Note on Uniqueness of the Isotropic Solution of the 2D Doi-Onsager Model

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Abstract. In this short note we prove a new uniqueness result for the 2D Doi-Onsager model for the isotropic-nematic phase transition in liquid crystals. Our result applies to the model with general interaction kernels. In particular, for the Onsager kernel we prove that the trivial solution is unique for $\lambda < \sqrt{\pi}$. This improves the previous bound of $\frac{\pi}{2}$ obtained in [M. A. Niksirat, X. Yu, On stationary solutions of the 2D Doi-Onsager model, J. Math. Anal. Appl. 430 (2015) 152–165].

1. Introduction

Liquid crystals are characterized by phase transitions, when the internal organization of the molecules undergo sudden changes. The mathematical study of such changes started in 1949 when Lars Onsager proposed in [Ons49] a model for the phase transition in dilute colloidal solutions of rod-like molecules between the so-called isotrophic phase, where the molecules are random in both location and direction, and the nematic phase, where the molecules are still randomly located but become more or less aligned with a "preferred" direction.

Onsager's model involves a probability density function $f(\boldsymbol{r})\colon \mathbb{S}^2 \mapsto [0,\infty)$, where $\mathbb{S}^2$ is the unit sphere in $\mathbb{R}^3$, which models the distribution of directions of the molecules. It can be generalized to the d-dimensional unit sphere $\mathbb{S}^{d-1}$ for any dimension $d \geqslant 2$ in a straightforward manner. We present the generalized model below.

Let $f(\boldsymbol{r})\colon \mathbb{S}^{d-1} \mapsto [0,\infty)$ be the probability density function characterizing the directions of the molecules, that is

$$P(\text{the rod is along } \boldsymbol{r} \in A \subseteq \mathbb{S}^{d-1}) = \int_A f(\boldsymbol{r})\,\mathrm{d}\sigma(\boldsymbol{r}) \tag{1}$$

where $\sigma(\boldsymbol{r})$ is the volume element on $\mathbb{S}^{d-1}$. The following requirements are natural.

$$f(\boldsymbol{r}) \geqslant 0, \qquad \int_{\mathbb{S}^{d-1}} f(\boldsymbol{r})\,\mathrm{d}\sigma(\boldsymbol{r}) = 1. \tag{2}$$

We further assume that there is no distinction between the two ends of the molecules. Such assumption leads to

$$f(\boldsymbol{r}) = f(-\boldsymbol{r}) \qquad \forall \boldsymbol{r} \in \mathbb{S}^{d-1}. \tag{3}$$

By limiting consideration to the interaction of two or less molecules, Onsager derived that the equilibrium distribtions should be critical points of the energy functional

$$E(f) := \int_{\mathbb{S}^{d-1}} (\log f(\boldsymbol{r}))\, f(\boldsymbol{r})\,\mathrm{d}\sigma(\boldsymbol{r}) + \frac{1}{2}\int_{\mathbb{S}^{d-1}} (U(f)(\boldsymbol{r}))\, f(\boldsymbol{r})\,\mathrm{d}\sigma(\boldsymbol{r}) \tag{4}$$

where the interaction potential $(U(f))$ is given by

$$U(f)(\boldsymbol{r}) := \lambda \int_{\mathbb{S}^{d-1}} K(\boldsymbol{r},\boldsymbol{r}')\, f(\boldsymbol{r}')\,\mathrm{d}\sigma(\boldsymbol{r}'). \tag{5}$$

The parameter λ in (5) represents the concentration of the molecules in the carrier fluid. It can also be interpreted as the inverse of the absolute temperature.

One of the most important result of [Ons49] is the derivation of the interaction kernel

$$K(\boldsymbol{r}, \boldsymbol{r}') := \sqrt{1 - (\boldsymbol{r} \cdot \boldsymbol{r}')^2}, \tag{6}$$

which we will refer to as the Onsager kernel in the remaining of this note. On the other hand, from a mathematical point of view it is natural to consider general kernels satisfying the following symmetry properties.

$$K(-\boldsymbol{r}, \boldsymbol{r}') = K(\boldsymbol{r}, \boldsymbol{r}'); \quad K(\boldsymbol{r}, \boldsymbol{r}') = K(\boldsymbol{r}', \boldsymbol{r}); \quad K(\boldsymbol{r}, \boldsymbol{r}') = K(T\boldsymbol{r}, T\boldsymbol{r}') \quad \forall T \in O(d). \tag{7}$$

Under the above assumptions, the quantitative understanding of Onsager's model reduces to the study of the following nonlinear functional equation which is the Euler-Lagrange equation of (2)–(5).

$$f(\boldsymbol{r}) = \frac{e^{-U(f)(\boldsymbol{r})}}{\int_{\mathbb{S}^{d-1}} e^{-U(f)(\boldsymbol{r})} \, \mathrm{d}\sigma(\boldsymbol{r})}, \qquad f(\boldsymbol{r}) = f(-\boldsymbol{r}). \tag{8}$$

From (8) it is immediately seen that $f(\boldsymbol{r}) \equiv \frac{1}{|\mathbb{S}^{d-1}|}$ is a trivial solution for all λ. This solution describes the isotropic phase where all directions are equally likely to be taken. To understand the isotropic-nematic phase transition we need to study the appearance of non-trivial solutions as λ varies, that is the bifurcation structure of (8). This is very difficult to do for the general kernel (7). Nevertheless, much progress has been made for kernels having a finite spherical harmonic expansion (Fourier expansion when $d = 2$), see e.g. [CLW10], [CKT04], [CV05], [FS05a], [FS05b], [LZZ05a], [LV10], [LZZ05b], [WH08], [ZWFW05], [ZWWF07]. For such kernels the corresponding potential U lives in a finite dimensional function space and (8) can be reduced to a finite system of nonlinear equations.

In contrast, study of the model with the Onsager kernel (6) is less successful. In [WZ08], the first three bifurcations from the trivial solution are computed numerically for the two-dimensional problem. Later in [NY15], local bifurcation structure from the trivial solution is obtained for $d = 2$ through a new method based on the Leray-Schauder degree theory. It is also proved in [NY15] that when $\lambda < \lambda_0$ for some $\lambda_0 > 0$ depending on K, the only solution is the trivial one. Very recently, similar uniqueness and bifurcation analysis for $d = 3$ has been carried out in the preprint [Vol15] through variational method.

In the following we focus on the two-dimensional problem which could be written as

$$f(\theta) = \frac{e^{-U(f)(\theta)}}{\int_{-\pi}^{\pi} e^{-U(f)(\theta)} \, \mathrm{d}\theta}, \quad f(\theta) = f(\pi + \theta), \quad U(f)(\theta) = \lambda \int_{-\pi}^{\pi} K(\theta - \theta') \, f(\theta') \, \mathrm{d}\theta'. \tag{9}$$

We also denote by k_m the Fourier coefficients of K, that is

$$K(\theta) = \sum_{m=0}^{\infty} k_m \cos(2\, m\, \theta). \tag{10}$$

For (9) the following uniqueness result has been proved in [NY15].

Theorem 1. ([NY15]) *Let $K \in W^{1,\infty}([-\pi, \pi])$. The problem (9) has a unique solution, which must be the trivial solution, when $0 < \lambda < (\sum_{m=1}^{\infty} |k_m|)^{-1}$.*

The goal of this note is to improve Theorem 1 to the following theorem for a large class of kernels including the Onsager kernel.

Theorem 2. *Let $K \in W^{1,\infty}([-\pi,\pi])$. Then problem (9) has a unique solution, which must be the trivial solution, when*

i. $0<\lambda<(\sum_{m=1}^{\infty}|k_m|)^{-1/2}(\sum_{m\text{ odd}}|k_m|)^{-1/2}$, *if* $|k_m|\geqslant 4|k_{2m}|$ *for all* m;

ii. $0<\lambda<\frac{2}{\sqrt{3}}(\sum_{m=1}^{\infty}|k_m|)^{-1}$, *if* $|k_m|<4|k_{2m}|$ *for all* m.

Remark 3. By (6), $K(\theta)=|\sin\theta|$ for the Onsager kernel. This gives $k_m=-\frac{4}{\pi(4m^2-1)}$ which satisfies $|k_m|\geqslant 4|k_{2m}|$. As $\sum_{m\text{ odd}}\frac{4}{\pi(4m^2-1)}=\frac{1}{2}$, in this case we improve the range of λ guaranteeing the uniqueness of solutions from $\lambda<\frac{\pi}{2}$ to $\lambda<\sqrt{\pi}$.

In the following two sections we will prove Theorem 2. Although many preparatory steps of the proof are the same as those in the proof of Theorem 1 in [NY15], we choose not to omit them to make the paper reasonably self-contained. On the other hand, we will avoid repetition by presenting these materials in a more compact manner as detailed presentation can be found in [NY15].

2. Preparations

Similar to [NY15], we convolve the equation for f in (9) by K to obtain the the following equation for the potential U.

$$U(\theta)=\frac{\int_{-\pi}^{\pi}\lambda K(\theta-\theta')\,e^{-U(\theta')}\,\mathrm{d}\theta'}{\int_{-\pi}^{\pi}e^{-U(\theta)}\,\mathrm{d}\theta},\qquad U(\theta)=U(\theta+\pi). \tag{11}$$

Next we define $\overline{K}:=\frac{1}{2\pi}\int_{-\pi}^{\pi}K(\theta)\,\mathrm{d}\theta$ and write

$$\tilde{K}(\theta):=K(\theta)-\overline{K},\qquad V(\theta):=U(\theta)-\lambda\overline{K}. \tag{12}$$

From (11) the equation for V can be easily derived as

$$V(\theta)=\frac{\int_{-\pi}^{\pi}\lambda\tilde{K}(\theta-\theta')\,e^{-V(\theta')}\,\mathrm{d}\theta'}{\int_{-\pi}^{\pi}e^{-V(\theta)}\,\mathrm{d}\theta},\quad \int_{-\pi}^{\pi}V(\theta)\,\mathrm{d}\theta=0,\quad V(\theta)=V(\theta+\pi). \tag{13}$$

Denoting

$$H:=\left\{V(\theta)\in H^1([0,2\pi]);V(\theta)=V(\theta+\pi)\ a.e.;\int_{-\pi}^{\pi}V(\theta)\,\mathrm{d}\theta=0;\ V(\theta)=V(2\pi-\theta)\ a.e.\right\}, \tag{14}$$

$$\Gamma(V)(\theta):=\frac{\int_{-\pi}^{\pi}\tilde{K}(\theta-\theta')\,e^{-V(\theta')}\,\mathrm{d}\theta'}{\int_{-\pi}^{\pi}e^{-V(\theta)}\,\mathrm{d}\theta}, \tag{15}$$

we rewrite (13) into a fixed-point problem.

$$V(\theta)=\lambda\Gamma(V)(\theta),\qquad V(\theta)\in H. \tag{16}$$

Note that the restriction $V(\theta)=V(2\pi-\theta)$ in (14) corresponds to the a priori axisymmetry of solutions which was proved in [WZ08] and [CLW10].

We will need the following results for Γ and H. For their proofs see [NY15].

Proposition 4. **([NY15])** *Assume $K\in W^{1,\infty}([-\pi,\pi])$.*

a) The problems (9) and (16) are equivalent.

b) H *is a Hilbert space.*

c) $\Gamma: H \mapsto H$ *is compact.*

d) Γ *is Fréchet differentiable.*

e) Let $m,\ n \in \mathbb{N}$*. The* $m,\ n$ *entry of the matrix representation* A *of the Jacobian* $D\Gamma$ *is* $\frac{k_m A_{mn} (1 + 4 m n)}{\sqrt{4 m^2 + 1} \sqrt{4 n^2 + 1}}$ *where*

$$A_{mn} := \int_{-\pi}^{\pi} \cos(2 m \theta)\, \mathrm{d}\mu_V \cdot \int_{-\pi}^{\pi} \cos(2 n \theta)\, \mathrm{d}\mu_V - \int_{-\pi}^{\pi} \cos(2 m \theta) \cos(2 n \theta)\, \mathrm{d}\mu_V \tag{17}$$

with the probability measure $\mathrm{d}\mu_V$ *defined through*

$$\mathrm{d}\mu_V := \left(\int_{-\pi}^{\pi} e^{-V(\theta)}\, \mathrm{d}\theta \right)^{-1} e^{-V(\theta)}\, \mathrm{d}\theta. \tag{18}$$

A crucial part in the proof of Theorem 1 in [NY15] is the following Gruess-type inequality which gives $|A_{mn}| \leqslant 1$ for all $m, n \in \mathbb{N}$.

Lemma 5. ([NY15]) *Let* μ *be a probability measure over a domain* Ω*. Let* $f, g \in L^\infty(\Omega)$ *satisfy* $a \leqslant f \leqslant A, b \leqslant g \leqslant B$ *a.e., then*

$$\left| \int_\Omega f(x)\, g(x)\, \mathrm{d}\mu - \left(\int_\Omega f(x)\, \mathrm{d}\mu \right) \left(\int_\Omega g(x)\, \mathrm{d}\mu \right) \right| \leqslant \frac{(A - a)\,(B - b)}{4}. \tag{19}$$

In such generality (19), and consequently the estimate $|A_{mn}| \leqslant 1$, is sharp. Nevertheless improvement is possible due to the following observation. What we should estimate is not $|A_{mn}|$ per se, but the infinite sum $\sum_{m=1}^\infty \frac{k_m A_{mn} (1 + 4 m n)}{\sqrt{4 m^2 + 1} \sqrt{4 n^2 + 1}}$. The goal of this note is to reveal a hidden structure in this sum that leads to significant cancellations.

We end this preparatory section with the following simple lemma.

Lemma 6. *Let* A_{mn} *be defined as in (17). Then* $|A_{mn}| \leqslant A_{mm}^{1/2} A_{nn}^{1/2}$*.*

Proof. This follows immediately from

$$|A_{mn}| = \frac{1}{2} \left| \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} [\cos(2 m \theta) - \cos(2 m \theta')]\, [\cos 2 n \theta - \cos(2 n \theta')]\, \mathrm{d}\mu_V(\theta)\, \mathrm{d}\mu_V(\theta') \right| \tag{20}$$

and the Cauchy-Schwartz inequality. □

3. PROOF OF THEOREM 2

Following [NY15], we apply the classical Leray-Schauder degree theory to the fixed point problem

$$(I - \lambda \Gamma)(V) = 0, \qquad V \in H \tag{21}$$

where Γ and H are defined in (15) and (14), respectively. The idea is to show the existence of $\Lambda > 0$ such that when $0 < \lambda < \Lambda$, both the degree of the mapping $I - \lambda \Gamma$ and the index at each possible solution are 1. Once these solutions are shown to be isolated, uniqueness readily follows from the fact that degree is the sum of indices.

The most important part of the proof is the following estimate.

Proposition 7. *Let $\lambda_{\max}$ be the maximal eigenvalue of the Jacobian $D\Gamma$. Then*

$$\lambda_{\max} \leqslant \begin{cases} \left(\sum_{m \text{ odd}}^{\infty} |k_m|\right)^{1/2} \left(\sum_{m=1}^{\infty} |k_m|\right)^{1/2} & |k_m| \geqslant 4\,|k_{2m}| \text{ for all } m \\ \frac{\sqrt{3}}{2} \sum_{m=1}^{\infty} |k_m| & |k_m| < 4\,|k_{2m}| \text{ for all } m \end{cases}. \tag{22}$$

Proof. Following Proposition 4 we have

$$(D\Gamma)_{mn} = \frac{k_m\,A_{mn}\,(1 + 4\,m\,n)}{\sqrt{4\,m^2 + 1}\,\sqrt{4\,n^2 + 1}} \tag{23}$$

which gives

$$\lambda_{\max} \leqslant \sum_{m=1}^{\infty} |k_m\,A_{mn}|. \tag{24}$$

Thanks to Lemmas 5 and 6 we have $|A_{mn}| \leqslant A_{mm}^{1/2}\,A_{nn}^{1/2} \leqslant A_{mm}^{1/2}$. Therefore (24) implies

$$\lambda_{\max} \leqslant \left(\sum_{m=1}^{\infty} |k_m|\,A_{mm}\right)^{1/2} \left(\sum_{m=1}^{\infty} |k_m|\right)^{1/2}. \tag{25}$$

To estimate $\sum_{m=1}^{\infty} |k_m|\,A_{mm}$ we recall (17) and calculate

$$\begin{aligned} \sum_{m=1}^{\infty} |k_m|\,A_{mm} &= \sum_{m=1}^{\infty} |k_m| \left[\int_{-\pi}^{\pi} \cos^2(2\,m\,\theta)\,\mathrm{d}\mu_V - \left(\int_{-\pi}^{\pi} \cos(2\,m\,\theta)\,\mathrm{d}\mu_V\right)^2\right] \\ &= \sum_{m=1}^{\infty} |k_m| \left[\frac{1}{2} + \frac{1}{2}\int_{-\pi}^{\pi} \cos(4\,m\,\theta)\,\mathrm{d}\mu_V - \left(\int_{-\pi}^{\pi} \cos(2\,m\,\theta)\,\mathrm{d}\mu_V\right)^2\right. \\ &=: \sum_{m=1}^{\infty} |k_m| \left[\frac{1}{2} + \frac{\mu_{2m}}{2} - \mu_m^2\right] \\ &= \sum_{m=1}^{\infty} \frac{|k_m|}{2} + \sum_{m=1}^{\infty} \left(\frac{|k_m|}{2}\,\mu_{2m} - |k_{2m}|\,\mu_{2m}^2\right) - \sum_{m \text{ odd}} |k_m|\,\mu_m^2, \end{aligned} \tag{26}$$

where $\mu_m := \int_{-\pi}^{\pi} \cos(2\,m\,\theta)\,\mathrm{d}\mu_V$. We notice that $|\mu_m| \leqslant 1$.

To bound the middle term in (26), we calculate

$$\max_{\mu \in [-1,1]} \left[\frac{|k_m|}{2}\,\mu - |k_{2m}|\,\mu^2\right] = \begin{cases} \frac{|k_m|}{2} - |k_{2m}| & \frac{|k_m|}{4\,|k_{2m}|} \geqslant 1 \\ \frac{|k_m|^2}{16\,|k_{2m}|} < \frac{|k_m|}{4} & \frac{|k_m|}{4\,|k_{2m}|} < 1 \end{cases}. \tag{27}$$

Now we discuss the two cases.

- $|k_m| \geqslant 4\,|k_{2m}|$ for all m. In this case we have $\frac{|k_m|}{2}\,\mu_{2m} - |k_{2m}|\,\mu_{2m}^2 \leqslant \frac{|k_m|}{2} - |k_{2m}|$ for all m and consequently

  $$\sum_{m=1}^{\infty} |k_m|\,A_{mm} \leqslant \sum_{m \text{ odd}}^{\infty} |k_m|\,(1 - \mu_m^2) \leqslant \sum_{m \text{ odd}}^{\infty} |k_m|, \tag{28}$$

  which gives

  $$\lambda_{\max} \leqslant \left(\sum_{m \text{ odd}}^{\infty} |k_m|\right)^{1/2} \left(\sum_{m=1}^{\infty} |k_m|\right)^{1/2}. \tag{29}$$

- $|k_m| < 4\,|k_{2m}|$ for all m. In this case we have $\frac{|k_m|}{2}\,\mu_{2m} - |k_{2m}|\,\mu_{2m}^2 \leqslant \frac{|k_m|}{4}$ for all m and consequently
$$\sum_{m=1}^{\infty} |k_m|\,A_{mm} \leqslant \frac{3}{4}\sum_{m=1}^{\infty} |k_m| \tag{30}$$
which gives
$$\lambda_{\max} \leqslant \frac{\sqrt{3}}{2}\sum_{m=1}^{\infty} |k_m|. \tag{31}$$

Thus ends the proof. □

Corollary 8. *For the Onsager kernel* $\lambda_{\max} \leqslant \sqrt{\pi}$.

Proof. For the Onsager kernel we have $k_m = -\frac{4}{\pi\,(4\,m^2-1)}$ which belongs to the case $k_m \geqslant 4\,k_{2m}$. □

Now we are ready to prove Theorem 2.

Proof. (of Theorem 2) We follow [NY15] and divide the proof into four steps. Let $\Lambda := (\sum_{m\text{ odd}}^{\infty} |k_m|)^{-1/2}\,(\sum_{m=1}^{\infty} |k_m|)^{-1/2}$ when $|k_m| \geqslant 4\,|k_{2m}|$ for all m, and $\Lambda := \frac{2}{\sqrt{3}}\,(\sum_{m=1}^{\infty} |k_m|)^{-1}$ when $|k_m| < 4\,|k_{2m}|$ for all m.

1. There is a bounded open set $\Omega \subset H$ such that $(I - \lambda\,\Gamma)(V) = 0$ has no solution outside Ω for all $0 < \lambda < \Lambda$. To see this , let $R := \Lambda^{-1}\,\|\tilde{K}\|_{W^{1,\infty}}$. Then it is clear that $\lambda\,\Gamma(V) \in B(0,R)$ and we can simply take $\Omega = B(0,R)$.
2. $\deg(I - \lambda\,\Gamma, \Omega, 0) = 1$. We consider the homotopy $H(t) := I - t\,\lambda\,\Gamma$ with $t \in [0,1]$. It is clear that $H(t)(V) = 0$ has no solution on $\partial\Omega$ for any $t \in [0,1]$. The conclusion now follows from $\deg(I, \Omega, 0) = 1$.
3. The solutions are isolated. By Proposition 4 Γ is Fréchet differentiable and compact. By Proposition 7 there holds $\lambda_{\max}(D\Gamma) \leqslant \Lambda^{-1}$ which implies $\ker(I - \lambda\,D\Gamma) = \{0\}$. Therefore by Fredholm alternative (see e.g. [AP93]) $I - \lambda\,D\Gamma$ is a homeomorphism. Consquently the solutions are isolated.
4. The index of any solution is 1. By Proposition 7 there holds $\lambda_{\max}(D\Gamma) \leqslant \Lambda^{-1}$. Thus for $0 < \lambda < \Lambda$, all the eigenvalues of $I - \lambda\,D\Gamma$ are bounded below by the positive constant $1 - \frac{\lambda}{\Lambda}$. Consequently the index of the map $I - \lambda\,\Gamma$ is 1 everywhere.

As the solutions are all isolated, we have
$$\deg(I - \lambda\,\Gamma, \Omega, 0) = \sum \text{indices at solutions in } \Omega \tag{32}$$
and uniqueness follows. □

Remark 9. Further improvement can be obtained exploring the factor $|A_{nn}|^{1/2}$ that has been discarded in (25) using the rough bound $|A_{nn}|^{1/2} \leqslant 1$ coming from Lemma 5. We observe that as V solves (16), there is a priori L^∞ bounds (depending on λ) on the probability density of the measure $\mathrm{d}\mu_V$ defined in (18). Such bounds implies $|A_{nn}| \lesssim \rho < 1$ for some absolute constant ρ. However the analysis is very technical and the improvement is minor (ρ is close to 1). Therefore we will not present it here.

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