Note on the Number of Steady States for a 2D Smoluchowski Equation

Peter Constantin†and Jesenko Vukadinovic‡

† Department of Mathematics, The University of Chicago, Chicago, Il 60637, USA. email: const@cs.uchicago.edu

‡ Department of Mathematics, Van Vleck Hall, 480 Lincoln Dr., Madison, WI 53706, email: vukadino@math.wisc.edu

Abstract. Dynamics of concentrated polymer solutions are modeled by a Smoluchowski equation. At high concentrations, such solutions form liquid crystalline polymers of nematic structure. We prove that at high intensities the 2D Smoluchowski equation possesses exactly two steady states corresponding to the isotropic and the nematic phase.

AMS classification scheme numbers: 35Kxx, 70Kxx

1. Introduction

Rigid rodlike polymers are known to form a liquid crystalline phase of nematic structure in high concentration solutions. The scientific interest in such lyotropic liquid crystals has increased in recent years due to the possibility of spinning high strength fibers from this highly ordered phase. The dynamics of such polymers are modeled by the Smoluchowski equation (due to Doi [3]) involving the probability distribution function $\psi(u)$ for the orientation of a test polymer viewed as a cylinder of diameter d, length L and axis parallel to the unit vector u. This is a nonlinear integro-differential equation phrased on the unit $n-1$-dimensional sphere. In case of a spatially homogenous solution, and in the absence of a macroscopic flow and any external fields, the equation has the form of a Fokker-Planck equation:

$$\partial_t \psi = \Delta_g \psi + \nabla_g \cdot (\psi \nabla_g V).$$

Here V represents the mean-field potential accounting for the molecule interactions in form of the excluded volume effects due to the steric forces. It was first derived by Onsager in his seminal work [5], however it is accepted that a good qualitative analysis is possible after truncating, using the Maier-Saupe potential:

$$V(u, [\psi]) = -b(u \otimes u) :< u \otimes u >_\psi ,$$

where the parameter $b \propto cd^2 L$ represents the nondimensional intensity of the potential, c represents the concentration, and $< \cdot >_\psi$ denotes the average over the distribution ψ.

The static equation, which preceded the kinetic equation historically, was also derived by Onsager from the formula for the free energy, and it has the distribution for the mean-field potential:

$$\psi(u) = Z(\psi)^{-1} \exp(-V(u, [\psi])), \tag{1.1}$$

where

$$Z(\psi) = \int_{S^{n-1}} \exp(-V(u, [\psi]))\ \sigma(du).$$

A rigorous treatment of this equation in both two and three dimensions was conducted in [1] and [2]. In two dimensions, in addition to the solution $\psi = 1/2\pi$ corresponding to the isotropic phase, at high intensities $b > 4$ Constantin at al. obtained an additional solution corresponding to the nematic phase. It was proven that (modulo rotation) there can be at most $2[b/4]$ solutions. The question as of the exact number of steady states modulo rotation remained open.

In this paper, we prove using a very simple argument based on ideas of [1] that at intensities $b > 4$ we have exactly two steady states: the isotropic and the nematic one.

One of the authors of the present paper was aware of the existence of the preprint ([4]) in which the same result is claimed, using a different proof based on a continued-fractions analysis.

2. Main Result

We represent the orientation $u = (\cos\phi, \sin\phi)$ using a local coordinate $\phi \in [0, 2\pi]$. We also represent the probability distribution in terms of ϕ as $\psi(\phi)$. Under equilibrium conditions, the orientation distribution is symmetric about an orientation called the director, which we will assume to be $(1, 0)$. This means that ψ is even in ϕ. One can easily see that under such symmetry the potential can be given through

$$V(\phi) = -\frac{b}{2} < \cos 2\phi >_{\psi} \cos 2\phi.$$

Denoting $r = \frac{b}{2} < \cos 2\phi >_{\psi}$, the equation (1.1) becomes

$$\psi(\phi) = \frac{\exp(r\cos 2\phi)}{\int_0^{2\pi} \exp(r\cos 2\phi)}.$$

Putting these two relations together, we can view the problem of finding steady states as finding the solutions to the equation ([1]):

$$\frac{2r}{b} = \frac{\int_0^{2\pi} \cos\phi \exp(r\cos\phi) d\phi}{\int_0^{2\pi} \exp(r\cos\phi) d\phi}.$$

For simplicity, for a continuous 2π-periodic function f we introduce the notation $[f](r) := \int_0^{2\pi} f(\phi) \exp(r\cos\phi) d\phi / \int_0^{2\pi} \exp(r\cos\phi) d\phi$, and the equation becomes

$$[\cos](r) = \frac{2r}{b}. \tag{2.2}$$

From [1] we adopt the following facts:

Lemma 1 *For any analytic 2π-periodic function $f(\phi)$, the function $[f](r)$ is continuous on $[0,\infty)$, and obeys*

$$\lim_{r\to\infty}[f](r) = f(0).$$

We have

$$[\cos]'(r) = [\cos^2](r) - [\cos]^2(r) = [\cos - [\cos](r)]^2(r) > 0, \tag{2.3}$$

so $[\cos]$ is an increasing function such that $0 \le [\cos](r) \to 1$ when $r \to \infty$.

Theorem 1 *For $b \le 4$ the trivial solution $r = 0$ is the only solution of the equation (2.2). For $b > 4$ there are exactly two solutions: the trivial and a nontrivial one.*

Proof : Integrating by parts in the numerator of $[\cos](r)$, one arrives at the identity

$$[\cos](r) = r\left(1 - [\cos^2](r)\right), \tag{2.4}$$

and the equation (2.2) becomes

$$r\left(1 - [\cos^2](r)\right) = \frac{2r}{b}.$$

$r = 0$ is a solution for all $b > 0$. Dividing by r, one obtains the equation for the nontrivial solution:

$$[\cos^2](r) = 1 - \frac{2}{b}.$$

It is an easy calculation that $[\cos^2](0) = 1/2$ and that $\lim_{r\to\infty}[\cos^2](r) = 1$. Showing that $y(r) = [\cos^2](r)$ is strictly increasing would prove the theorem.

Taking d/dr in (2.4), and using (2.2) and (2.4) one obtains a closed ordinary differential equation on y:

$$\frac{dy}{dr} = ry^2 - 2(r + \frac{1}{r})y + r + \frac{1}{r} = r(y - y_1(r))(y - y_2(r)), \tag{2.5}$$

where

$$1/2 \le y_1(r) = \frac{\sqrt{r^2+1}}{\sqrt{r^2+1}+1} \le 1 \le y_2(r) = \frac{\sqrt{r^2+1}}{\sqrt{r^2+1}-1}.$$

Observe that from (2.4) $1 - 1/r < y(r) \le 1$. Since $y(0) = y_1(0) = 1/2$, $y'(0) = y_1'(0) = 0$ and $y''(0) = 1/8 < y_1''(0) = 1/4$. Therefore, for small r, $y(r)$ belongs the interval $(1/2, y_1(r))$. Since $y_1(r)$ is strictly for increasing for $r > 0$, and since, in view of (2.5), $y'(r)$ vanishes when $y(r) = y_1(r)$, it follows that $y(r)$ remains in the interval $(1/2, y_1(r))$ for all $r > 0$. On this interval dy/dr is positive. This completes the proof. □

3. References

[1] Constantin P, Kevrekidis I and Titi E S 2004 Remarks on a Smoluchowski equation *Discrete and Continuous Dynamical Systems*, vol **11** (1), 101-112.

[2] Constantin P, Kevrekidis I and Titi E S 2004 Asymptotic states of a Smoluchowski equation *Archive for Rational Mechanics and Analysis*, to appear

[3] Doi M 1981 Molecular dynamics and rheological properties of concentrated solutions of rodlike polymers in isotropic and liquid crystalline phases, *J. Polym. Sci., Polym. Phys. Ed.* vol **19** p 229–243

[4] Luo C, Zhang H and Zhang P 2004 The structure of equilibrium solutions of one dimensional Doi equation *Nonlinearity*, to appear.

[5] Onsager L 1949 The effects of shape on the interaction of colloidal particles *Ann. N. Y. Acad. Sci* v **51** p 627–659