_x\right)^{\frac{1}{m-1}}}{dw_d\int_0^\pi \left(1-\cos\theta\right)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta}, \qquad \forall x \in \mathbb{S}^d. \tag{3.42}$$

Here, θ_x represents the angle measured from a fixed (but arbitrary) direction $x_0 \in \mathbb{S}^d$, which represents the normalized centre of mass of $\bar{\rho}$:

$$x_0 = \frac{c_{\bar{\rho}}}{\|c_{\bar{\rho}}\|}. \tag{3.43}$$

We also denote

$$\bar{s} = \|c_{\bar{\rho}}\|, \tag{3.44}$$

and corresponding to (2.22) we have

$$\bar{s} = \frac{\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \mathrm{d}\theta}{\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta}. \tag{3.45}$$

With notation (3.42), the measure-valued equilibria (2.10) has the form

$$\mu_\alpha = \alpha\delta_{x_0} + (1-\alpha)\bar{\rho}\,\mathrm{d}S. \tag{3.46}$$

The only parameter that needs to be determined (in terms of κ) is α, the strength of the singular part. Using (2.23) in (2.19) – with $\bar{\rho}$ instead of ρ, along with notation (3.44), we arrive at the following equation for α:

$$\kappa(\alpha + (1-\alpha)\bar{s}) = (dw_d)^{1-m} \frac{m(1-\alpha)^{m-1}}{1-m} \left(\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \,\mathrm{d}\theta\right)^{1-m}. \tag{3.47}$$

By the considerations above, at $\kappa = \kappa_2$, a solution of (3.47) is $\alpha = 0$. Hence, (3.47) can be simplified into

$$\kappa(\bar{s} + \alpha(1-\bar{s})) = (1-\alpha)^{m-1}\kappa_2\bar{s}. \tag{3.48}$$

Denote the l.h.s. and the r.h.s. of (3.48) by

$$f_\kappa(\alpha) = \kappa(\bar{s} + \alpha(1-\bar{s})), \qquad \text{and} \qquad g(\alpha) = (1-\alpha)^{m-1}\kappa_2\bar{s}. \tag{3.49}$$

We are now concerned with finding the number of solutions $\alpha \in (0,1)$ to $f_\kappa(\alpha) = g(\alpha)$, for a given value of κ. Note that f_κ is a linear function of α, while g is an increasing function of α which becomes infinite as $\alpha \to 1$. We also note that the expression for $\bar{s}$ can be simplified using the Gamma function (see Appendix E) to

$$\bar{s} = \frac{1}{(1-m)d - 1}. \tag{3.50}$$

Since $0 < m < 1 - \frac{2}{d}$, it holds indeed that $0 < \bar{s} < 1$.

Lemma 3.3. *Assume $d \geqslant 3$, and consider the ranges of m identified in Section 3.1; note that for $d = 3$ only cases i) and ii) apply. Then,*

- *Case i) $1 - \frac{2}{d} < m < 1$. For any κ, equation (3.47) has no solutions in the interval $(0,1)$.*
- *Case ii) $1 - \frac{2}{d-1} < m < 1 - \frac{2}{d}$. There exists κ_2 introduced in (3.38) such that:*
  - *for $0 < \kappa < \kappa_2$, equation (3.47) has no solutions in the interval $(0,1)$.*
  - *for $\kappa > \kappa_2$, equation (3.47) has a unique solution $\alpha_\kappa \in (0,1)$.*
- *Case iii) $0 < m < 1 - \frac{2}{d-1}$. There exists a critical value $\kappa_3 \in (0, \kappa_2)$ such that:*
  - *for $0 < \kappa < \kappa_3$, equation (3.47) has no solutions in the interval $(0,1)$.*

– *for* $\kappa_3 < \kappa < \kappa_2$*, there exist two solutions* $0 < \tilde{\alpha}_\kappa < \alpha_\kappa < 1$ *of* (3.47)*. At* $\kappa = \kappa_3$*, the two solutions* $\tilde{\alpha}_\kappa$ *and* α_κ *coincide. Also, as* $\kappa \nearrow \kappa_2$ *we have* $\tilde{\alpha}_\kappa \searrow 0$.
– *for* $\kappa > \kappa_2$*,* (3.47) *has a unique solution* $\alpha_\kappa \in (0,1)$.

Proof. We consider the three cases separately.

• *Case i)* $1 - \frac{2}{d} < m < 1$. Let assume that there exist $\alpha \in (0,1)$ satisfying (3.47). From (3.50) and the given range of m, we get

$$\bar{s} > \frac{1}{\left(1 - \left(1 - \frac{2}{d}\right)\right) d - 1} = 1.$$

However, by the expression of $\bar{s}$ in (3.45), it holds that $\bar{s} < 1$. Hence, we get a contradiction and we conclude that there is no solution in the interval $(0,1)$.

• *Case ii)* $1 - \frac{2}{d-1} < m < 1 - \frac{2}{d}$. We note that both $f_\kappa(0)$ and $f'_\kappa(0)$ are increasing functions of κ. Therefore, if we show that for $\kappa = \kappa_2$, $\alpha = 0$ is the only solution of (3.48), then we can infer the uniqueness of the solution for $\kappa > \kappa_2$ – see Figure 2(a) for an illustration of this case. From the same property, we can also infer that (3.48) has no solutions for $0 < \kappa < \kappa_2$.

We know that $f_{\kappa_2}(0) = g(0)$, and we will show that $f'_{\kappa_2}(0) < g'(0)$. Given that f_{κ_2} is linear and g is increasing, this shows that $\alpha = 0$ is the only solution of (3.48) for $\kappa = \kappa_2$. Indeed, the slope of the tangent line of $g(\alpha)$ at $\alpha = 0$ can be calculated as

$$g'(0) = (1 - m)\kappa_2 \bar{s}.$$

Also, $f'_{\kappa_2}(0) = \kappa_2(1 - \bar{s})$. By a simple calculation we find that

$$\kappa_2(1 - \bar{s}) < (1 - m)\kappa_2 \bar{s},$$

as this is equivalent to

$$1 < (2 - m)\bar{s},$$

which after using (3.50), is equivalent to

$$m > 1 - \frac{2}{d - 1}.$$

The latter inequality is satisfied by the assumption on m.

Therefore, for any $\kappa > \kappa_2$ there exists a unique solution $0 < \alpha_\kappa < 1$ of $f_\kappa(\alpha) = g(\alpha)$ for this case. Similarly, we can also conclude that for any $0 < \kappa < \kappa_2$, there exists no solution of (3.48) in the interval $(0,1)$.

• *Case iii)* $0 < m < 1 - \frac{2}{d-1}$. From a similar argument (reverse the inequality sign in the calculation above), in this case we have

$$f'_{\kappa_2}(0) > g'(0).$$

Therefore, in addition to $\alpha = 0$, the equation $f_{\kappa_2}(\alpha) = g(\alpha)$ has an additional solution in the interval $(0,1)$ – see Figure 2(b) for an illustration.

Recall that both $f_\kappa(0)$ and $f'_\kappa(0)$ are increasing functions of κ. Hence, for $\kappa > \kappa_2$, there exists a unique solution in $(0,1)$ of (3.47). Also, by decreasing the values of κ down from

κ_2, we infer that there exists $\kappa_3 < \kappa_2$ such that $f_{\kappa_3}(\alpha)$ and $g(\alpha)$ are tangent to each other at some $\overline{\alpha} \in (0, 1)$. To find κ_3 and $\overline{\alpha}$ one needs to solve

$$\begin{cases} f_{\kappa_3}(\overline{\alpha}) = g(\overline{\alpha}), \\ f'_{\kappa_3}(\overline{\alpha}) = g'(\overline{\alpha}). \end{cases}$$

Using the expressions of f_κ and g, the system above becomes

$$\begin{cases} \kappa_3(\bar{s} + \overline{\alpha}(1 - \bar{s})) = (1 - \overline{\alpha})^{m-1}\kappa_2\bar{s}, \\ \kappa_3(1 - \bar{s}) = (1 - m)(1 - \overline{\alpha})^{m-2}\kappa_2\bar{s}, \end{cases}$$

and solving the system we find

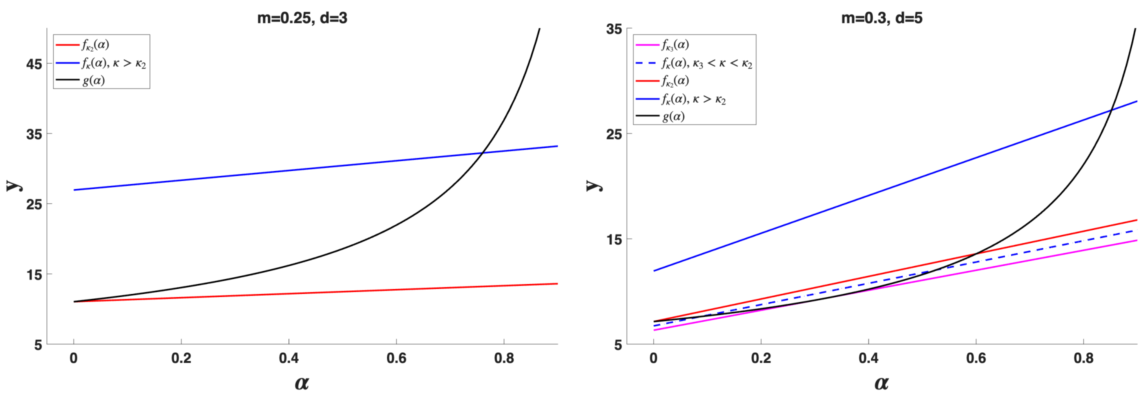
$$\overline{\alpha} = \frac{1 - 2\bar{s} + m\bar{s}}{(1 - \bar{s})(2 - m)},$$

and

$$\kappa_3 = \kappa_2 \frac{(1 - m)\bar{s}}{1 - \bar{s}}(1 - \overline{\alpha})^{m-2}, \tag{3.51}$$

with $\bar{s}$ given by (3.50).

For $\kappa_3 < \kappa < \kappa_2$, there exist two solutions $0 < \tilde{\alpha}_\kappa < \alpha_\kappa < 1$ of (3.47). At $\kappa = \kappa_3$, the two solutions $\tilde{\alpha}_\kappa$ and α_κ are equal to $\overline{\alpha}$. For $\kappa < \kappa_3$ there exist no solutions. □



(a) (b)

FIGURE 2. Plots of f_κ and g from (3.49). (a) Case $1 - \frac{2}{d-1} < m < 1 - \frac{2}{d}$: for any $\kappa > \kappa_2$, equation (3.47) has a unique solution $\alpha_\kappa \in (0, 1)$. (b) Case $0 < m < 1 - \frac{2}{d-1}$: for $\kappa_3 < \kappa < \kappa_2$, there exist two solutions $0 < \tilde{\alpha}_\kappa < \alpha_\kappa < 1$ of (3.47). At $\kappa = \kappa_3$, the two solutions $\tilde{\alpha}_\kappa$ and α_κ coincide. For $\kappa > \kappa_2$, (3.47) has a unique solution in the interval $(0, 1)$. The numerical simulations correspond to (a) $m = 0.25$ and $d = 3$, and (b) $m = 0.3$ and $d = 5$.

In each of the cases of Lemma 3.3, for every solution α_κ of (3.47) it corresponds an equilibrium μ_{α_κ} in the form (3.46), where the density $\bar{\rho}$ is given by (3.42).

The findings in this section can be put together in the following Proposition; see also Table 2 for a summary of these results.

Proposition 3.1 (Phase transitions and equilibria)**.** *Given a dimension $d \geqslant 1$, we distinguish three ranges of $0 < m < 1$: i) $1-\frac{2}{d} < m < 1$, ii) $1-\frac{2}{d-1} < m < 1-\frac{2}{d}$, and iii) $0 < m < 1-\frac{2}{d-1}$. Note that for $d=1$ and $d=2$, cases ii) and iii) do not apply, while for $d=3$ case iii) is not applicable. Then,*

a) In all three cases, at $\kappa = \kappa_1$ (see (2.25)*), an equilibrium fully supported on $\mathbb{S}^d$ bifurcates from the uniform distribution ρ_{uni}. This equilibrium, in the form* (2.8)*, is given by*

$$\rho_\kappa(x) = \left(\frac{m}{1-m}\right)^{\frac{1}{1-m}} \left(-\lambda_\kappa - \kappa s_\kappa \cos\theta_x\right)^{\frac{1}{m-1}}, \qquad \forall x \in \mathbb{S}^d, \tag{3.52}$$

where s_κ and λ_κ are uniquely determined by κ (see (3.33) *and* (3.34)*), as given by:*

$$s_\kappa = \frac{\int_0^\pi (\eta_\kappa - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \mathrm{d}\theta}{\int_0^\pi (\eta_\kappa - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta}, \tag{3.53}$$

$\lambda_\kappa = -\kappa s_\kappa \eta_\kappa$, with η_κ being the unique solution of $H(\eta_\kappa) = \kappa^{-1}$.

In case i), the equilibria ρ_κ exist for all $\kappa \in (\kappa_1, \infty)$. In case ii), they exist only for $\kappa \in (\kappa_1, \kappa_2)$, where $\kappa_2 > \kappa_1$, and in case iii) they exist for $\kappa \in (\kappa_2, \kappa_1)$. For both cases ii) and iii), κ_2 is given by (3.38).

b) In cases ii) and iii), at $\kappa = \kappa_2$ the equilibria (3.52) *transition from density-valued to measure-valued.*

- *case ii) $1-\frac{2}{d-1} < m < 1-\frac{2}{d}$. By Lemma 3.3, for any $\kappa > \kappa_2$, equation* (3.47) *has a unique solution $0 < \alpha_\kappa < 1$. Hence, for any $\kappa > \kappa_2$, there exists a unique equilibrium in the form* (3.46)*, given by*

$$\mu_{\alpha_\kappa} = \alpha_\kappa \delta_{x_0} + (1-\alpha_\kappa)\bar{\rho}\, \mathrm{d}S, \tag{3.54}$$

  where the density $\bar{\rho}$ (which does not depend on κ) is given by (3.42)*. Here, $x_0 \in \mathbb{S}^d$ is a fixed (arbitrary) unit vector; see also* (3.43).
- *case iii) $0 < m < 1-\frac{2}{d-1}$. In this case, there exists a third critical value $\kappa_3 < \kappa_2$ (see* (3.51) *and Lemma 3.3) such that:*
  - *at $\kappa = \kappa_3$ a pair of equilibria in the form* (2.10) *gets born. For any $\kappa_3 < \kappa < \kappa_2$, there exist two solutions $0 < \tilde{\alpha}_\kappa < \alpha_\kappa < 1$ of* (3.47)*. To each of the two values $\tilde{\alpha}_\kappa$ and α_κ, it corresponds a measure-valued equilibrium in the form* (3.54)*, with $\bar{\rho}$ given by* (3.42)*. At $\kappa = \kappa_3$, the two solutions $\tilde{\alpha}_\kappa$ and α_κ (and hence the corresponding equilibria) coincide.*
  - *as $\kappa \nearrow \kappa_2$ we have $\tilde{\alpha}_\kappa \searrow 0$, and its corresponding equilibrium $\mu_{\tilde{\alpha}_\kappa}$ changes at $\kappa = \kappa_2$ from measure-valued to an equilibrium density in the form* (3.52)*. On the other hand, μ_{α_κ} undergoes no transition at $\kappa = \kappa_2$ and retains the form* (3.54)*. As κ increases to infinity, μ_{α_κ} approaches δ_{x_0}.*

3.3. **Numerical illustrations.** We illustrate Proposition 3.1 with numerical results. For case i) we used $m = 0.5$ and $d = 2$. Figure 3(a) shows the bifurcation at κ_1 – for this choice of m and d we have $\kappa_1 \approx 5.3174$. Blue colour corresponds to the uniform distribution (with centre of mass at the origin), which is unstable for $\kappa > \kappa_1$ (Proposition 2.1). In red we plot $s_\kappa = \|c_{\rho_\kappa}\|$ for the fully supported equilibria (3.52), which for case i) exist for all $\kappa > \kappa_1$. In Figure 4(a) we plot the equilibria ρ_κ at several values of κ (at $\kappa = \kappa_1$, ρ_κ is the uniform

Case	Range of m	Equilibria
i)	$1-\frac{2}{d}<m<1$	ρ_{uni} $(\kappa>0)$ and ρ_κ $(\kappa>\kappa_1)$
ii)	$1-\frac{2}{d-1}<m<1-\frac{2}{d}$	ρ_{uni} $(\kappa>0)$, ρ_κ $(\kappa_1<\kappa<\kappa_2)$ and μ_{α_κ} $(\kappa>\kappa_2)$
iii)	$0<m<1-\frac{2}{d-1}$	ρ_{uni} $(\kappa>0)$, ρ_κ $(\kappa_2<\kappa<\kappa_1)$, $\mu_{\tilde{\alpha}_\kappa}$ $(\kappa_3<\kappa<\kappa_2)$ and μ_{α_κ} $(\kappa>\kappa_3)$

TABLE 2. The table shows the various equilibria established in Proposition 3.1, for the three ranges of m. In each case, the uniform distribution ρ_{uni} is an equilibrium for all $\kappa>0$, and a fully supported density ρ_κ bifurcates from ρ_{uni} at $\kappa=\kappa_1$. At $\kappa=\kappa_2$ (cases ii) and iii)), ρ_κ transitions to a measure-valued equilibrium; note that $\kappa_1<\kappa_2$ for case ii), while $\kappa_1>\kappa_2$ for case iii). In case iii), a pair of measure-valued equilibria gets born at κ_3: $\mu_{\tilde{\alpha}_\kappa}$ which changes at $\kappa=\kappa_2$ from measure-valued to a density, and μ_{α_κ} which undergoes no further transition and exists for all $\kappa>\kappa_3$.

distribution). As κ increases, ρ_k concentrates around $\theta=0$, behaviour which can also be inferred from Figure 3(a) since $\|c_{\rho_\kappa}\|$ approaches 1 as $\kappa\to\infty$.

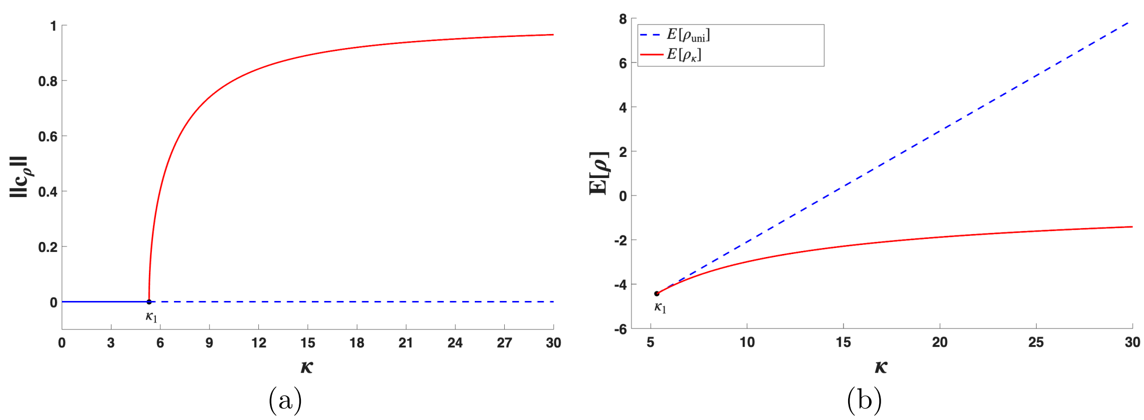
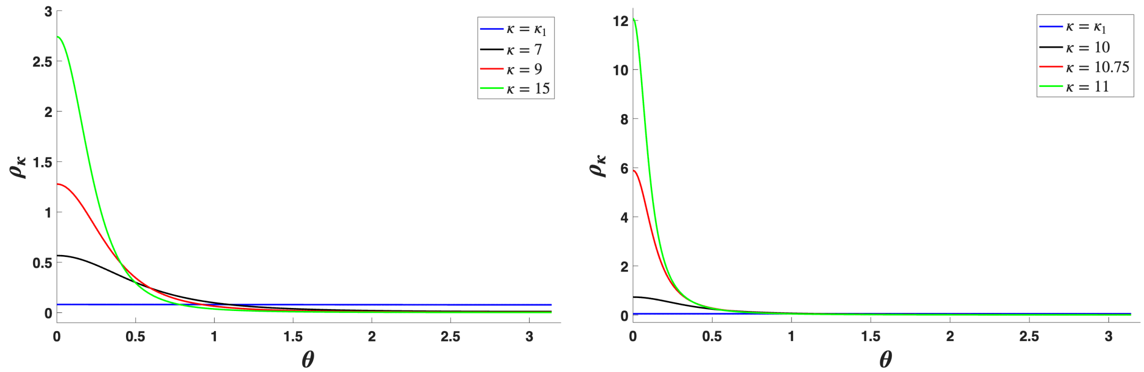


FIGURE 3. Case i) $1-2/d<m<1$. (a) Plot of the norm of the centre of mass of equilibria. b) Plot of the energies of equilibria for $\kappa>\kappa_1$. In both plots, blue corresponds to ρ_{uni} and red to ρ_κ – see Proposition 3.1 part a). At $\kappa=\kappa_1$, a fully supported equilibrium ρ_κ in the form (3.52) emerges from the uniform distribution, and then it exists for all $\kappa>\kappa_1$. The equilibrium ρ_κ is the global energy minimizer when $\kappa>\kappa_1$ – see Theorem 4.1 part a). The numerical simulations correspond to $m=0.5$ and $d=2$.



(a) (b)

FIGURE 4. Plot of equilibrium densities ρ_κ from (3.52). (a) $m = 0.5$, $d = 2$. These values correspond to case i) from Proposition 3.1. The equilibrium densities ρ_κ exist for all $\kappa > \kappa_1$. (b) $m = 0.25$, $d = 3$. These values correspond to case ii) from Proposition 3.1. The equilibrium densities ρ_κ exist for $\kappa_1 < \kappa < \kappa_2$ in this case (here $\kappa_2 \approx 12.4453$). For both plots, $\kappa = \kappa_1$ corresponds to the uniform distribution, and ρ_κ concentrates around $\theta = 0$ as κ increases.

For case ii) we used $m = 0.25$ and $d = 3$. Figure 5(a) illustrates the bifurcation at $\kappa_1 \approx 9.3648$ and the transition to measure-valued equilibria at $\kappa_2 \approx 12.4453$. Blue corresponds to the uniform distribution, the red line represents $\|c_{\rho_\kappa}\|$ ($\kappa_1 < \kappa < \kappa_2$) – see (3.52), and the black line corresponds to $\|c_{\mu_{\alpha_\kappa}}\|$ ($\kappa > \kappa_2$) – see (3.54) and (3.42). Figure 4(b) shows the equilibria ρ_κ at several values of $\kappa < \kappa_2$ (so before the equilibria become measure-valued), where $\kappa = \kappa_1$ corresponds to the uniform distribution. For $\kappa \geqslant \kappa_2$, the regular part $\bar{\rho}$ of the equilibrium μ_{α_κ} (see (3.42)) is infinite at $\theta = 0$, so we could not provide good illustrations for this range. As κ increases, $\alpha_\kappa \nearrow 1$ (see Figure 2(a)) and the equilibria μ_{α_κ} approach a delta Dirac.

Finally, for case iii) we used $m = 0.3$ and $d = 5$. Figure 6(a) shows the bifurcation at $\kappa_1 \approx 19.9199$, the transition to measure-valued equilibria at $\kappa_2 \approx 17.8623$, and the bifurcation at $\kappa_3 \approx 15.8088$, where two measure valued-equilibria emerge. Blue corresponds to the uniform distribution, and the solid black line represents $\|c_{\mu_{\alpha_\kappa}}\|$ (which exists for all $\kappa > \kappa_3$). Also, the dashed black line represents $\|c_{\mu_{\tilde{\alpha}_\kappa}}\|$ for $\kappa_3 < \kappa < \kappa_2$ (see (3.54) and (3.42)), and the dashed red corresponds to $\|c_{\rho_\kappa}\|$ for $\kappa_2 < \kappa < \kappa_1$ (see (3.52)). At $\kappa = \kappa_2$ the equilibrium $\mu_{\tilde{\alpha}_\kappa}$ changes from measure-valued to an equilibrium density ρ_κ in the form (3.52); this transition is indicated by a black diamond. At $\kappa = \kappa_1$, ρ_κ merges with the uniform distribution and vanishes. We do not provide separate illustrations of ρ_κ here, as the qualitative behaviour is similar to Figure 4(b), except that ρ_κ now concentrates as κ decreases from κ_1 to κ_2. Finally, as κ increases to infinity, the equilibrium μ_{α_κ} on the upper branch approaches a delta Dirac (as $\alpha_\kappa \nearrow 1$).

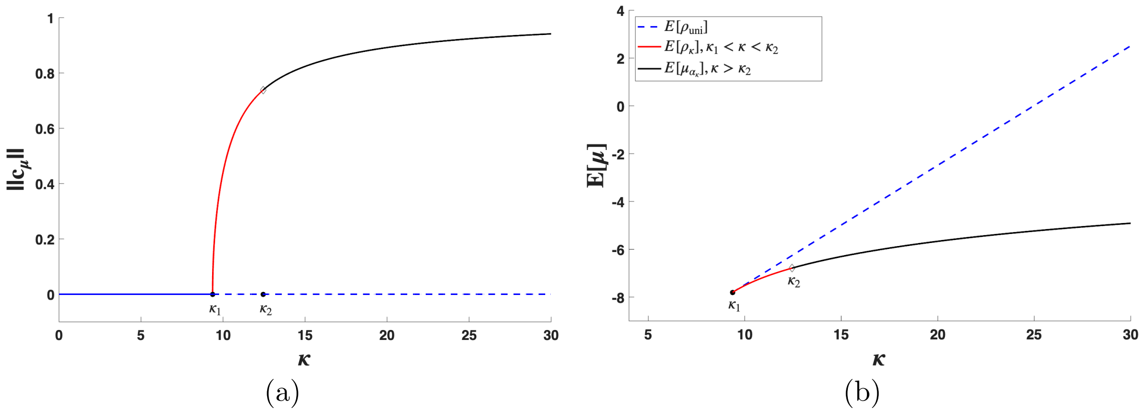


FIGURE 5. Case ii) $1-2/(d-1) < m < 1-2/d$. (a) Plot of the norm of the centre of mass of equilibria. (b) Plot of the energies of equilibria for $\kappa > \kappa_1$. In both plots, blue corresponds to ρ_{uni}, red to ρ_κ, and black to μ_{α_κ} – see Proposition 3.1. At $\kappa = \kappa_1$, a fully supported equilibrium ρ_κ in the form (3.52) emerges from the uniform distribution. At $\kappa = \kappa_2$, ρ_κ changes to a measure-valued equilibrium μ_{α_κ} – see (3.54) and (3.42); this transition is indicated by a black diamond. The global minimizer when $\kappa_1 < \kappa < \kappa_2$ is ρ_κ, and when $\kappa > \kappa_2$, the ground state is μ_{α_κ} – see Theorem 4.1 part a). The numerical simulations correspond to $m = 0.25$, $d = 3$.

4. Energy minimizers

In this section we investigate which of the equilibria identified in Proposition 3.1 are global energy minimizers. The result is given by the following theorem.

Theorem 4.1 (Global energy minimizers)**.** *Consider the uniform distribution together with the equilibria established in Proposition 3.1, for a fixed* $d \geqslant 1$*. Note that we examined three ranges of* $0 < m < 1$ *there, where for* $d = 1, 2$ *and* 3 *only some of the ranges are applicable. Then,*

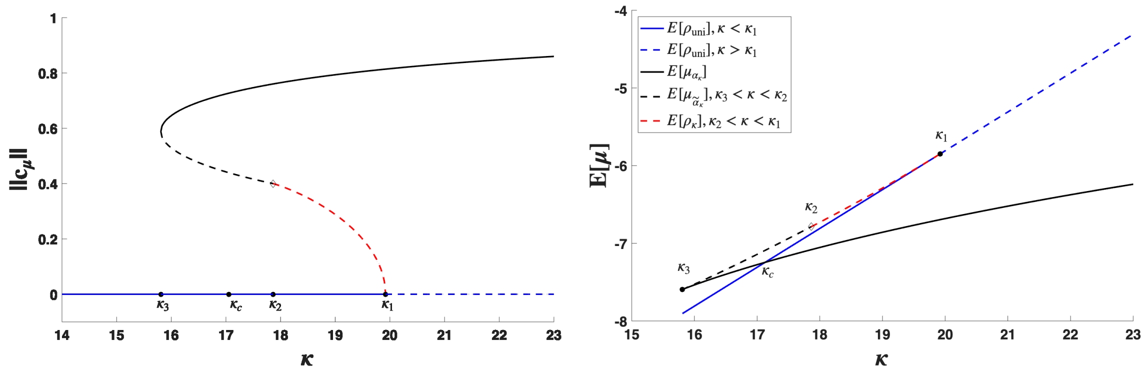
a) In cases i) and ii), the uniform distribution ρ_{uni} *is the global energy minimizer on* $\mathcal{P}(\mathbb{S}^d)$ *for all* $\kappa < \kappa_1$*. For* $\kappa > \kappa_1$*, we have*

- *case i)* $1 - \frac{2}{d} < m < 1$*. The global minimizer for any* $\kappa > \kappa_1$ *is given by the equilibrium* ρ_κ *in* (3.52),
- *case ii)* $1 - \frac{2}{d-1} < m < 1 - \frac{2}{d}$*. The global minimizer for* $\kappa_1 < \kappa < \kappa_2$ *is given by* ρ_κ *in* (3.52)*, while for* $\kappa > \kappa_2$*, the ground state is the measure-valued equilibrium* μ_{α_κ} *from* (3.54).

Moreover, in both cases the energy differences $E[\rho_{uni}] - E[\rho_\kappa]$ *and* $E[\rho_{uni}] - E[\mu_{\alpha_\kappa}]$ *increase with* κ *for* $\kappa > \kappa_1$.

b) In case iii) $1 - \frac{2}{d-1} < m < 1 - \frac{2}{d}$*, there exists* $\kappa_3 < \kappa_c < \kappa_1$ *such that the global energy minimizer on* $\mathcal{P}(\mathbb{S}^d)$ *is*

- *the uniform distribution* ρ_{uni} *when* $\kappa < \kappa_c$,
- *the measure-valued equilibrium* μ_{α_κ} *in the form* (3.54)*, as identified in Proposition 3.1, when* $\kappa > \kappa_c$.



(a) (b)

FIGURE 6. Case iii) $0 < m < 1-2/(d-1)$. (a) Plot of the norm of the centre of mass of equilibria. (b) Plot of the energies of equilibria. In both plots, blue corresponds to ρ_{uni} and the solid black to the measure-valued equilibrium μ_{α_κ} (which exists for all $\kappa > \kappa_3$). Also, the dashed black corresponds to $\mu_{\tilde{\alpha}_\kappa}$ (for $\kappa_3 < \kappa < \kappa_2$) and the dashed red corresponds to ρ_κ (for $\kappa_2 < \kappa < \kappa_1$) – see Proposition 3.1. At $\kappa = \kappa_3$, a pair of measure-valued equilibria in the form (3.54) emerges. At $\kappa = \kappa_2$, the measure-valued equilibrium $\mu_{\tilde{\alpha}_\kappa}$ on the lower branch changes to a fully supported density-valued equilibrium ρ_κ in the form (3.52); this transition is indicated by a black diamond. At $\kappa = \kappa_1$, the equilibrium ρ_κ merges with the uniform distribution and vanishes. As $\kappa \to \infty$, the equilibria μ_{α_κ} on the upper branch approaches a delta Dirac. A fourth critical value $\kappa_c \in (\kappa_1, \kappa_3)$ exists in this case. The global energy minimizer is ρ_{uni} for $\kappa < \kappa_c$ and μ_{α_κ} for $\kappa > \kappa_c$ – see Theorem 4.1 part b). The numerical simulations correspond to $m = 0.3$, $d = 5$.

Moreover, the energy difference $E[\rho_{uni}] - E[\mu_{\alpha_\kappa}]$ increases with κ for $\kappa > \kappa_3$.

Proof. We will compare the energies of the various equilibria that exist in each case, for various ranges of κ.

Step 1: Compare $E[\rho_{uni}]$ with $E[\rho_\kappa]$. This calculation applies to case i) when $\kappa > \kappa_1$, to case ii) when $\kappa_1 < \kappa < \kappa_2$, and to case iii) when $\kappa_2 < \kappa < \kappa_1$.

By (2.3) we write

$$E[\rho_{\text{uni}}] - E[\rho_\kappa] = \frac{1}{m-1}\int_{\mathbb{S}^d} \rho_{\text{uni}}^m(x)\mathrm{d}S - \frac{1}{m-1}\int_{\mathbb{S}^d} \rho_\kappa(x)^m \mathrm{d}S(x) + \frac{\kappa}{2}\|c_{\rho_\kappa}\|^2. \tag{4.55}$$

The first term in the r.h.s. above is a constant, and it does not change with κ. We will investigate how the other two terms change with κ.

Using (3.34) and (3.52), we compute
(4.56)

$$
\begin{aligned}
\frac{\kappa}{2}\|c_{\rho_\kappa}\|^2 - \frac{1}{m-1}\int_{\mathbb{S}^d}\rho_\kappa^m(x)\mathrm{d}S &= \frac{m}{2(1-m)(dw_d)^{m-1}}\frac{\int_0^\pi(\eta_\kappa-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta\mathrm{d}\theta}{\left(\int_0^\pi(\eta_\kappa-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\right)^m}\\
&\quad - \frac{1}{(m-1)(dw_d)^{m-1}}\frac{\int_0^\pi(\eta_\kappa-\cos\theta)^{\frac{m}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta}{\left(\int_0^\pi(\eta_\kappa-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\right)^m}\\
&:= g_1(\eta_\kappa)g_2(\eta_\kappa),
\end{aligned}
$$

where

$$
\begin{aligned}
g_1(\eta) &= m\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta\mathrm{d}\theta + 2\int_0^\pi(\eta-\cos\theta)^{\frac{m}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta,\\
g_2(\eta) &= \frac{1}{2(1-m)(dw_d)^{m-1}}\frac{1}{\left(\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\right)^m}.
\end{aligned}
$$

Calculate

$$
\begin{aligned}
g_1'(\eta) &= \frac{m}{m-1}\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\cos\theta\mathrm{d}\theta + \frac{2m}{m-1}\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\\
&= \frac{m}{m-1}\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\cos\theta\mathrm{d}\theta\\
&\quad + \frac{2m}{m-1}\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}(\eta-\cos\theta)\sin^{d-1}\theta\mathrm{d}\theta\\
&= \frac{2m\eta}{m-1}\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\mathrm{d}\theta - \frac{m}{m-1}\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\cos\theta\mathrm{d}\theta,
\end{aligned}
$$

and

$$
g_2'(\eta) = \frac{m}{2(1-m)^2(dw_d)^{m-1}}\frac{\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\mathrm{d}\theta}{\left(\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\right)^{m+1}}.
$$

Then,

$$
\begin{aligned}
&(g_1(\eta)g_2(\eta))' = g_1'(\eta)g_2(\eta) + g_1(\eta)g_2'(\eta)\\
&\quad= \frac{\frac{m}{1-m}\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\mathrm{d}\theta}{2(1-m)(dwd)^{m-1}\left(\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\right)^m}\times\\
&\qquad\Bigg(-2\eta + \frac{\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\cos\theta\mathrm{d}\theta}{\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\mathrm{d}\theta}\\
&\qquad\quad+\frac{m\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta\mathrm{d}\theta + 2\int_0^\pi(\eta-\cos\theta)^{\frac{m}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta}{\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta}\Bigg).
\end{aligned}
$$

Now write

$$\int_0^\pi (\eta-\cos\theta)^{\frac{m}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta = \int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}(\eta-\cos\theta)\sin^{d-1}\theta \mathrm{d}\theta$$
$$= \eta\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta - \int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta,$$

to simplify

(4.57)

$$(g_1(\eta)g_2(\eta))' = \frac{\frac{m}{1-m}\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta \mathrm{d}\theta}{2(1-m)(dwd)^{m-1}\left(\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta\right)^m}\times$$
$$\left(\frac{\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta}{\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta \mathrm{d}\theta} + (m-2)\frac{\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta}{\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta}\right).$$

By a direct calculation using the expression of $H(\eta)$ in (3.35), we compute

(4.58)

$$\frac{H'(\eta)}{H(\eta)} = \frac{1}{m-1}\frac{\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta}{\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta} + \frac{m-2}{m-1}\frac{\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta \mathrm{d}\theta}{\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta}.$$

Then, by combining (4.57) and (4.58), we write

$$(g_1(\eta)g_2(\eta))' = -(1-m)h(\eta)\frac{H'(\eta)}{H(\eta)}, \tag{4.59}$$

where

$$h(\eta) := \frac{m}{2(1-m)^2(dw_d)^{m-1}}\frac{\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta}{\left(\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta\right)^m}. \tag{4.60}$$

Note that $h(\eta) > 0$. To show this, we only need to investigate the sign of $\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta$. Since $\frac{1}{m-1} < 0$, we find $(\eta-\cos\theta)^{\frac{1}{m-1}} - (\eta+\cos\theta)^{\frac{1}{m-1}} > 0$ for all $0 \leqslant \theta < \frac{\pi}{2}$ and $\eta > 1$. Therefore, we have

$$\int_0^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta$$
$$= \int_0^{\pi/2} (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta + \int_{\pi/2}^\pi (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta$$
$$= \int_0^{\pi/2} (\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta - \int_0^{\pi/2} (\eta+\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta$$
$$= \int_0^{\pi/2} \left((\eta-\cos\theta)^{\frac{1}{m-1}} - (\eta+\cos\theta)^{\frac{1}{m-1}}\right)\sin^{d-1}\theta\cos\theta \mathrm{d}\theta > 0,$$

where for the second equal sign we made a change of variable $\tilde\theta = \pi - \theta$.

Since $h(\eta) > 0$ and $H(\eta) > 0$, the sign of $(g_1(\eta)g_2(\eta))'$ is opposite to the sign of $H'(\eta)$. For cases i) and ii), $H(\eta)$ is increasing with $\eta > 1$, while for case iii), $H(\eta)$ is decreasing

– see Lemma 3.1. Consequently, $g_1(\eta)g_2(\eta)$ is decreasing with η in cases i) and ii), and increasing with η in case iii).

From (4.55) and (4.56), we have

$$E[\rho_{\rm uni}] - E[\rho_\kappa] = \text{const.} + g_1(\eta_\kappa)g_2(\eta_\kappa). \tag{4.61}$$

In cases i) and ii), η_κ decreases as κ increases from κ_1 (since $H(\eta)$ is increasing). Therefore, by the considerations above, $g_1(\eta_\kappa)g_2(\eta_\kappa)$ (and hence the energy difference $E[\rho_{\rm uni}]-E[\rho_\kappa]$) increases with κ. Note that since ρ_κ forms at $\kappa=\kappa_1$, the energy difference starts from value 0. We also point out that for $\kappa<\kappa_1$ in cases i) and ii), the uniform distribution is the only critical point, and therefore the global minimizer. We have now partially shown part a) of the proposition: case i) is complete, and case ii) is shown for $\kappa_1<\kappa<\kappa_2$. For a numerical illustration we refer to Figures 3(b) and 5(b).

In case iii), η_κ increases as κ increases from κ_2 to κ_1 (since $H(\eta)$ is decreasing). Then, by the monotonicity of $g_1(\eta)g_2(\eta)$, $g_1(\eta_\kappa)g_2(\eta_\kappa)$ (and hence the energy difference $E[\rho_{\rm uni}]-E[\rho_\kappa]$) increases as κ ranges from κ_2 to κ_1. Since at $\kappa=\kappa_1$, ρ_κ coincides with $\rho_{\rm uni}$, we conclude that $E[\rho_{\rm uni}]-E[\rho_\kappa]$ increases from a negative value at $\kappa=\kappa_2$ to value 0 at $\kappa=\kappa_1$; see Figure 6(b) for a numerical illustration.

Step 2: Compare $E[\rho_{uni}]$ with $E[\mu_{\alpha_\kappa}]$ and $E[\mu_{\tilde\alpha_\kappa}]$. This calculation applies to case ii) when $\kappa>\kappa_2$, and to case iii). Note that for case iii), there exist two measure-valued solutions: μ_{α_κ} (for $\kappa>\kappa_3$) and $\mu_{\tilde\alpha_\kappa}$ (for $\kappa_3<\kappa<\kappa_2$), where $0<\tilde\alpha_\kappa<\alpha_\kappa<1$. Recall that both $\mu_{\tilde\alpha_\kappa}$ and μ_{α_κ} are in the form (3.54), where the density $\bar\rho$ does not depend on κ – see (3.42). Also recall notation (3.44).

By (2.12), we have

$$\begin{aligned}E[\rho_{\rm uni}] - E[\mu_{\alpha_\kappa}] &= \frac{1}{m-1}\int_{\mathbb{S}^d}\rho_{\rm uni}^m(x)\mathrm{d}S - \frac{1}{m-1}\int_{\mathbb{S}^d}(1-\alpha_\kappa)^m\bar\rho(x)^m\mathrm{d}S(x) + \frac{\kappa}{2}\|c_{\mu_{\alpha_\kappa}}\|^2\\ &= \frac{1}{m-1}\int_{\mathbb{S}^d}\rho_{\rm uni}^m(x)\mathrm{d}S - \frac{1}{m-1}\int_{\mathbb{S}^d}(1-\alpha_\kappa)^m\bar\rho(x)^m\mathrm{d}S(x)\\ &\quad+\frac{\kappa}{2}\left(\alpha_\kappa+(1-\alpha_\kappa)\bar s\right)^2.\end{aligned} \tag{4.62}$$

Take a derivative with κ in (4.62) to get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\kappa}\left(E[\rho_{\rm uni}]-E[\mu_{\alpha_\kappa}]\right) &= \frac{m}{m-1}\left(\int_{\mathbb{S}^d}(1-\alpha_\kappa)^{m-1}\bar\rho(x)^m\mathrm{d}S(x)\right)\frac{\mathrm{d}\alpha_\kappa}{\mathrm{d}\kappa}\\ &\quad+\frac{1}{2}\left(\alpha_\kappa+(1-\alpha_\kappa)\bar s\right)^2+\kappa(1-\bar s)\left(\alpha_\kappa+(1-\alpha_\kappa)\bar s\right)\frac{\mathrm{d}\alpha_\kappa}{\mathrm{d}\kappa}.\end{aligned} \tag{4.63}$$

We will show that the terms containing $\frac{\mathrm{d}\alpha_\kappa}{\mathrm{d}\kappa}$ cancel each other. Indeed, using (3.42) we have

$$\frac{m}{m-1}\int_{\mathbb{S}^d}(1-\alpha_\kappa)^{m-1}\bar\rho(x)^m\mathrm{d}S(x) = \frac{m}{m-1}(dw_d)^{1-m}(1-\alpha_\kappa)^{m-1}\frac{\int_0^\pi(1-\cos\theta)^{\frac{m}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta}{\left(\int_0^\pi(1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\right)^m}. \tag{4.64}$$

By combining (2.19) and (2.23) – use $\bar{\rho}$ instead of ρ and α_κ instead of α there, we find (4.65)

$$\begin{aligned}\kappa\left(\alpha_\kappa+(1-\alpha_\kappa)\bar{s}\right) &= -\frac{\lambda}{1-\alpha_\kappa} \\ &= \frac{m}{1-m}(dw_d)^{1-m}(1-\alpha_\kappa)^{m-1}\frac{1}{\left(\int_0^\pi(1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\right)^{m-1}},\end{aligned}$$

which used in (4.64) leads to

$$\frac{m}{m-1}\int_{\mathbb{S}^d}(1-\alpha_\kappa)^{m-1}\bar{\rho}(x)^m\mathrm{d}S(x) = -\kappa\left(\alpha_\kappa+(1-\alpha_\kappa)\bar{s}\right)\cdot\frac{\int_0^\pi(1-\cos\theta)^{\frac{m}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta}{\int_0^\pi(1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta}.$$

Now write

$$\int_0^\pi(1-\cos\theta)^{\frac{m}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta = \int_0^\pi(1-\cos\theta)^{\frac{1}{m-1}}(1-\cos\theta)\sin^{d-1}\theta\mathrm{d}\theta,$$

and then by (3.45) we get

$$\begin{aligned}\frac{\int_0^\pi(1-\cos\theta)^{\frac{m}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta}{\int_0^\pi(1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta} &= 1-\frac{\int_0^\pi(1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta\mathrm{d}\theta}{\int_0^\pi(1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta} \\ &= 1-\bar{s}.\end{aligned} \tag{4.66}$$

By using (4.65) and (4.66) in (4.64), we then find

$$\frac{m}{m-1}\int_{\mathbb{S}^d}(1-\alpha_\kappa)^{m-1}\bar{\rho}(x)^m\mathrm{d}S(x) = -\kappa(1-\bar{s})\left(\alpha_\kappa+(1-\alpha_\kappa)\bar{s}\right).$$

Return now to the r.h.s of (4.63) and note that the terms containing $\frac{\mathrm{d}\alpha_\kappa}{\mathrm{d}\kappa}$ cancel each other. Hence, we get

$$\frac{\mathrm{d}}{\mathrm{d}\kappa}\left(E[\rho_{\mathrm{uni}}]-E[\mu_{\alpha_\kappa}]\right) = \frac{1}{2}\left(\alpha_\kappa+(1-\alpha_\kappa)\bar{s}\right)^2, \tag{4.67}$$

which is positive for all $0\leqslant\alpha_\kappa\leqslant 1$.

We conclude that $E[\rho_{\mathrm{uni}}]-E[\mu_{\alpha_\kappa}]$ increases with κ. Together with the previous considerations, this completes the conclusion of the theorem in case ii) – See Figure 5(b) for an illustration, and hence, part (a) of the theorem is now shown.

Similar to (4.67) - just replace α_κ with $\tilde{\alpha}_\kappa$ in the derivation above, we find

$$\frac{\mathrm{d}}{\mathrm{d}\kappa}\left(E[\rho_{\mathrm{uni}}]-E[\mu_{\tilde{\alpha}_\kappa}]\right) = \frac{1}{2}\left(\tilde{\alpha}_\kappa+(1-\tilde{\alpha}_\kappa)\bar{s}\right)^2,$$

which is also positive for all $0\leqslant\tilde{\alpha}_\kappa\leqslant 1$. We infer that the energy difference $E[\rho_{\mathrm{uni}}]-E[\mu_{\tilde{\alpha}_\kappa}]$ increases with κ, for $\kappa_3<\kappa<\kappa_2$. Note that at $\kappa=\kappa_2$, $\mu_{\tilde{\alpha}_\kappa}$ coincides with ρ_κ, and we know from the previous calculations that $E[\rho_{\mathrm{uni}}]-E[\rho_\kappa]<0$ at $\kappa=\kappa_2$. Hence, $E[\rho_{\mathrm{uni}}]-E[\mu_{\tilde{\alpha}_\kappa}]$ increases from a negative value at $\kappa=\kappa_3$, and for all $\kappa_3<\kappa<\kappa_2$ we have $E[\rho_{\mathrm{uni}}]<E[\mu_{\tilde{\alpha}_\kappa}]$. Also see Figure 6(b) for a numerical illustration.

Regarding μ_{α_κ}, first note that it coincides with $\mu_{\tilde{\alpha}_\kappa}$ at $\kappa=\kappa_3$, and by the above, ρ_{uni} is more energetically favourable at κ_3. Hence, $E[\rho_{\mathrm{uni}}]-E[\mu_{\alpha_\kappa}]$ increases from a negative value at $\kappa=\kappa_3$. By (4.67), the rate of change of $E[\rho_{\mathrm{uni}}]-E[\mu_{\alpha_\kappa}]$ is strictly positive, so there exists a $\kappa_c > \kappa_3$ (a fourth critical value of κ) where $E[\rho_{\text{uni}}] - E[\mu_{\alpha_\kappa}] = 0$, and past $\kappa > \kappa_c$, we have $E[\mu_{\alpha_\kappa}] < E[\rho_{\text{uni}}]$. To conclude part (b) and hence the proof, it remains to compare the energies of the two measure-valued solutions $\mu_{\tilde{\alpha}_\kappa}$ and μ_{α_κ} (for $\kappa_3 < \kappa < \kappa_2$) and the energies of ρ_κ and μ_{α_κ} (for $\kappa_2 < \kappa < \kappa_1$).

Step 3: Compare $E[\mu_{\tilde{\alpha}_\kappa}]$ and $E[\mu_{\alpha_\kappa}]$. This part concerns case iii) only, with $\kappa_3 < \kappa < \kappa_2$. By (2.14) and (3.54) we have

$$\begin{aligned} E[\mu_{\tilde{\alpha}_\kappa}] - E[\mu_{\alpha_\kappa}] &= \frac{1}{m-1}\int_{\mathbb{S}^d} (1-\tilde{\alpha}_\kappa)^m \bar{\rho}(x)^m \mathrm{d}S(x) - \frac{\kappa}{2}\left(\tilde{\alpha}_\kappa + (1-\tilde{\alpha}_\kappa)\bar{s}\right)^2 \\ &\quad - \frac{1}{m-1}\int_{\mathbb{S}^d} (1-\alpha_\kappa)^m \bar{\rho}(x)^m \mathrm{d}S(x) + \frac{\kappa}{2}\left(\alpha_\kappa + (1-\alpha_\kappa)\bar{s}\right)^2 . \end{aligned}$$

From a calculation similar to that leading from (4.63) to (4.67), we get

$$\frac{\mathrm{d}}{\mathrm{d}\kappa}\left(E[\mu_{\tilde{\alpha}_\kappa}] - E[\mu_{\alpha_\kappa}]\right) = \frac{1}{2}\left(\alpha_\kappa + (1-\alpha_\kappa)\bar{s}\right)^2 - \frac{1}{2}\left(\tilde{\alpha}_\kappa + (1-\tilde{\alpha}_\kappa)\bar{s}\right)^2 .$$

Since $\tilde{\alpha}_\kappa < \alpha_\kappa$, the r.h.s. above is positive, and we infer that $E[\mu_{\tilde{\alpha}_\kappa}] - E[\mu_{\alpha_\kappa}]$ increases with κ. For the range $\kappa_3 < \kappa < \kappa_2$ (where $\mu_{\tilde{\alpha}_\kappa}$ exists) we then have $E[\mu_{\tilde{\alpha}_\kappa}] > E[\mu_{\alpha_\kappa}]$.

Step 4: Compare $E[\rho_\kappa]$ and $E[\mu_{\alpha_\kappa}]$. This calculations applies to case iii), for $\kappa_2 < \kappa < \kappa_1$. Using (4.61) and (4.67), we get

$$\frac{\mathrm{d}}{\mathrm{d}\kappa}\left(E[\rho_\kappa] - E[\mu_{\alpha_\kappa}]\right) = \frac{1}{2}\left(\alpha_\kappa + (1-\alpha_\kappa)\bar{s}\right)^2 - \frac{\mathrm{d}}{\mathrm{d}\kappa}(g_1(\eta_\kappa)g_2(\eta_\kappa)). \tag{4.68}$$

We will show that the r.h.s. above is positive.

By chain rule we have

$$\frac{\mathrm{d}}{\mathrm{d}\kappa}(g_1(\eta_\kappa)g_2(\eta_\kappa)) = \frac{\mathrm{d}}{\mathrm{d}\eta_\kappa}(g_1(\eta_\kappa)g_2(\eta_\kappa))\frac{\mathrm{d}\eta_\kappa}{\mathrm{d}\kappa}. \tag{4.69}$$

Now differentiate

$$H(\eta_\kappa)^{-1} = \kappa,$$

with respect to κ, to get

$$-\frac{H'(\eta_\kappa)}{H^2(\eta_\kappa)}\frac{\mathrm{d}\eta_\kappa}{\mathrm{d}\kappa} = 1. \tag{4.70}$$

Then, using (4.69) together with (4.59) and (4.70), we find

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\kappa}(g_1(\eta_\kappa)g_2(\eta_\kappa)) &= -(1-m)h(\eta_\kappa)\frac{H'(\eta_\kappa)}{H^2(\eta_\kappa)}\left(-\frac{H^2(\eta_\kappa)}{H'(\eta_\kappa)}\right) \\ &= \frac{1}{2}\left(\frac{\int_0^\pi (\eta_\kappa - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta\cos\theta\mathrm{d}\theta}{\int_0^\pi (\eta_\kappa - \cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta\mathrm{d}\theta}\right)^2, \end{aligned}$$

where for the second equal sign we used the expressions of $h(\eta)$ and $H(\eta)$ from (4.60) and (3.35).

From (3.53) we find from the above that

$$\frac{\mathrm{d}}{\mathrm{d}\kappa}(g_1(\eta_\kappa)g_2(\eta_\kappa)) = \frac{1}{2}s_\kappa^2. \tag{4.71}$$

Here, η_κ ranges from 1 (for $\kappa = \kappa_2$) to ∞ (for $\kappa = \kappa_1$). By using (4.71) in (4.68), we get

$$\frac{\mathrm{d}}{\mathrm{d}\kappa}\left(E[\rho_\kappa] - E[\mu_{\alpha_\kappa}]\right) = \frac{1}{2}\left(\alpha_\kappa + (1-\alpha_\kappa)\bar{s}\right)^2 - \frac{1}{2}s_\kappa^2. \tag{4.72}$$

Note that $\bar{s} = s_{\kappa_2}$ (see (3.39) and (3.45)), as $\eta_{\kappa_2} = 1$. Now, since $\alpha_\kappa > 0$ we have

$$\alpha_\kappa + (1-\alpha_\kappa)\bar{s} > \bar{s},$$

and to show that the r.h.s. of (4.72) is positive, it is enough to show that s_κ decreases with increasing κ (or equivalently, with increasing η_κ), as this implies $\bar{s} > s_\kappa$, for all $\kappa_2 < \kappa < \kappa_1$. This behaviour was in fact observed numerically – see the red dashed line in Figure 6(a).

We can show that s_κ is a decreasing function of η_κ by using the expression of H from (3.35), and express s_κ in terms of $H(\eta_\kappa)$ as

$$s_\kappa = \left(\frac{m}{(1-m)(dw_d)^{m-1}}H(\eta_\kappa)\right)\left(\int_0^\pi (\eta_\kappa - \cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta\right)^{1-m}.$$

From Lemma 3.1, we know that H is a decreasing function for $0 < m < 1 - \frac{2}{d-1}$. Since $\frac{1}{m-1} < 0$ and $1-m > 0$, we also infer that $\left(\int_0^\pi (\eta_\kappa - \cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta\right)^{1-m}$ is a decreasing function of η_κ. Therefore, as a product of two positive decreasing functions, s_κ is also a decreasing function.

We deduce that the r.h.s. of (4.72) is positive for $\kappa_2 < \kappa < \kappa_1$. We have $E[\rho_\kappa] - E[\mu_{\alpha_\kappa}] > 0$ at $\kappa = \kappa_2$ (as ρ_κ coincides with $\mu_{\tilde{\alpha}_\kappa}$ there, and use Step 3), and from there on, the energy difference will increase to a larger positive value at $\kappa = \kappa_1$. Since ρ_κ coincides with ρ_{uni} at $\kappa = \kappa_1$, we find that $E[\rho_{\text{uni}}] > E[\mu_{\alpha_\kappa}]$ at κ_1. By Step 2, $E[\rho_{\text{uni}}] < E[\mu_{\alpha_\kappa}]$ at $\kappa = \kappa_3$, which implies that the fourth critical value κ_c is between κ_3 and κ_1. By the considerations in Steps 2-4, we now conclude part b) of the proof. □

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Appendix A. Proof of Lemma 2.1

Assume that μ in the form (2.4) is a critical point of the energy $E[\mu]$, where $\alpha > 0$ and μ_s is not a Dirac delta measure concentrated at one point. By (2.3) and (2.4), we write

$$E[\mu] = \frac{1}{m-1}\int_{\mathbb{S}^d}(1-\alpha)^m\rho(x)^m\mathrm{d}S(x) - \frac{\kappa}{2}\|\alpha c_{\mu_s} + (1-\alpha)c_\rho\|^2 + \frac{\kappa}{2}, \tag{A.73}$$

where

$$c_{\mu_s} = \int_{\mathbb{S}^d} x\mathrm{d}\mu_s(x), \qquad \text{and} \qquad c_\rho = \int_{\mathbb{S}^d} x\rho(x)\mathrm{d}S(x).$$

As we can see from (A.73), c_{μ_s} is the only term that depends on the singular measure μ_s. To show that μ cannot be a ground state, we will provide a change of μ_s which decreases the total energy, i.e., increases $\|\alpha c_{\mu_s} + (1-\alpha)c_\rho\|$.

First, if $\|c_\rho\| \neq 0$ and the directions of c_ρ and c_{μ_s} are not aligned, then a rotation that aligns the two directions decreases the energy. Indeed, assume c_ρ and c_{μ_s} are not parallel.

Denote by $\tilde{\mu}_s$ the singular measure obtained by rotating μ_s so that c_ρ and $c_{\tilde{\mu}_s}$ are aligned, i.e., $c_\rho = \|c_\rho\| z$ and $c_{\tilde{\mu}_s} = \|c_{\tilde{\mu}_s}\| z$, for some unit vector $z \in \mathbb{S}^d$. Also denote

$$\tilde{\mu} = \alpha \tilde{\mu}_s + (1-\alpha)\rho \, \mathrm{d}S.$$

Then, we have

$$\begin{aligned} \|\alpha c_{\mu_s} + (1-\alpha) c_\rho\| &< \alpha \|c_{\mu_s}\| + (1-\alpha)\|c_\rho\| \\ &= \alpha \|c_{\tilde{\mu}_s}\| + (1-\alpha)\|c_\rho\| \\ &= \|\alpha c_{\tilde{\mu}_s} + (1-\alpha) c_\rho\|, \end{aligned}$$

where we used the triangle inequality, the fact that a rotation preserves the norm of the centre of mass, and finally, that c_ρ and $c_{\tilde{\mu}_s}$ are aligned. From this calculation we infer that by the rotation, $\|\alpha c_{\mu_s} + (1-\alpha)c_\rho\|$ increases, and hence, the total energy will be decreased (i.e., $E[\tilde{\mu}] \leqslant E[\mu]$).

Based on the considerations above, the cases we have to consider are: either $\|c_\rho\| = 0$ or $\|c_\rho\| \neq 0$, in which case directions of c_ρ and c_{μ_s} are aligned. For both cases, we can assume that $c_\rho = \|c_\rho\| z$ and $c_{\mu_s} = \|c_{\mu_s}\| z$ for some unit vector $z \in \mathbb{S}^d$.

Consider the map $f_z^t : \mathbb{S}^d \to \mathbb{S}^d$ defined for all $0 \leqslant t < 1$ by

$$f_z^t(x) = \frac{x + tz}{\|x + tz\|}, \qquad \forall x \in \mathbb{S}^d,$$

and the push-forward measure $(f_z^t)_\# \mu_s$ of μ_s under this map. Then, we have

$$\langle c_{(f_z^t)_\#\mu_s}, z \rangle = \left\langle \int_{\mathbb{S}^d} x \mathrm{d}(f_z^t)_\#\mu_s(x), z \right\rangle = \left\langle \int_{\mathbb{S}^d} \frac{x+tz}{\|x+tz\|} \mathrm{d}\mu_s(x), z \right\rangle = \int_{\mathbb{S}^d} \frac{\langle x+tz, z\rangle}{\|x+tz\|} \mathrm{d}\mu_s(x),$$

and by taking a derivative with respect to t in the above, we find

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle c_{(f_z^t)_\#\mu_s}, z \rangle = \int_{\mathbb{S}^d} \left(\frac{1}{\|x+tz\|} - \frac{\langle x+tz, z\rangle^2}{\|x+tz\|^3} \right) \mathrm{d}\mu_s(x). \tag{A.74}$$

Evaluate (A.74) at $t = 0$ to get

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle c_{(f_z^t)_\#\mu_s}, z \rangle \Big|_{t=0} = \int_{\mathbb{S}^d} \left(1 - \langle x, z\rangle^2\right) \mathrm{d}\mu_s(x).$$

If μ_s is not concentrated on $\{z, -z\}$, then $\frac{\mathrm{d}}{\mathrm{d}t} \langle c_{(f_z^t)_\#\mu_s}, z \rangle \big|_{t=0} > 0$, and this implies

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \left\| \alpha c_{(f_z^t)_\#\mu_s} + (1-\alpha) c_\rho \right\|^2 \Big|_{t=0} &= 2 \left\langle \alpha \frac{\mathrm{d}}{\mathrm{d}t} c_{(f_z^t)_\#\mu_s} \Big|_{t=0}, (\alpha\|c_{\mu_s}\| + (1-\alpha)\|c_\rho\|) z \right\rangle \\ &= 2\alpha(\alpha\|c_{\mu_s}\| + (1-\alpha)\|c_\rho\|) \frac{\mathrm{d}}{\mathrm{d}t} \langle c_{(f_z^t)_\#\mu_s}, z \rangle \Big|_{t=0} \\ &> 0. \end{aligned}$$

Therefore, a perturbation $\mu^t = \alpha (f_z^t)_\#\mu_s + (1-\alpha)\rho \mathrm{d}S$ of μ decreases its energy.

Consider now the case when μ_s is concentrated on $\{z, -z\}$. Since we already assumed μ_s is not concentrated at one point, we can assume that $\alpha\mu_s = \alpha_1 \delta_z + \alpha_2 \delta_{-z}$, where $\alpha_1 \geqslant \alpha_2 > 0$ and $\alpha = \alpha_1 + \alpha_2$. Take a perturbation of $\alpha\mu_s$ given by

$$\alpha \mu_s^t = \alpha_1 \delta_z + \alpha_2 \delta_{-(\cos t) z + (\sin t) w}, \qquad \text{for } 0 \leqslant t \leqslant \frac{\pi}{2},$$

for some $w \in \mathbb{S}^d$ that satisfies $\langle w, z\rangle = 0$. Then, we have

$$\begin{aligned}\alpha c_{\mu_s^t} + (1-\alpha)c_\rho &= \alpha_1 z + \alpha_2\left(-(\cos t)z + (\sin t)w\right) + (1-\alpha)\|c_\rho\| z \\ &= (\alpha_1 - \alpha_2\cos t + (1-\alpha)\|c_\rho\|)z + \alpha_2(\sin t)w \\ &= (\alpha\|c_{\mu_s}\| + \alpha_2(1-\cos t) + (1-\alpha)\|c_\rho\|)z + \alpha_2(\sin t)w,\end{aligned}$$

where we used $\alpha_1 - \alpha_2 = \alpha\|c_{\mu_s}\|$. It yields

$$\|\alpha c_{\mu_s^t} + (1-\alpha)c_\rho\|^2 = (\alpha\|c_{\mu_s}\| + \alpha_2(1-\cos t) + (1-\alpha)\|c_\rho\|)^2 + \alpha_2^2\sin^2 t,$$

and this function is increasing in t, for $0 \leqslant t \leqslant \frac{\pi}{2}$. For this reason, a perturbation $\mu^t = \alpha\mu_s^t + (1-\alpha)\rho\mathrm{d}S$ of μ decreases its energy, and we infer again that μ cannot be a ground state.

Appendix B. Proof of Lemma 3.1

We will investigate the sign of $H'(\eta)$ for $\eta > 1$. From integration by parts, we have

$$\begin{aligned}&\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta\,\mathrm{d}\theta \\ &\quad= \left[\frac{1}{d}(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^d\theta\mathrm{d}\theta\right]_0^\pi - \frac{1}{d(m-1)}\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d+1}\theta\mathrm{d}\theta \\ &\quad= \frac{1}{d(1-m)}\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d+1}\theta\mathrm{d}\theta,\end{aligned}$$

which we use in (3.35) to rewrite H as

$$H(\eta) = \frac{1}{dm}(dw_d)^{m-1}\left(\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d+1}\theta\mathrm{d}\theta\right)\left(\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\right)^{m-2}.$$

Then, the derivative of $\ln H(\eta)$ can be written as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\eta}\ln H(\eta) &= \frac{H'(\eta)}{H(\eta)} \\ &= \left(\frac{2-m}{m-1}\right)\left(\frac{\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-2}\sin^{d+1}\theta\mathrm{d}\theta}{\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d+1}\theta\mathrm{d}\theta}\right) \\ &\quad+\left(\frac{m-2}{m-1}\right)\left(\frac{\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\mathrm{d}\theta}{\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta}\right).\end{aligned}$$

Since $\frac{m-2}{m-1} > 0$ for any $0 < m < 1$, the sign of $H'(\eta)$ is the same as the sign of

(B.75)
$$\begin{aligned}\mathcal{H}_1(\eta, m, d) := &\left(\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta\mathrm{d}\theta\right)\left(\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-1}\sin^{d+1}\theta\mathrm{d}\theta\right) \\ &-\left(\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}-2}\sin^{d+1}\theta\mathrm{d}\theta\right)\left(\int_0^\pi(\eta-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\mathrm{d}\theta\right).\end{aligned}$$

We will study the sign of $\mathcal{H}_1$ using tables of integrals that involve associated Legendre functions of the first kind, available in [33]. From Section 3.666, equation (2) of [33], we have:

$$\int_0^\pi (\cosh\beta + \sinh\beta\cos\theta)^{\mu+\nu}\sin^{-2\nu}\theta \mathrm{d}\theta = \frac{\sqrt{\pi}}{2^\nu}\sinh^\nu\beta\,\Gamma\left(\frac{1}{2}-\nu\right)P_\mu^\nu(\cosh\beta) \quad \forall \mathrm{Re}(\nu) < \frac{1}{2},$$

where P_μ^ν denotes the associated Legendre function of the first kind. By factoring out $\sinh\beta$ from the l.h.s., the equation can be written as

$$\int_0^\pi (\coth\beta + \cos\theta)^{\mu+\nu}\sin^{-2\nu}\theta \mathrm{d}\theta = \frac{\sqrt{\pi}}{2^\nu}\sinh^{-\mu}\beta\,\Gamma\left(\frac{1}{2}-\nu\right)P_\mu^\nu(\cosh\beta). \tag{B.76}$$

Denote $\mu_0 = \frac{1}{m-1} - 2 + \frac{d+1}{2}$, $\nu_0 = -\frac{d+1}{2}$ and substitute $\eta = \coth\beta$ in (B.75), and use (B.76) to simplify each integral in $\mathcal{H}_1(\eta, m, d)$ as follows:

$$\begin{cases}
\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}-1}\sin^{d-1}\theta \mathrm{d}\theta & = \frac{\sqrt{\pi}}{2^{\nu_0+1}}\sinh^{-\mu_0}\beta\,\Gamma\left(\frac{1}{2}-(\nu_0+1)\right)P_{\mu_0}^{\nu_0+1}(\cosh\beta),\\
\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}-1}\sin^{d+1}\theta \mathrm{d}\theta & = \frac{\sqrt{\pi}}{2^{\nu_0}}\sinh^{-(\mu_0+1)}\beta\,\Gamma\left(\frac{1}{2}-\nu_0\right)P_{\mu_0+1}^{\nu_0}(\cosh\beta),\\
\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}-2}\sin^{d+1}\theta \mathrm{d}\theta & = \frac{\sqrt{\pi}}{2^{\nu_0}}\sinh^{-\mu_0}\beta\,\Gamma\left(\frac{1}{2}-\nu_0\right)P_{\mu_0}^{\nu_0}(\cosh\beta),\\
\int_0^\pi (\eta - \cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta & = \frac{\sqrt{\pi}}{2^{\nu_0+1}}\sinh^{-(\mu_0+1)}\beta\,\Gamma\left(\frac{1}{2}-(\nu_0+1)\right)P_{\mu_0+1}^{\nu_0+1}(\cosh\beta).
\end{cases}$$

Hence, we can write $\mathcal{H}_1(\eta, m, d)$ as

$$\begin{aligned}
\mathcal{H}_1(\eta, m, d) = {} & \frac{\pi}{2^{2\nu_0+1}}\sinh^{-(2\mu_0+1)}\beta\,\Gamma\left(\frac{1}{2}-\nu_0\right)\Gamma\left(-\frac{1}{2}-\nu_0\right)\\
& \times \left(P_{\mu_0}^{\nu_0+1}(\cosh\beta)P_{\mu_0+1}^{\nu_0}(\cosh\beta) - P_{\mu_0}^{\nu_0}(\cosh\beta)P_{\mu_0+1}^{\nu_0+1}(\cosh\beta)\right).
\end{aligned}$$

The sign of $\mathcal{H}_1(\eta, m, d)$ is the same as the sign of

$$\mathcal{H}_2(\beta, m, d) := P_{\mu_0}^{\nu_0+1}(\cosh\beta)P_{\mu_0+1}^{\nu_0}(\cosh\beta) - P_{\mu_0}^{\nu_0}(\cosh\beta)P_{\mu_0+1}^{\nu_0+1}(\cosh\beta),$$

where β ranges in $(0, \infty)$.

Equation (1) in Section 8.715 of [33] provides the following integral representation of the associated Legendre function of the first kind:

$$P_\mu^\nu(\cosh\beta) = \frac{\sqrt{2}\sinh^\nu\beta}{\sqrt{\pi}\Gamma\left(\frac{1}{2}-\nu\right)}\int_0^\beta \frac{\cosh\left(\mu+\frac{1}{2}\right)t}{(\cosh\beta - \cosh t)^{\nu+\frac{1}{2}}}\mathrm{d}t.$$

By using the integral expression above, we can rewrite $\mathcal{H}_2(\beta, m, d)$ as

$$\begin{aligned}\mathcal{H}_2(\beta, m, d) = &\frac{2\sinh^{2\nu_0+1}\beta}{\pi\Gamma\left(\frac{1}{2}-\nu_0\right)\Gamma\left(-\frac{1}{2}-\nu_0\right)} \\ &\times \left(\int_0^\beta \frac{\cosh\left(\mu_0+\frac{1}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{3}{2}}}\mathrm{d}t \int_0^\beta \frac{\cosh\left(\mu_0+\frac{3}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{1}{2}}}\mathrm{d}t\right. \\ &\quad \left. - \int_0^\beta \frac{\cosh\left(\mu_0+\frac{1}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{1}{2}}}\mathrm{d}t \int_0^\beta \frac{\cosh\left(\mu_0+\frac{3}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{3}{2}}}\mathrm{d}t\right).\end{aligned}$$

Finally, we will investigate the sign of

$$\begin{aligned}\mathcal{H}_3(\beta, m, d) := &\int_0^\beta \frac{\cosh\left(\mu_0+\frac{1}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{3}{2}}}\mathrm{d}t \int_0^\beta \frac{\cosh\left(\mu_0+\frac{3}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{1}{2}}}\mathrm{d}t \\ &- \int_0^\beta \frac{\cosh\left(\mu_0+\frac{1}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{1}{2}}}\mathrm{d}t \int_0^\beta \frac{\cosh\left(\mu_0+\frac{3}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{3}{2}}}\mathrm{d}t,\end{aligned}$$

for $\beta \in (0, \infty)$. The sign of

$$A := \mu_0 + 1 = \frac{1}{m-1} + \frac{d-1}{2}$$

will be crucial in determining the sign of $\mathcal{H}_3$ (and hence, of H).

We express $\mathcal{H}_3$ using A instead of μ_0 as follows:

$$\begin{aligned}\mathcal{H}_3(\beta, m, d) = &\int_0^\beta \frac{\cosh\left(A-\frac{1}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{3}{2}}}\mathrm{d}t \int_0^\beta \frac{\cosh\left(A+\frac{1}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{1}{2}}}\mathrm{d}t \\ &- \int_0^\beta \frac{\cosh\left(A-\frac{1}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{1}{2}}}\mathrm{d}t \int_0^\beta \frac{\cosh\left(A+\frac{1}{2}\right)t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{3}{2}}}\mathrm{d}t \\ = &\int_0^\beta \frac{\cosh\left|A-\frac{1}{2}\right|t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{3}{2}}}\mathrm{d}t \int_0^\beta \frac{\cosh\left|A+\frac{1}{2}\right|t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{1}{2}}}\mathrm{d}t \\ &- \int_0^\beta \frac{\cosh\left|A-\frac{1}{2}\right|t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{1}{2}}}\mathrm{d}t \int_0^\beta \frac{\cosh\left|A+\frac{1}{2}\right|t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{3}{2}}}\mathrm{d}t,\end{aligned}$$

where in the second equality we used that $\cosh(\cdot)$ is an even function.

Now define, for $t > 0$:

$$\mathrm{d}\xi := \left(\frac{\cosh\left|A+\frac{1}{2}\right|t}{(\cosh\beta-\cosh t)^{\nu_0+\frac{3}{2}}}\right)\mathrm{d}t, \quad f(t) = \cosh\beta - \cosh t, \quad g(t) = \frac{\cosh\left|A-\frac{1}{2}\right|t}{\cosh\left|A+\frac{1}{2}\right|t}.$$

Hence, we write

$$\mathcal{H}_3(\beta, m, d) = \int_0^\beta f(t)\mathrm{d}\xi \int_0^\beta g(t)\mathrm{d}\xi - \int_0^\beta f(t)g(t)\mathrm{d}\xi \int_0^\beta \mathrm{d}\xi.$$

The function f is decreasing on $t \geqslant 0$. Also, g' can be calculated from

$$\frac{g'(t)}{g(t)} = \left|A - \frac{1}{2}\right| \tanh \left|A - \frac{1}{2}\right| t - \left|A + \frac{1}{2}\right| \tanh \left|A + \frac{1}{2}\right| t,$$

which is positive for $A < 0$, negative for $A > 0$ and zero for $A = 0$. We distinguish between the following cases:
(Case 1: $A = 0$) In this case, $g(t) = 1$ and $\mathcal{H}_3 \equiv 0$.

(Case 2: $A > 0$) Since f and g are both decreasing, $\mathcal{H}_3 < 0$ from the Chebyshev inequality.

(Case 3: $A < 0$) For this case, since f is decreasing and g is increasing, $\mathcal{H}_3 > 0$ from the Chebyshev inequality.

Therefore, we can finally conclude that H is increasing for $1 - \frac{2}{d-1} < m < 1$, decreasing for $0 < m < 1 - \frac{2}{d-1}$, and constant for $m = 1 - \frac{2}{d-1}$, which concludes the proof of Lemma 3.1.

Appendix C. Proof of Lemma 3.2

We show that

$$\lim_{\eta \to \infty} H(-\eta) = \kappa_1^{-1},$$

where κ_1 is given by (2.25) and the function H by (3.35). By factoring out η from each of the terms in (3.35), we have
(C.77)

$$H(\eta) = \frac{1-m}{m}(dw_d)^{m-1}\eta \left(\int_0^\pi \left(1 - \frac{\cos\theta}{\eta}\right)^{\frac{1}{m-1}} \sin^{d-1}\theta \cos\theta \mathrm{d}\theta \right) \left(\int_0^\pi \left(1 - \frac{\cos\theta}{\eta}\right)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta \right)^{m-2}.$$

We will use Newton's generalized binomial theorem: for any $r \in \mathbb{R}$ and $x \in \mathbb{R}$ with $|x| < 1$, it holds that

$$(1+x)^r = \sum_{k=0}^{\infty} \binom{r}{k} x^k,$$

where $\binom{r}{k} = \frac{r(r-1)....(r-k+1)}{k!}$, with the convention $\binom{r}{0} = 1$. Then, as the binomial series is uniformly convergent, we get from (C.77):

$$\begin{aligned} H(\eta) &= \frac{1-m}{m}(dw_d)^{m-1}\eta \left(\sum_{k=0}^{\infty} (-1)^k \binom{\frac{1}{m-1}}{k} \frac{1}{\eta^k} \int_0^\pi \cos^{k+1}\theta \sin^{d-1}\theta \mathrm{d}\theta \right) \\ &\quad \times \left(\sum_{k=0}^{\infty} (-1)^k \binom{\frac{1}{m-1}}{k} \frac{1}{\eta^k} \int_0^\pi \cos^{k}\theta \sin^{d-1}\theta \mathrm{d}\theta \right)^{m-2} \\ &= \frac{1-m}{m}(dw_d)^{m-1} \left(\sum_{k=1}^{\infty} (-1)^k \binom{\frac{1}{m-1}}{k} \frac{1}{\eta^{k-1}} \int_0^\pi \cos^{k+1}\theta \sin^{d-1}\theta \mathrm{d}\theta \right) \\ &\quad \times \left(\sum_{k=0}^{\infty} (-1)^k \binom{\frac{1}{m-1}}{k} \frac{1}{\eta^k} \int_0^\pi \cos^{k}\theta \sin^{d-1}\theta \mathrm{d}\theta \right)^{m-2}, \end{aligned}$$

where for the second equal sign we used that the $k = 0$ term in the first binomial sum, vanishes.

Then, in the limit η tends to infinity, we find

$$\begin{aligned}
\lim_{\eta\to\infty} H(\eta) &= \frac{1-m}{m}(dw_d)^{m-1}\left(-\binom{\frac{1}{m-1}}{1}\int_0^\pi \cos^2\theta \sin^{d-1}\theta \mathrm{d}\theta\right)\left(\binom{\frac{1}{m-1}}{0}\int_0^\pi \sin^{d-1}\theta\right)^{m-2} \\
&= \frac{1-m}{m}(dw_d)^{m-1}\frac{1}{1-m}\times\frac{1}{d+1}\left(\int_0^\pi \sin^{d-1}\theta\right)^{m-1} \\
&= \frac{|\mathbb{S}^d|^{m-1}}{m(d+1)},
\end{aligned}$$

where for the last equal sign we used

$$|\mathbb{S}^d| = |\mathbb{S}^{d-1}|\int_0^\pi \sin^{d-1}\theta \mathrm{d}\theta,$$

and $|\mathbb{S}^{d-1}| = dw_d$. This proves the claim.

Appendix D. Derivation of κ_2

We will derive the explicit expression of κ_2 given in Remark 3.4. We calculate $H(1)$ first (see (3.35) and (3.38)):

$$\begin{aligned}
H(1) &= \frac{1-m}{m}(dw_d)^{m-1}\frac{\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta\cos\theta \mathrm{d}\theta}{\left(\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}}\sin^{d-1}\theta \mathrm{d}\theta\right)^{2-m}} \\
&= \frac{1-m}{m}(dw_d)^{m-1}\frac{\int_0^\pi 2^{\frac{1}{m-1}}\sin^{\frac{2}{m-1}}\left(\frac{\theta}{2}\right)\sin^{d-1}\theta\cos\theta \mathrm{d}\theta}{\left(\int_0^\pi 2^{\frac{1}{m-1}}\sin^{\frac{2}{m-1}}\left(\frac{\theta}{2}\right)\sin^{d-1}\theta \mathrm{d}\theta\right)^{2-m}} \\
&= 2\left(\frac{1-m}{m}\right)(dw_d)^{m-1}\frac{\int_0^\pi \sin^{\frac{2}{m-1}}\left(\frac{\theta}{2}\right)\sin^{d-1}\theta\cos\theta \mathrm{d}\theta}{\left(\int_0^\pi \sin^{\frac{2}{m-1}}\left(\frac{\theta}{2}\right)\sin^{d-1}\theta \mathrm{d}\theta\right)^{2-m}}.
\end{aligned} \tag{D.78}$$

Using the identity

$$\int_0^\pi \cos^a\left(\frac{\theta}{2}\right)\sin^b\left(\frac{\theta}{2}\right)\mathrm{d}\theta = \frac{\Gamma\left(\frac{a+1}{2}\right)\Gamma\left(\frac{b+1}{2}\right)}{\Gamma\left(\frac{a+b+2}{2}\right)}, \tag{D.79}$$

the property $\Gamma(z+1) = z\Gamma(z)$ for all $z > 0$, and the elementary trig identities

$$\sin(\theta) = 2\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right), \qquad \cos\theta = 2\cos^2\left(\frac{\theta}{2}\right) - 1,$$

we can simplify the numerator and denominator in (D.78) as

$$\begin{aligned}
&\int_0^\pi \sin^{\frac{2}{m-1}}\left(\frac{\theta}{2}\right)\sin^{d-1}\theta\cos\theta \mathrm{d}\theta \\
=&2^{d-1}\int_0^\pi \left(\sin^{\frac{2}{m-1}+d-1}\left(\frac{\theta}{2}\right)\cos^{d+1}\left(\frac{\theta}{2}\right) - \sin^{\frac{2}{m-1}+d+1}\left(\frac{\theta}{2}\right)\cos^{d-1}\left(\frac{\theta}{2}\right)\right)\mathrm{d}\theta \\
=&2^{d-1}\left(\frac{\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d+2}{2}\right) - \Gamma\left(\frac{1}{m-1}+\frac{d+2}{2}\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{1}{m-1}+d+1\right)}\right) \\
=&2^{d-1}\left(\frac{\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{1}{m-1}+d+1\right)}\right)\left(\frac{d}{2} - \left(\frac{1}{m-1}+\frac{d}{2}\right)\right) \\
=&\frac{2^{d-1}\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d}{2}\right)}{(1-m)\Gamma\left(\frac{1}{m-1}+d+1\right)},
\end{aligned}$$

and

$$\begin{aligned}
\int_0^\pi \sin^{\frac{2}{m-1}}\left(\frac{\theta}{2}\right)\sin^{d-1}\theta \mathrm{d}\theta &= 2^{d-1}\int_0^\pi \sin^{\frac{2}{m-1}+d-1}\left(\frac{\theta}{2}\right)\cos^{d-1}\left(\frac{\theta}{2}\right)\mathrm{d}\theta \\
&= \frac{2^{d-1}\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{1}{m-1}+d\right)}.
\end{aligned}$$

Then, we can simplify $H(1)$ from (D.78) as follows:

$$\begin{aligned}
H(1) &= 2\left(\frac{1-m}{m}\right)(dw_d)^{m-1}\frac{\left(\frac{2^{d-1}\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d}{2}\right)}{(1-m)\Gamma\left(\frac{1}{m-1}+d+1\right)}\right)}{\left(\frac{2^{d-1}\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{1}{m-1}+d\right)}\right)^{2-m}} \\
&= \frac{2^{1+(d-1)(m-1)}}{m\left(\frac{1}{m-1}+d\right)}(dw_d)^{m-1}\left(\frac{\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{1}{m-1}+d\right)}\right)^{m-1}.
\end{aligned}$$

Finally, use $|\mathbb{S}^d| = \frac{dw_d\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{d+1}{2}\right)}$ to write the above expression as

$$H(1) = \frac{2^{1+(d-1)(m-1)}|\mathbb{S}^d|^{m-1}}{m\left(\frac{1}{m-1}+d\right)}\left(\frac{\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d+1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{1}{m-1}+d\right)}\right)^{m-1}.$$

The explicit expression for κ_2 listed in Remark 3.4, follows then from $\kappa_2 = H(1)^{-1}$.

Appendix E. Calculation of $\bar{s}$

We calculate from (3.45) using simple trig identities:

$$\begin{aligned}
\bar{s} &= 1 - \frac{\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta (1-\cos\theta) \mathrm{d}\theta}{\int_0^\pi (1-\cos\theta)^{\frac{1}{m-1}} \sin^{d-1}\theta \mathrm{d}\theta} \\
&= 1 - \frac{\int_0^\pi \left(2\sin^2\frac{\theta}{2}\right)^{\frac{1}{m-1}+1} \left(2\sin\frac{\theta}{2}\cos\frac{\theta}{2}\right)^{d-1} \mathrm{d}\theta}{\int_0^\pi \left(2\sin^2\frac{\theta}{2}\right)^{\frac{1}{m-1}} \left(2\sin\frac{\theta}{2}\cos\frac{\theta}{2}\right)^{d-1} \mathrm{d}\theta} \\
&= 1 - 2\,\frac{\int_0^\pi \sin^{\frac{2}{m-1}+d+1}\frac{\theta}{2}\cos^{d-1}\frac{\theta}{2}\mathrm{d}\theta}{\int_0^\pi \sin^{\frac{2}{m-1}+d-1}\frac{\theta}{2}\cos^{d-1}\frac{\theta}{2}\mathrm{d}\theta}.
\end{aligned}$$

Then, using the Gamma function and its properties (see (D.79)) we find

$$\begin{aligned}
\bar{s} &= 1 - 2\,\frac{\frac{\Gamma\left(\frac{1}{m-1}+\frac{d}{2}+1\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{1}{m-1}+d+1\right)}}{\frac{\Gamma\left(\frac{1}{m-1}+\frac{d}{2}\right)\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{1}{m-1}+d\right)}} \\
&= 1 - 2\,\frac{\frac{1}{m-1}+\frac{d}{2}}{\frac{1}{m-1}+d} \\
&= 1 - \frac{2+d(m-1)}{1+d(m-1)} \\
&= \frac{1}{(1-m)d-1}.
\end{aligned}$$

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