The spectrum of the torus profile to a geometric variational problem with long range interaction

Xiaofeng Ren [a,*], Juncheng Wei [b]

[a] *Department of Mathematics, The George Washington University, Washington, DC 20052, USA*
[b] *Department of Mathematics, University of British Columbia, Vancouver, BC, Canada V6T 1Z2*

HIGHLIGHTS

- The profile problem is a nonlocal geometric variational problem on sets.
- The energy is perimeter plus a Newtonian potential related long range term.
- The linearized operator decomposes into a family of operators indexed by the mode.
- Each operator in the family becomes stable when the minor radius is small.
- No matter how small the radius is there is a mode with an unstable operator.

ABSTRACT

The profile problem for the Ohta–Kawasaki diblock copolymer theory is a geometric variational problem. The energy functional is defined on sets in $\mathbb{R}^3$ of prescribed volume and the energy of an admissible set is its perimeter plus a long range interaction term related to the Newtonian potential of the set. This problem admits a solution, called a torus profile, that is a set enclosed by an approximate torus of the major radius 1 and the minor radius q. The torus profile is both axially symmetric about the z axis and reflexively symmetric about the xy-plane. There is a way to set up the profile problem in a function space as a partial differential-integro equation. The linearized operator $\mathcal{L}$ of the problem at the torus profile is decomposed into a family of linear ordinary differential-integro operators $\mathcal{L}^m$ where the index $m = 0, 1, 2, \ldots$ is called a mode. The spectrum of $\mathcal{L}$ is the union of the spectra of the $\mathcal{L}^m$'s. It is proved that for each m, when q is sufficiently small, $\mathcal{L}^m$ is positive definite. (0 is an eigenvalue for both $\mathcal{L}^0$ and $\mathcal{L}^1$, due to the translation and rotation invariance.) As q tends to 0, more and more $\mathcal{L}^m$'s become positive definite. However no matter how small q is, there is always a mode m of which $\mathcal{L}^m$ has a negative eigenvalue. This mode grows to infinity like $q^{-3/4}$ as $q \to 0$.

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1. Introduction

The Ohta–Kawasaki theory [1] for diblock copolymers is an archetypal example of binary inhibitory systems. In the strong segregation limit, where the two constituents are fully separated by sharp interfaces, Nishiura and Ohnishi [2] simplified the theory to a geometric variational problem where the free energy of the system can be written as

$$\mathcal{J}_D(\Omega) = \frac{1}{2}\mathcal{P}_D(\Omega) + \frac{\gamma}{2}\int_D \left|(-\Delta)^{-1/2}(\chi_\Omega - \omega)\right|^2 dx. \tag{1.1}$$

Here D is a bounded domain in $\mathbb{R}^3$, and there are two parameters $\gamma > 0$ and $\omega \in (0, 1)$. The input of this functional is Ω, a Lebesgue measurable subset of D, whose measure $|\Omega|$ is fixed at

$$|\Omega| = \omega|D|. \tag{1.2}$$

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* Corresponding author. Fax: +1 202 994 6760.
  E-mail address: ren@gwu.edu (X. Ren).

The first term $\mathscr{P}_D(\Omega)$ is the perimeter of Ω in D. If D is bounded by smooth surfaces, then $\mathscr{P}_D(\Omega)$ is the total area of those surfaces that are inside D. These surfaces form the set $\partial\Omega \cap D$, which is called the interface of Ω because it separates Ω from $D \setminus \Omega$ in D.

The second term in the functional (1.1) is the most interesting. The nonlocal operator $(-\Delta)^{-1/2}$ is defined to be the positive square root of $(-\Delta)^{-1}$. For the latter operator, given $f \in L^2(D)$ and $\int_D f(x)\,dx = 0$, define $w = (-\Delta)^{-1}f$ by solving the Poisson's equation

$$-\Delta w = f \quad \text{in } D, \qquad \partial_\nu w = 0 \quad \text{on } \partial D, \qquad \int_D w(x)\,dx = 0. \tag{1.3}$$

In (1.3) $\partial_\nu w$ stands for the outward normal derivative of w on ∂D.

A stationary set of $\mathscr{J}_D$ is a solution of the equation

$$\mathcal{H}(\partial\Omega) + \gamma(-\Delta)^{-1}(\chi_\Omega - \omega) = \lambda \tag{1.4}$$

which holds on the interface $\partial\Omega \cap D$. Here $\mathcal{H}(\partial\Omega)$ is the mean curvature of $\partial\Omega$. The constant λ on the right side of (1.4) is a Lagrange multiplier corresponding to the volume constraint (1.2). If Ω shares boundary with D, then

$$\partial\Omega \cap D \perp \partial D; \tag{1.5}$$

namely the interface of Ω meets the domain boundary perpendicularly.

It is easy to show that the functional $\mathscr{J}_D$ admits a global minimizer. One can study its properties for various parameter ranges of γ and ω [3–6]. One may also construct stable stationary sets of (1.1) either by finding local minimizers of $\mathscr{J}_D$ [7,8], or by solving (1.4) [9–15].

Many morphological phases observed in nature are assemblies of small components with almost the same size and shape. These components arrange themselves in a very regular pattern. The most well known are the hexagonal pattern and the body centered cubic pattern. A cross section of a hexagonal pattern is a two dimensional assembly of small disks, and a body centered cubic pattern is a three dimensional assembly of small balls. These two patterns were found as stable stationary assemblies of (1.1) by the authors in [12,13].

The starting point of these constructions is an observation that (1.4) has a counterpart on the entire space $\mathbb{R}^3$ ($\mathbb{R}^2$, resp):

$$\mathcal{H}(\partial\Omega) + \gamma\mathcal{N}(\Omega) = \lambda \quad \text{on } \partial\Omega. \tag{1.6}$$

A solution Ω to (1.6) must have a prescribed volume:

$$|\Omega| = \mu \tag{1.7}$$

where $\mu > 0$ is one of the two parameters, the other being γ; λ on the right side of (1.6) is a Lagrange multiplier corresponding to (1.7). In (1.6), $\mathcal{N}(\Omega)$ is the Newtonian potential of Ω:

$$\mathcal{N}(\Omega)(x) = \int_\Omega \frac{1}{4\pi|x-y|}\,dy. \tag{1.8}$$

Eq. (1.6) has its own variational structure. A solution of (1.6) is a stationary set of the functional

$$\mathscr{J}(\Omega) = \frac{1}{2}\mathscr{P}(\Omega) + \frac{\gamma}{2}\int_\Omega \mathcal{N}(\Omega)(x)\,dx. \tag{1.9}$$

Here $\mathscr{P}(\Omega)$ is the perimeter of Ω in $\mathbb{R}^3$, i.e. the area of $\partial\Omega$.

We term (1.6) the *profile equation* of the Ohta–Kawasaki model; a solution of (1.6) is called a *profile*. A ball of volume μ is a profile, because its boundary has constant mean curvature and its Newtonian potential is a radially symmetric function, hence also constant on its boundary. This ball is used as an approximation for a component in a stationary assembly constructed in [13]. In that assembly each component is close to a scaled version of the ball, and the locations of the components are determined by the geometry of D via the Green's function of Poisson's equation (1.3). Similarly in two dimensions, a disk of area μ is a profile and it serves as a component for the hexagonal stationary assembly [12].

The method of building stationary assemblies from profiles is a general one, which has been lately successfully applied to other inhibitory systems [16,17]. In addition to balls and disks, a few other profiles have been found [9,18,14,19,20].

In this paper we study a profile that shapes like a solid torus in $\mathbb{R}^3$. This profile was found in [19] and is a set enclosed by a surface which is a slightly perturbed torus. Our interest in a torus shaped profile partially comes from a discovery by Pochan et al. [21] of a block copolymer morphology phase of toroidal supramolecule assemblies. This phase was found by combining dilute solution characteristics critical for both bundling of like-charged biopolymers and block copolymer micelle formation. The key to toroid versus classic cylinder micelle formation is the interaction of the negatively charged hydrophilic block of an amphiphilic triblock copolymer with a positively charged divalent organic counterion. This produces a self-attraction of cylindrical micelles that leads to toroid formation, a mechanism akin to the toroidal bundling of semiflexible charged biopolymers such as DNA. Non-constant mean curvature surfaces are also found in some local second order variational problems; see Doelman et al. [22], Dai and Promislow [23], and Promislow and Wu [24].

A perfect torus is a surface characterized by a major radius p and a minor radius q with $0 < q < p$. The profile found in [19] is bounded by an approximate torus. Nevertheless this approximate torus still has well defined major radius and minor radius, and it encloses the same volume as the perfect torus with the same radii does; see the comments after Proposition 3.1. The profile problem (1.6) has μ and γ as parameters so the radii p and q of the torus profile are dependent on μ and γ. In [19] we took $\mu = 1$. This assumption is harmless because one can always transform μ to 1 by a change of space variable x and a change of γ. The two radii of the torus profile were then denoted by p_γ and q_γ, both dependent on γ. This profile exists when γ is sufficiently large. As $\gamma \to \infty$, $p_\gamma \to \infty$ and $q_\gamma \to 0$.

However it is more convenient in this paper to take the radii p and q as parameters and treat μ and γ as derived quantities. Moreover, without the loss of generality we let

$$p = 1. \tag{1.10}$$