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On minimizers of interaction functionals with competing attractive and repulsive potentials

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Abstract

We consider a family of interaction functionals consisting of power-law potentials with attractive and repulsive parts and use the concentration compactness principle to establish the existence of global minimizers. We consider various minimization classes, depending on the signs of the repulsive and attractive power exponents of the potential. In the special case of quadratic attraction and Newtonian repulsion we characterize in detail the ground state.

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1. Introduction

We consider the minimization of energies of the form

$$E[\rho] := \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} K(x-y)\rho(x)\rho(y)\,dx\,dy, \tag{1}$$

where

$$K(x) := \frac{1}{q}|x|^q - \frac{1}{p}|x|^p, \quad \text{for } -N < p < q. \tag{2}$$

These functionals are directly connected to a class of self-assembly/aggregation models which recently have received much attention (see for example, [1–13]). The aggregation models consist of the following active transport equation in $\mathbb{R}^N$ for the population density ρ:

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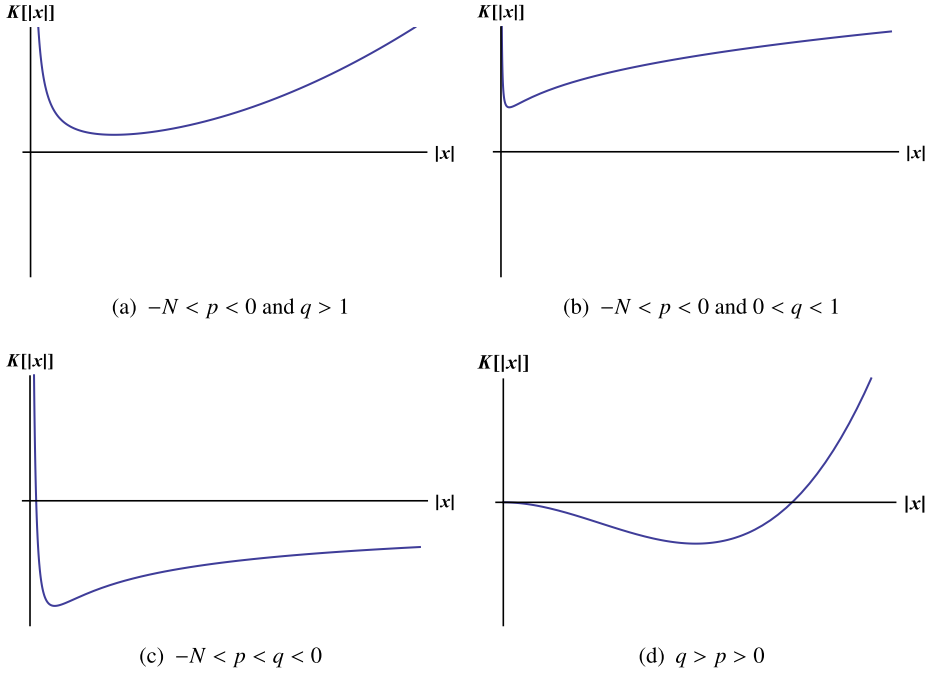

(a) $-N < p < 0$ and $q > 1$ (b) $-N < p < 0$ and $0 < q < 1$

(c) $-N < p < q < 0$ (d) $q > p > 0$

Fig. 1. Generic examples of K for various values of p and q.

$$\rho_t + \nabla \cdot (\rho \mathbf{v}) = 0, \quad \mathbf{v} = -\nabla K * \rho, \tag{3}$$

where K represents the interaction potential and $*$ denotes spatial convolution. This partial differential equation is the gradient flow of the energy (1) with respect to the 2-Wasserstein metric [14,15]. Indeed, the evolution equation (3) can be written in the form

$$\partial_t \rho = \nabla \cdot \left(\rho \nabla \frac{\delta E[\rho]}{\delta \rho} \right),$$

which is the standard form for the 2-Wasserstein gradient flow [14] of the energy (1).

Model (3) appears in the study of many phenomena, including biological swarms [11,12], granular media [1,13], self-assembly of nanoparticles [7,8] and molecular dynamics simulations of matter [16]. The study of solutions to (3) (well-posedness, finite or infinite time blow-up, long-time behavior) has been a very active area of research during the past decade [2–5,10]. It is important to note that the analysis and behavior of solutions to (3) depend essentially on the properties of the potential K. In the context of biological swarms, K incorporates social interactions (attraction and repulsion) between group individuals. Potentials which are attractive in nature typically lead to blow-up [2,9], while attractive–repulsive potentials may generate finite-size, confined aggregations [6,10].

By inspecting the equation for $\mathbf{v}$ in (3) one notes that the nature of a symmetric potential $K(x) = K(|x|)$ is dictated by the sign of its derivative ($K' > 0$ corresponds to attraction and $K' < 0$ to repulsion). Hence, for K given by (2), the exponent q refers to attraction and p to repulsion (p and q can be of any sign). The condition $q > p$ is needed to ensure that the potential is repulsive at short ranges and attractive in the far field – see Figs. 1(a)–1(c) for a generic illustration of K with $p < 0$ and Fig. 1(d) for an example of K with $p > 0$. Note that in the regime $p < 0$ when $q \geqslant 1$, the potential K is positive, convex and $K \to \infty$ as $|x| \to \infty$ whereas when $0 < q < 1$, K is still positive and grows indefinitely with $|x|$; however, it is not convex. Finally for $-N < q < 0$, K becomes negative, approaches 0 as $|x| \to \infty$ and is not convex.

Potentials in power-law form have been frequently considered in the recent literature on the aggregation model (3) [17,18,6,19,20]. As shown in these works, the delicate balance between attraction and repulsion often leads to complex equilibrium configurations, supported on sets of various dimensions. Indeed, a simple particle model simulation in two dimensions shows accumulation of the density in different states depending on the powers of the interaction potential K (see Figs. 2 and 3). The dimensionality of local minimizers of (1) with K given by (2) was recently