Some Problems on the Dynamics of Nematic Liquid Crystals



Mark Wilkinson

St Edmund Hall

University of Oxford

A thesis submitted for the degree of

Doctor of Philosophy in Mathematics

Trinity 2013

To Charlie, Pauline and Karin.

Acknowledgements

I would like to thank my supervisor, John Ball, for his expert guidance and support over the past four years. It has been an honour for me to have worked as his student and as a member of the OxPDE centre.

It is also with my deepest gratitude that I acknowledge my supervisor, Arghir Zarnescu, for his insight and guidance during my time in Oxford. I am grateful to have been his first student. I only hope I can be the supportive and generous supervisor for my future students that he has been for me.

During my third year, I spent some time at the University of Sussex, Brighton, as a Visiting Research Fellow. I also had the pleasure of being a visitor at the Hausdorff Institute, Bonn, for three months. I would like to express my appreciation to both of these institutions for having offered me very comfortable research environments. I am also grateful to Professor Laure Saint-Raymond for several invitations to Paris during my final year in Oxford.

I am particularly thankful to Professor Ball for the opportunity to study as a member of the vibrant OxPDE centre. Besides benefitting from its wonderful seminar series, the student travel funding it provided allowed me to travel frequently throughout my DPhil years. The experience was a formative one.

I would like to thank my mentor and friend, Professor Adam McBride, for his wonderful support and guidance both during and beyond my undergraduate years at the University of Strathclyde. Were it not for that fateful meeting in the summer of 2005, I certainly would be nowhere close to the point at which I stand today.

Special words of thanks go to François Genoud, Gabriel Koch and Tianyi Wang who offered me brotherhood. I would like to extend my appreciation to my colleagues Giovanni Alberti, Chuei-Yee Chen, Judith Campos, Michael Helmers, Christof Heuer, Christopher Hopper, Tom Hudson, Kostas Koumatos, Adrian Martin, Norman Metzner, Anton Mühlemann, Michaela Nieuwenhuis, Parth Soneji, Peter Pang and Xiang Wei for their friendship during my time at Oxford.

Most of all, I thank my mother, father and sister for their support and love. I dedicate this thesis to you.

Oxford, August 2013

"*If people do not believe that mathematics is simple,*
it is only because they do not realise how complicated life is."
John von Neumann

Contents

1 Introduction **1**

1.1 Nematic Order Parameters 2
1.2 Landau-de Gennes Theory 7
1.3 Dynamic Theory of Beris and Edwards 15
1.4 Overview of this Thesis 23

2 Dynamics and Eigenvalue Constraints **26**

2.1 Introduction 27
2.2 The Ball-Majumdar Singular Potential f 34
2.3 The Modified Beris-Edwards Model 39
2.4 Statement of Main Results 43
2.5 Energy Dissipation of the Beris-Edwards Equations 45
2.6 A Formal Maximum Principle for $f(Q)$ 50
2.7 Existence of Strictly Physical Weak Solutions 51
2.8 Existence of Global Strong Solutions in Dimension 2 71
2.9 Comments on the Existence Theory for $\xi \neq 0$ 77
2.10 Discussion 78
2.11 Appendix: Properties of the Ball-Majumdar Potential f 80

3 Dynamic Statistical Scaling **84**

3.1 Introduction 85
3.2 Some Preliminary Results 92
3.3 A Representation Formula 98
3.4 The Scaling Regime $L(t) = t^{1/2}$ 107
3.5 The Scaling Regime $L(t) = t$: An Observation 116
3.6 Closing Remarks 117

4 Concluding Remarks **118**

Bibliography **119**

Chapter 1

Introduction

Outline. In this chapter, we introduce the Q-tensor order parameter for nematic liquid crystals. Following this, we present a derivation of the two main models of dynamics of nematics employed in this thesis, namely the $L^2(\mathbb{R}^3)$-gradient flow of the *Landau-de Gennes* energy and the hydrodynamic theory of Beris and Edwards [13]. To conclude, we present the main results of this thesis which are to appear in the journal articles Wilkinson [85] and Kirr, Wilkinson and Zarnescu [50].

1.1 Nematic Order Parameters

The systems of condensed matter in which we are interested in this thesis are *thermotropic nematic liquid crystals*. We shall often refer to this class of materials simply as *nematics*. Nematics form a class of organic compounds whose constituent molecules are typically long and rod-like. The principle interest in such materials, especially for those who work in the display industry, relates to the *local ordering phenomenon* they exhibit when quenched from a high temperature state to a suitably low one.

In the high temperature state, known commonly as the *isotropic* phase, both molecular orientations and molecular centres of mass can be considered as randomly distributed throughout the material. Yet in the low temperature state, to which we subsequently refer as the *nematic* phase, the rod-like molecules tend to align locally with one another, with no such discernable order attributed to their centres of mass. Therefore, in the appropriate temperature interval depending on the nematic material of interest, this local molecular alignment endows nematics with optical properties reminiscent of crystals, while the lack of ordering in the molecular centres of mass permits these materials to flow like liquids. We discuss further details and the modelling of this temperature-dependent *phase transition* in section 1.2 below.

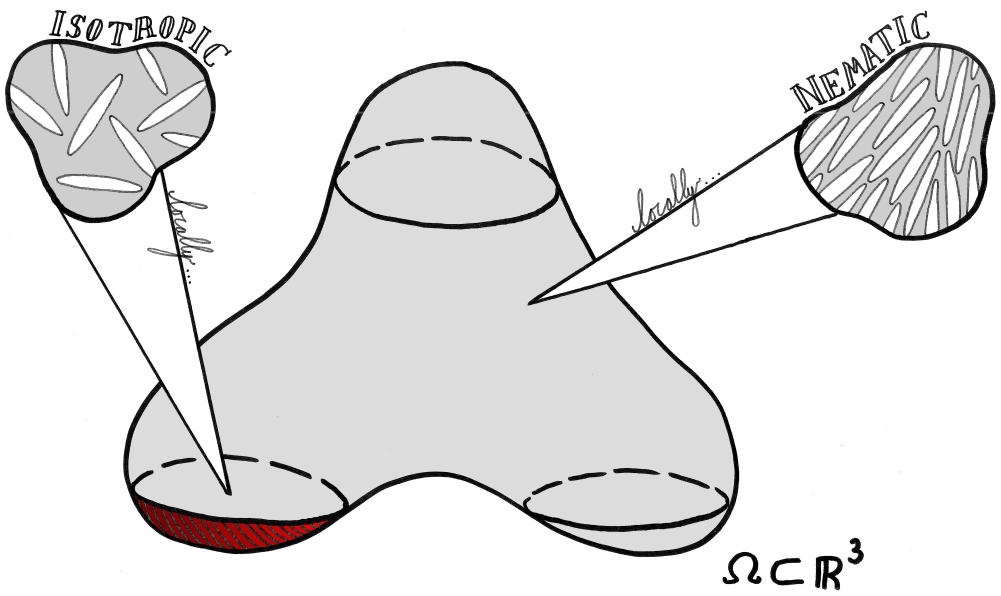


Figure 1.1: Nematic sample filling domain Ω with locally 'hot' boundary conditions (in red)

Aside from their well-known technological importance in the display industry, the modelling of nematic liquid crystals raises many interesting and often difficult mathematical problems, both in statistical mechanics and in the theory of partial differential equations.

However, before one can begin the study of any one equation or variational theory, it is necessary to specify an object that allows one to distinguish between randomness and order in molecular orientations for these materials. Such an object is known as an *order parameter* in the condensed matter physics literature.

There are a number of commonly-employed order parameters in the literature describing nematic liquid crystal systems. One could, for instance, employ a probability density function ϱ on the unit sphere $\mathbb{S}^2$ to express the likelihood of observing a molecule with a certain orientation at a given place and time. The most popular theory built using this order parameter is the Maier-Saupe theory, which is a variational theory for the equilibrium configurations of nematic systems. One could also choose to model molecular orientations by a unit vector field n, as is the case in the well-known Oseen-Frank and Ericksen-Leslie theories. However, in this thesis we focus on the mathematical analysis of two models for the dynamics of nematic liquid crystals which employ the *Q-tensor order parameter*.

The Q-tensor is a symmetric and traceless matrix $Q \in \mathbb{R}^{3\times 3}$ that allows one not only to model the isotropic and nematic phases of nematic liquid crystals, but it also describes biaxial configurations of uniaxial particles. We invite the reader to consult Mottram and Newton [62] for further information on uniaxial and biaxial configurations of both uniaxial and biaxial molecules. The two models of interest here that employ the order parameter Q are the $L^2(\mathbb{R}^3)$-gradient flow of the so-called *Landau-de Gennes* energy (section 1.2), and the hydrodynamic theory of Beris and Edwards (section 1.3)

As one might imagine, the literature on thermotropic nematic liquid crystals is vast. There are a number of excellent texts, such as Chandrasekhar [20] or De Gennes and Prost [24], which present the general theory of nematics in a very careful and thorough manner. It is for this reason we do not try to present the reader with an introduction to nematics in this thesis. Regarding the mathematical analysis of liquid crystal models, those interested in the static theory are recommended to consult Virga [84], while a good introduction to aspects of the dynamic theory can be found in Sonnet and Virga [79] and Stewart [80]. Let us now, however, offer the reader a more careful introduction to the order parameter Q of interest throughout this thesis.

The Q-tensor Order Parameter

The following discussion of the Q-tensor order parameter is merely heuristic. It remains an open problem to demonstrate to what extent an equation governing the Q-tensor (be it static or dynamic) can be understood to capture the leading order asymptotics of an underlying kinetic theory. We do not develop this idea here; however, we refer the reader to the work of Cercignani, Illner and Pulvirenti [19], Golse [40] and Saint-Raymond

[74] for results on how evolution equations governing the observable properties of particle systems in the gaseous phase can be understood as approximating moments of a kinetic equation, namely the Boltzmann equation.

Let us turn our thoughts firmly to thermotropic nematic liquid crystal systems. It is known that particles possessing different symmetries can give rise to the nematic phase. We shall work throughout with *uniaxial* nematic particles, namely those with $\mathbb{Z}^2 \times \mathbb{S}^1$ symmetry, whose $\mathbb{S}^2$-axis of symmetry can be considered the long molecular axis. The microscopic spatial configuration of such particles is completely specified by a centre of mass (a vector in $\mathbb{R}^3$) and the orientation of a long axis (an element of $\mathbb{S}^2$). A concrete example of a uniaxial particle is the ellipsoid of revolution $\mathcal{E}$ given by

$$\mathcal{E} := \left\{ z \in \mathbb{R}^3 \, : \, \left(\frac{z_1}{a}\right)^2 + z_2^2 + z_3^2 \leq 1 \right\},$$

for some $a > 1$. In liquid crystal theory, it is also common to consider systems composed of so-called *biaxial* particles, which possess fewer symmetries than that of their uniaxial counterparts. One example of a biaxial particle is the right parallelepiped, which has $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. The Q-tensor theory corresponding to biaxial particle systems requires more than just a single 3×3 matrix order parameter: see Sonnet and Virga [79] (chapter 4, section 2). We exclude this more complicated case from our subsequent discussions, and consider only the Q-tensor order parameter corresponding to *uniaxial* particles in what follows.

Suppose that a spatial domain $\Omega \subseteq \mathbb{R}^3$ is filled densely with a number N of uniaxial particles. When in motion, the microscopic configuration of each particle is characterised by the vector

$$(x, \theta, v, \omega) \in \mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^3 \times \mathbb{R}^3,$$

where x represents the centre of mass of a particle, θ its orientation, v the linear velocity of its centre of mass and ω its angular speed. We also stipulate that the particles possess no polarity, so that the particle characterised by (x, θ, v, ω) is identified with $(x, -\theta, v, \omega)$. Suppose further that such particles are *hard*, i.e. they do not interpenetrate, and experience elastic collision upon mutual contact. In the absense of external forces and intermolecular potentials, the equations of motion for this system is of the following shape,

$$\begin{cases} \dfrac{dx_i}{dt} = v_i & \dfrac{dv_i}{dt} = 0 \\ \dfrac{d\theta_i}{dt} = \omega_i & \dfrac{d\omega_i}{dt} = 0 \end{cases}$$

for $i = 1, ..., N$, for which the dynamic coupling between particles is achieved through the elastic collision boundary conditions.

Adhering to the common practice of statistical physics, as it is not possible for individual microscopic states of every molecule in a given system to be measured and tracked during their evolution without error, it is appropriate that a model of such a complex system be probabilistic. It is typical to replace the study of the above system of coupled ODEs by the study of the evolution of a probability density $\varrho = \varrho(x, \theta, v, \omega, t)$ whose law of evolution is compatible with that of the microscopic equations. For simplicity, we henceforth drop x-, v-, ω- and t-dependence on ϱ.

The probability density ϱ is not deemed to be an observable quantity of the particle system. On the other hand, suitable *moments* of the density ϱ are thought of as being experimentally-measurable. This then begs the natural question, "*What is an appropriate observable θ-moment of the probability density ϱ?*" It was the idea of the Nobel prize-winning physicist Pierre-Gilles de Gennes that the normalised matrix of second-order moments of ϱ, termed *the Q-tensor order parameter*, captures the essential information contained within ϱ with respect to molecular orientations. For a given ϱ, its associated Q-tensor is defined by

$$Q(\varrho) := \int_{\mathbb{S}^2} \left(\theta \otimes \theta - \frac{1}{3} I \right) \varrho(\theta) \, d\theta. \tag{1.1}$$

It is immediate from the definition (1.1) that Q is a symmetric and traceless 3×3 matrix with real entries. Note that the second moments are the first non-vanishing moments of ϱ, due to the symmetry assumption that $\varrho(-\theta) = \varrho(\theta)$ for all $\theta \in \mathbb{S}^2$. Moreover, the subtracted multiple of the identity tensor in (1.1) contributes no information to the order parameter Q, since

$$\frac{1}{3} \int_{\mathbb{S}^2} \varrho(\theta) \, d\theta I = \frac{1}{3} I, \tag{1.2}$$

and so this contribution to Q is indeed independent of ϱ. It is included by convention, so as to ensure Q is zero in the isotropic phase, namely when the underlying probability density is uniform,

$$\varrho_{\text{uniform}}(\theta) := \frac{1}{|\mathbb{S}^2|} \qquad \text{for all} \qquad \theta \in \mathbb{S}^2. \tag{1.3}$$

This expresses the fact that at a certain point in a nematic material, no one particle orientation is preferred over another. We invite the reader to consult De Gennes and Prost [24] (chapter 2) for details related to how this nematic order parameter is measured in the laboratory.

We remark in passing that one can show the eigenvalues λ_i of any Q satisfying (1.1) for some ϱ are constrained by the following set of inequalities,

$$-\frac{1}{3} < \lambda_i(Q) < \frac{2}{3} \qquad \text{for} \qquad i = 1, 2, 3. \tag{1.4}$$

This observation plays a significant role in chapter 2 of this thesis, and we shall explore this remark in greater detail in due course. In what is to come, we work simply with traceless

and symmetric matrices Q, without necessarily turning our thoughts to the probability measure to which they might correspond. When working with static and dynamic theories of nematics, our basic objects are those maps from a spatial domain taking values in the set of matrices

$$\mathrm{Sym}_0(3) := \left\{ Q \in \mathbb{R}^{3\times 3} \,:\, Q^T = Q \text{ and } \mathrm{tr}(Q) = 0 \right\},$$

to which we refer as the space of *Q-tensors*. Finally, as it will be of importance in what is to come, we make the following definitions.

Definition 1.1. *The zero matrix* $0 \in \mathrm{Sym}_0(3)$ *is defined to be the* **isotropic** *Q-tensor, in accord with* (1.3)*. Those elements of the diagonal form*

$$\begin{pmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & -2\lambda \end{pmatrix}$$

for some $\lambda \neq 0$ *after conjugation by an element of* $\mathrm{O}(3)$ *are defined to be* **uniaxial** *Q-tensors, i.e.* Q *is uniaxial if and only if there exists* $\mathsf{R} \in \mathrm{O}(3)$ *such that* $\mathsf{R}Q\mathsf{R}^T = \mathrm{diag}(\lambda, \lambda, -2\lambda)$*. Finally, elements of* $\mathrm{Sym}_0(3)$ *which are conjugate to matrices of the form*

$$\begin{pmatrix} \lambda & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & -\lambda-\mu \end{pmatrix}$$

for non-zero $\lambda \neq \mu$ *are defined to be* **biaxial** *Q-tensors.*

For a discussion on the role of uniaxiality and biaxiality in Q-tensor theory, we refer the reader to Majumdar [60]. For comments regarding uniaxiality and biaxiality in optics, see Virga [84] (chapter 1). Let us now define how a *map* into $\mathrm{Sym}_0(3)$ models liquid crystalline behaviour.

Definition 1.2. *Let* $\Omega \subseteq \mathbb{R}^3$*. For a given map* $Q : \Omega \to \mathrm{Sym}_0(3)$*, we define the set*

$$\{x \in \Omega \,:\, Q(x) \neq 0\}$$

to be the nematic region of the liquid crystal occupying the domain Ω*. The complement of this set in* Ω *is defined to be the isotropic region of the liquid crystal.*

Strictly speaking, we think of a liquid crystal filling Ω as in the nematic phase only if the corresponding Q-map is non-zero on a subset of of Ω of non-zero Lebesgue measure. With the basic features of the Q-tensor established, we now introduce the most prominent theory in liquid crystal science that employs this nematic order parameter.

1.2 Landau-de Gennes Theory

As we suggested in the opening section, one particularly interesting property of thermotropic nematic liquid crystals is their ability to undergo the *isotropic-nematic* phase transition when the temperature of the material is reduced from a high-temperature state to a suitably low one. However, this disorder-to-order transition is not unique to thermotropic systems. We refer the reader to the important paper of Onsager [64] for properties of the isotropic-nematic phase transition in lyotropic systems, in which the concentration of nematic particles in an ambient fluid plays the role that temperature does for thermotropic systems.

If one wishes to build a mathematical model that can predict such a phase transition in thermotropics, it is first of all necessary to say exactly what one means by *phase*, and then how one might describe its *transition* from one given phase to another. The notion of phase using the Q-tensor was set out in definitions 1.1 and 1.2 above. Let us now consider how one might model the *change* from the isotropic to the nematic phase.

Although phase transitions are inherently dynamic phenomena on the microscopic level, if a material is sufficiently close to thermodynamic equilibrium, the well-known *Landau theory of phase transitions* advocates modelling such phenomena as a bifurcation problem in the calculus of variations. For a choice of temperature parameter ϑ, one studies a physically-relevant variational theory of the sort

$$\begin{cases} \text{Minimise} & \displaystyle\int_\Omega f(\nabla Q(x), Q(x), x; \vartheta)\, dx, \\ \text{subject to} & Q \in \mathcal{A}(\overline{Q}) \quad \text{for} \quad \overline{Q} : \partial\Omega \to \mathrm{Sym}_0(3). \end{cases}$$

As such, the observable equilibrium profiles are deemed to be minimisers $Q^* \in \mathcal{A}^*_\vartheta(\overline{Q})$ of a certain energy (with density f) among a class of natural candidate maps $\mathcal{A}(\overline{Q})$. These candidate maps are subject to prescribed boundary conditions $\overline{Q}$, and the temperature ϑ is to be considered as a bifurcation parameter.

The notion of phase transition in this framework relates to the structure of the set of minimisers $\mathcal{A}^*_\vartheta(\overline{Q})$ as the temperature parameter ϑ is varied. In particular, one would like a theory such that for large values of the temperature parameter ϑ, the class of minimisers $\mathcal{A}^*_\vartheta(\overline{Q})$ is the singleton containing the isotropic map. On the other hand, for appropriately-small values of ϑ, one would like the class of minimisers to contain only nematic maps, i.e. maps Q which differ from 0 on a set of positive measure.

The Landau theory which has received the most attention in the mathematical community is the Ginzburg-Landau theory of superconductivity. In the absence of an external field, the Ginzburg-Landau energy E_{GL} corresponding to a given complex-valued map $u : \Omega \to \mathbb{C}$

is given by

$$E_{\mathrm{GL}}[u] := \int_\Omega \left(\frac{1}{2}|\nabla u|^2 + \frac{1}{4}(1-|u|^2)^2 \right) dx.$$

For more information on the rigorous analysis of this model in two spatial dimensions, especially with regards to the structure of singularities of minimisers, see Sandier and Serfaty [75] or Bethuel, Brezis and Hélein [14]. In the following section, we present what one might say is the analogue of the Ginzburg-Landau theory for Q-tensor-valued maps.

Derivation of the Landau-de Gennes Theory

We derive the model here in the case where the underlying nematic molecules may assume any orientation in $\mathbb{S}^2$. However, the same arguments can be employed, subject to some simplifications, in the case when particle orientations are confined to a plane, yielding a traceless and symmetric matrix in $\mathbb{R}^{2\times 2}$.

The derivation of the Landau-de Gennes model runs as follows. It is assumed that spatial variations in the Q-tensor field are sufficiently small so that significant contributions to the system free energy come only from Q and its first-order derivatives ∇Q. With this in mind, we henceforth adopt the two basic suppositions of Landau theory (Landau and Lifschitz [51]) for the system free energy density f. Firstly, we assume that f is an analytic function of the Q-tensor in a neighbourhood of the isotropic phase $Q = 0$, namely

$$f(D,Q) = a + a^{(1,0)}_{ijk} D_{ijk} + a^{(1,1)}_{ijk\ell m} D_{ijk} Q_{\ell m} + a^{(0,1)}_{\ell m} Q_{\ell m} + \ldots,$$

when $|(D,Q)| < r$ for some radius of convergence $r > 0$. Secondly, we stipulate that f be both frame indifferent and invariant under local reflections in space, namely that it be an *isotropic* function satisfying

$$f(T(\mathsf{R})D, \mathsf{R}Q\mathsf{R}^T) = f(D,Q) \quad \text{for all} \quad \mathsf{R} \in \mathrm{O}(3),$$

where $(T(\mathsf{R})D)_{ijk} = \mathsf{R}_{i\ell}\mathsf{R}_{jm}\mathsf{R}_{kn}D_{\ell mn}$ for any rank 3 tensor D and Q is a member of $\mathrm{Sym}_0(3)$. We invite the reader to consult the lecture notes of Ball [4] for more on this point. For convenience, let us further decompose the map f into two pieces in the following fashion,

$$f(\nabla Q, Q) = \underbrace{f(0,Q)}_{\text{bulk density}} + \underbrace{\big(f(\nabla Q, Q) - f(0,Q)\big)}_{\text{elastic density}}$$

in order that we may treat its so-called bulk contribution $f_{\mathrm{B}}(Q) := f(0,Q)$ and its elastic contribution $w(\nabla Q, Q) := f(\nabla Q, Q) - f(0,Q)$ separately.

Once a map f satisfying the above conditions has been constructed, determining the equilibrium configurations of nematics becomes a matter of minimising the associated

Landau-de Gennes energy

$$E_{\mathrm{LdG}}[Q] := \int_\Omega \left(w(\nabla Q, Q) + f_{\mathrm{B}}(Q) \right) dx$$

over some appropriate class of admissible maps $Q : \Omega \to \mathrm{Sym}_0(3)$ subject to suitable boundary conditions. Determining explicit candidates for the free energy density f is now a problem of invariant theory. We refer the reader to HILBERT [45] for an introduction to this important topic.

Let us initially consider the problem of determining the form of the bulk term, which we denote by $\widetilde{f_{\mathrm{B}}}$ from now on. It can be shown that the only scalar functions φ satisfying $\varphi(\mathsf{R}Q\mathsf{R}^T) = \varphi(Q)$ subject to Q being traceless are functions of the invariants

$$\mathrm{tr}(Q^k) \quad \text{for} \quad k \geq 2.$$

Furthermore, by the Cayley-Hamilton theorem, one can show that

$$\mathrm{tr}(Q^k) = p_k \left(\mathrm{tr}(Q^2), \mathrm{tr}(Q^3) \right) \quad \text{for} \quad k \geq 4$$

for some explicit polynomial p_k. Thus, under the two basic assumptions of Landau theory introduced above, we have that the bulk density is necessarily of the form

$$\widetilde{f_{\mathrm{B}}}(Q) = a_0 + a_1 \mathrm{tr}\left(Q^2\right) + a_2 \mathrm{tr}\left(Q^3\right) + a_3 \left(\mathrm{tr}\left(Q^2\right)\right)^2 + a_4 \mathrm{tr}\left(Q^2\right) \mathrm{tr}\left(Q^3\right) + \ldots \tag{1.5}$$

for appropriate constants a_i and radius of convergence. Since it amounts to shifting the energy scale by a constant value, we neglect the constant contribution a_0 to the energy density. When it comes to performing explicit calculations to determine the qualitative properties of a system governed by $\widetilde{f_{\mathrm{B}}}$, such an infinite series is somewhat unwieldy. Crucially, we now seek to truncate the series in such a way that the resulting model predicts an isotropic-nematic phase transition.

We emphasise that we restrict our attention to thermotropic nematic liquid crystals, namely those nematic materials whose phase depends on temperature as opposed to density in a solvent. The coefficients a_i should therefore depend in an appropriate manner on temperature ϑ, which we subsequently consider as a bifurcation parameter. The isotropic-nematic phase transition within Q-tensor theory is then modelled as the following bifurcation phenomenon for the Landau-de Gennes energy $E_{\mathrm{LdG}} = E_{\mathrm{LdG}}[\cdot\,; \vartheta]$:

There exists a critical temperature $\vartheta_* > 0$, above which the set of global minimisers of $E_{\mathrm{LdG}}[\cdot\,; \vartheta]$ is the singleton $\{0\}$ containing the isotropic phase alone, and below which it contains at least one map $\overline{Q} : \Omega \to \mathrm{Sym}_0(3)$ which is non-zero on a set of positive Lebesgue measure.

Thus, the truncated bulk nonlinearity (which we now denote by f_{B} as opposed to $\widetilde{f_{\mathrm{B}}}$) should offer a competition between the isotropic phase and some prefered nematic state that is controlled by the temperature parameter ϑ.

If λ and μ denote the two essential eigenvalues of a given Q (the other eigenvalue is simply $-\lambda-\mu$), one can show by a diagonalisation argument that

$$\operatorname{tr}\left(Q^2\right) = 2\left(\lambda^2+\lambda\mu+\mu^2\right) \qquad \text{and} \qquad \operatorname{tr}\left(Q^3\right) = -3\lambda\mu(\lambda+\mu).$$

Up to quartic order, one in turn discovers that

$$f_{\mathrm{B}}(Q) = 2a_1\left(\lambda^2+\lambda\mu+\mu^2\right) - 3a_2\lambda\mu(\lambda+\mu) + 4a_3\left(\lambda^2+\lambda\mu+\mu^2\right)^2.$$

We now consider the critical point structure of the bulk potential, in the special uniaxial case when $\lambda=\mu$. considered as a graph over $\mathbb{R}^2$. Moreover, in order that f_B be bounded from below, we assume $a_3>0$. A simple computation reveals that the critical points of the resulting quartic polynomial in λ are

$$\lambda = 0 \ \text{(isotropic)} \qquad \text{and} \qquad \lambda = \frac{12a_2 \pm \sqrt{a_2^2-24a_1a_3}}{144a_3} \ \text{(nematic)}.$$

Clearly, the isotropic phase is a candidate for a global minimiser of f_B in the uniaxial regime if and only if $a_2^2-24a_1a_3\geq 0$, the case of equality corresponding to the situation where the isotropic and nematic phases are energetically on an equal footing.

One has some choice regarding introducing dependence on the temperature parameter ϑ. It has become commonplace in the literature (see, for instance, Majumdar [59]) to assume that a_1 depends linearly on ϑ, whilst a_2 and a_3 are independent of temperature. Therefore, setting

$$a_1 = \frac{1}{2}a(\vartheta) := \frac{1}{2}\alpha(\vartheta-\vartheta_*), \qquad a_2 = -\frac{b}{3}, \qquad a_3 = \frac{c}{4}$$

for $\alpha, b, c, \vartheta_* > 0$, by the above discussion it follows that the map

$$f_{\mathrm{B}}(Q) = \frac{a(\vartheta)}{2}\operatorname{tr}\left(Q^2\right) - \frac{b}{3}\operatorname{tr}\left(Q^3\right) + \frac{c}{4}\left(\operatorname{tr}\left(Q^2\right)\right)^2$$

predicts an isotropic-nematic phase transition, whilst agreeing with the required system symmetries.

Let us also briefly mention that if one wishes to employ a model which has biaxial critical points of the bulk minimiser, one needs to work with the six-term bulk energy density

$$f_{\mathrm{B}}(Q) + \frac{d_1}{5}\operatorname{tr}\left(Q^2\right)\operatorname{tr}\left(Q^3\right) + \frac{d_2}{6}\operatorname{tr}\left(Q^2\right)^3 + \frac{d_3}{6}\operatorname{tr}\left(Q^3\right)^2,$$

for appropriate constants d_i. For more on this, we refer the reader to Gramsbergen, Longa and De Jeu [41]. One has freedom to include as many terms of the expansion

(1.5) as one wishes. However, the aim is to work with a theory that is simple as possible that still captures the main qualitative features of interest.

The question of characterising the invariant elastic contributions to the energy density is much more involved. We refer the reader to Longa, Monselesan and Trebin [58] for more on this issue. Let us only remark that the terms

$$I_1(\nabla Q) := |\nabla Q|^2, \qquad I_2(\nabla Q) := Q_{ij,j}Q_{ik,k}$$
$$I_3(\nabla Q) := Q_{ik,j}Q_{ij,k} \quad \text{and} \quad I_4(\nabla Q, Q) := Q_{k\ell}Q_{ij,k}Q_{ij,\ell}$$

are among those commonly studied in the literature which are quadratic in the gradients of Q. In particular, when Q is of uniaxial form

$$Q(n) = s\left(n \otimes n - \frac{1}{3}\right),$$

the energy density

$$w(\nabla Q, Q) := \sum_{i=1}^{4} L_i I_i(\nabla Q, Q)$$

reduces to the well-known Oseen-Frank energy density, namely

$$w(\nabla Q(n), Q(n)) = w_{\mathrm{OF}}(\nabla n, n) := k_1 (\nabla \cdot n)^2 + k_2 (n \cdot \nabla \wedge n)^2 + k_3 |n \wedge \nabla \wedge n|^2 + (k_2 + k_4)\Big(\operatorname{tr}\left((\nabla n)^2\right) - (\nabla \cdot n)^2\Big), \tag{1.6}$$

where the Frank elastic constants k_i are given explicitly in terms of the Landau-de Gennes elastic constants by

$$k_1 = 2L_1 s^2 + L_2 s^2 + L_3 s^2 - \frac{2}{3}L_4 s^3, \qquad k_2 = 2L_1 s^2 - \frac{2}{3}L_4 s^3,$$
$$k_3 = 2L_1 s^2 + L_2 s^2 + L_3 s^2 + \frac{4}{3}L_4 s^3 \qquad \text{and} \qquad k_4 = L_3 s^2.$$

For more information on the Oseen-Frank theory, including the existence and partial regularity of its global minimisers in the $H^1(\Omega)$ setting, we refer the reader to Hardt, Kinderlehrer and Lin [42].

With the discussion of the form of the energy density now complete, let us define the Landau-de Gennes energy with which we work throughout the rest of this thesis.

Definition 1.3. For a suitable spatial domain $\Omega \subseteq \mathbb{R}^3$, temperature parameter $\vartheta \in \mathbb{R}$, material-dependent critical temperature $\vartheta_* \in \mathbb{R}^3$ and material-dependent constants $\alpha, b, c > 0$, we define the *quartic Landau-de Gennes energy* to be

$$E_{\mathrm{LdG}}[Q] := \int_\Omega \left(w(\nabla Q, Q) + \frac{a(\vartheta)}{2}\operatorname{tr}\left(Q^2\right) - \frac{b}{3}\operatorname{tr}\left(Q^3\right) + \frac{c}{4}\left(\operatorname{tr}\left(Q^2\right)\right)^2 \right) dx,$$

where $a(\vartheta) := \alpha(\vartheta - \vartheta_*)$, and the elastic energy density is given by

$$w(\nabla Q, Q) := L_1|\nabla Q|^2 + L_2 Q_{ij,j}Q_{ik,k} + L_3 Q_{ik,j}Q_{ij,k} + L_4 Q_{k\ell}Q_{ij,k}Q_{ij,\ell}$$

for the so-called elastic constants $L_1, L_2, L_3, L_4 \in \mathbb{R}$. We write E_{LdG} when the values of the constants L_i are left unspecified. When $L_2 = L_3 = L_4 = 0$ and L_1 is set to $L > 0$, we shall refer to $E_{\mathrm{LdG}} \equiv E^{(L)}_{\mathrm{LdG}}$ as the *one-constant* Landau-de Gennes energy functional. When all elastic constants are specified to be non-zero, $E_{\mathrm{LdG}} \equiv E_{4-\mathrm{LdG}}$ is be said to be the *four-constant* Landau-de Gennes functional.

Throughout this thesis, we shall often set $L_2 = L_3 = L_4 = 0$ in order to recover the Dirichlet energy, as it is much simpler to work with from an analyst's point of view. The full four-constant Landau-de Gennes theory, however, offers many interesting outstanding mathematical problems. We refer the reader to the end of chapter 2 for a brief outline of some of these problems.

We claimed that this derivation can also be performed for the case when $Q \in \mathrm{Sym}_0(2)$, where

$$\mathrm{Sym}_0(2) := \left\{ Q \in \mathbb{R}^{2\times 2} \,:\, \mathrm{tr}(Q) = 0 \ \text{ and } \ Q^T = Q \right\}.$$

Indeed, one can show that in this case the one-constant theory has the form

$$E^{(L)}_{\mathrm{LdG}}[Q] = \int_\Omega \left(\frac{L}{2}|\nabla Q|^2 - \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{c}{4}\left(\mathrm{tr}\left(Q^2\right)\right)^2 \right) dx,$$

since

$$\mathrm{tr}\left(Q^3\right) = \mathrm{tr}\left(\begin{pmatrix} \lambda^3 & 0 \\ 0 & -\lambda^3 \end{pmatrix} \right) = 0.$$

In particular, when the orientations of nematic particles are constrained to lie in $\mathbb{S}^1$, the Landau-de Gennes theory reduces in form to the planar Ginzburg-Landau theory of superconductivity.

Now that the work in setting up the static theory has been done, it is rather straightforward to define the equations of dynamics with which we work in chapter 3 of this thesis. The model, which we use to study a problem concerning the isotropic-nematic phase transition, is the $L^2(\mathbb{R}^3)$-gradient flow of the one-constant Landau-de Gennes energy

$$\int_{\mathbb{R}^3} \left(\frac{1}{2}|\nabla Q|^2 + \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\,\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\left(\mathrm{tr}\left(Q^2\right)\right)^2 \right) dx,$$

namely

$$\frac{\partial Q}{\partial t} = \Delta Q - a(\vartheta)Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}\left(Q^2\right) I \right) - c\,\mathrm{tr}\left(Q^2\right) Q,$$

for $x \in \mathbb{R}^3$ and $t > 0$. Due to the structure of the nonlinearity discussed above, this model is appropriate to describe this phase transition in the setting of dynamics.

On Landau-de Gennes Theory: Rigorous Results

We shall now pass comment on some of the more recent mathematical results on the Landau-de Gennes theory, most of which have come from the Oxford group. Our discussion of these recent results is far from exhaustive. We invite the reader to consult the lecture notes of Zarnescu [88] and also those of Ball [4, 5] for an introduction to various rigorous aspects of the theory.

The majority of research efforts have focussed on determining qualitative properties of either global minimisers or critical points of the one-constant theory

$$E^{(L)}_{\mathrm{LdG}}[Q] = \int_\Omega \left(\frac{L}{2}|\nabla Q|^2 - \frac{a}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\left(\mathrm{tr}\left(Q^2\right)\right)^2 \right) dx,$$

subject to $a, b, c > 0$. In the case where $\Omega = \mathbb{R}^3$, it is well known that the so-called *melting hedgehog* given by

$$Q_{\mathrm{mh}}(x) := s(|x|)\left(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}I \right)$$

is a solution of the Euler-Lagrange equations associated with $E^{(L)}_{\mathrm{LdG}}$, where the melting coefficient s satisfies the semilinear ODE

$$s''(r) + \frac{2}{r}s'(r) - \frac{6}{r^2}s(r) = -as(r) - \frac{b}{3}s(r)^2 + \frac{2c}{3}s(r)^3 \qquad \text{for } r > 0,$$

subject to the boundary conditions

$$s(0) = 0 \qquad \text{and} \qquad \lim_{r\to\infty} s(r) = s_+ := \frac{b + \sqrt{b^2 + 24ac}}{4c}.$$

It has been reported in Ignat, Nguyen, Slastikov and Zarnescu [46] that although the melting hedgehog does not have finite energy, i.e. $E^{(L)}_{\mathrm{LdG}}[Q_{\mathrm{mh}}] = \infty$, there exists $a_0 > 0$ such that it is a locally stable critical point of $E^{(L)}_{\mathrm{LdG}}$ for values of a strictly less than a_0. The problem of the stability of the hedgehog defect as a critical point of $E^{(L)}_{\mathrm{LdG}}$ is more challenging than the corresponding case in Ginzburg-Landau theory: see [46] (section 2) for a careful discussion of this issue.

We previously hinted at the fact that the four-constant Landau-de Gennes energy $E_{4-\mathrm{LdG}}$ has a formal connection with the Oseen-Frank theory E_{OF},

$$E_{\mathrm{OF}}[n] := \int_\Omega \Big(k_1(\nabla\cdot n)^2 + k_2(n\cdot\nabla\wedge n)^2 + k_3|n\wedge\nabla\wedge n|^2 \\ (k_2+k_4)\left(\mathrm{tr}\left((\nabla n)^2\right) - (\nabla\cdot n)^2\right)\Big)\, dx, \tag{1.7}$$

with n a unit vector field on Ω. In the special case where the Frank constants k_1, k_2, k_3 and k_4 are all equal to some $k > 0$, the Oseen-Frank energy reduces to the much simpler Dirichlet energy

$$E_{\mathrm{OF}}[n] = k\int_\Omega |\nabla n|^2\, dx. \tag{1.8}$$

Therefore, the problem of determining the equilibrium profiles of a liquid crystal filling Ω in this special case is reduced to the study of harmonic maps on Ω with values in $\mathbb{S}^2$: see, for instance, the book of Lin and Wang [56]. In [61], Majumdar and Zarnescu have shown that in the small elastic constant limit $L \to 0$, global minimisers of $E_{\mathrm{LdG}}^{(L)}$ in natural spaces of admissible maps tend, in the $W^{1,2}(\Omega)$-topology (and also in the $L^{\infty}_{\mathrm{loc}}(\Omega)$-topology, away from possible defects), to so-called *uniaxial harmonic maps* of the form

$$s_+ \left(n \otimes n - \frac{1}{3} I \right), \tag{1.9}$$

where n is a global minimiser of (1.8) subject to certain compatible boundary conditions. Moreover, this convergence was refined in Nguyen and Zarnescu [63] by demonstrating, among other results, that the convergence of global minimisers of $E_{\mathrm{LdG}}^{(L)}$ to suitable uniaxial harmonic maps (1.9) can be strengthened to the $C^{1,\alpha}_{\mathrm{loc}}(\Omega)$- and $C^{j}_{\mathrm{loc}}(\Omega)$-topologies, away from possible singularities of the uniaxial harmonic maps, where $\alpha \in (0,1)$ and $j \geq 2$. This connection between the Landau-de Gennes and Oseen-Frank theories will be discussed at greater length in chapter 2.

Finally, let us briefly discuss the work of Ball and Majumdar [7] related to the role of the eigenvalue constraints (1.4) on the Q-tensor order parameter within the calculus of variations. Much of what we touch upon here will be discussed in greater detail in chapter 2, so we choose only to offer a cursory discussion of their work here. Recall that when the Q-tensor order parameter was first introduced above, we claimed that if $Q \in \mathrm{Sym}_0(3)$ arises from an underlying probability density in the manner of (1.1), then its eigenvalues $\lambda_i = \lambda_i(Q)$ should be constrained by the following set of inequalities,

$$-\frac{1}{3} < \lambda_i(Q) < \frac{2}{3} \quad \text{for} \quad i = 1, 2, 3.$$

It is therefore a natural question to ask whether or not one can expect global minimisers Q^* of the Landau-de Gennes energy

$$E_{\mathrm{LdG}}[Q] = \int_{\Omega} \left(w(\nabla Q, Q) + \frac{a(\vartheta)}{2} \mathrm{tr}\left(Q^2\right) - \frac{b}{3} \mathrm{tr}\left(Q^3\right) + \frac{c}{4} \left(\mathrm{tr}\left(Q^2\right) \right)^2 \right) dx$$

to be physical in the sense that

$$-\frac{1}{3} < \lambda_i(Q^*(x)) < \frac{2}{3} \qquad \text{for} \quad i = 1, 2, 3 \quad \text{and almost every} \quad x \in \Omega,$$

once boundary conditions and a set of admissible maps has been specified. It has been shown by Majumdar in [59] that critical points of the quartic Landau-de Gennes bulk potential can break the above eigenvalue constraints when the temperature parameter ϑ is taken to be suitably small. Such an observation indicates that predictions of the quartic Landau-de Gennes theory are not always physically meaningful. Aside from concerns about

eigenvalues, it has also been shown by Ball and Majumdar in [7] that the minimisation of $E_{4-\mathrm{LdG}}$ is ill-posed on natural sets of candidate minimisers due to the presence of $b > 0$ and $L_4 \neq 0$. These observations related to analytical and modelling issues of the quartic Landau-de Gennes theory led Ball and Majumdar to construct an alternative, yet qualitatively similar energy functional given by

$$E[Q] := \int_\Omega \left(w(\nabla Q, Q) + \vartheta\, f(Q) - \frac{\kappa}{2}|Q|^2 \right) dx, \tag{1.10}$$

for $\vartheta, \kappa > 0$, where the map $f : \mathrm{Sym}_0(3) \to \mathbb{R} \cup \{\infty\}$ is defined by

$$f(Q) := \begin{cases} \inf\limits_{\rho \in \mathcal{A}(Q)} \displaystyle\int_{\mathbb{S}^2} \rho(\omega) \log \rho(\omega)\, d\omega, & \text{whenever } -\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}, \\ \infty & \text{otherwise,} \end{cases}$$

and

$$\mathcal{A}(Q) := \left\{ \rho : \mathbb{S}^2 \to [0,1] : \int_{\mathbb{S}^2} \rho = 1 \text{ and } \int_{\mathbb{S}^2} \left(\omega \otimes \omega - \frac{1}{3} I \right) \rho(\omega)\, d\omega = Q \right\}.$$

Although we do not give the precise conditions here under which the results were established, let us remark that the authors proved in [7] that not only do global minimisers of (1.10) respect the eigenvalue constraints pointwise on the underlying spatial domain, but also that the theory is well posed in the presence of a non-zero L_4 elastic constant on natural spaces of candidate minimisers. We refer the reader to chapter 2, section 2.2 for precise statements of these results. We conclude with the remark that the singular map f will be of great use to us in this thesis when we come to discuss the question whether or not models for the *dynamics* of Q respect the eigenvalue constraints (1.4).

With our introductory discussion on the Landau-de Gennes theory complete, let us now introduce the other model of interest in this thesis, namely the nemato-hydrodynamic theory of Beris and Edwards [13].

1.3 Dynamic Theory of Beris and Edwards

The theory of Beris and Edwards we study in this thesis is but one continuum theory for the hydrodynamics of nematic liquid crystals. Indeed, there are several well-established theories for the dynamics of nematics, which each claims to describe phenomena in nematic systems on different length scales and each using one of several choices of order parameter. The most well-known dynamic theory of nematics has grown from the Ericksen-Leslie equations attributed to Ericksen [30, 31] and Leslie [52]. In the absense of external forces,

the non-inertial form of the equations (taken from Stewart [80], chapter 4) is

$$(\mathrm{EL})\begin{cases} \rho\dfrac{\partial u}{\partial t} + (u\cdot\nabla)u + \nabla P + \nabla w_{\mathrm{OF}} = \mathrm{Div}\,\tau_0, \\ \gamma_1\left(\dfrac{\partial n_i}{\partial t} - (D_0)_{ij}n_j\right) + \gamma_2 D_{ij}n_j = \dfrac{\partial}{\partial x_j}\left(\dfrac{\partial w_{\mathrm{OF}}}{\partial n_{i,j}}\right) - \dfrac{\partial w_{\mathrm{OF}}}{\partial n_i} + \lambda n, \\ \nabla\cdot u = 0, \qquad \text{and} \qquad |n(x,t)| = 1, \end{cases}$$

where $w_{\mathrm{OF}} = w_{\mathrm{OF}}(\nabla n, n)$ denotes the Oseen-Frank energy density (1.6), $\rho > 0$, $\gamma_1, \gamma_2 \in \mathbb{R}$ and $\lambda = \lambda(\nabla n, n)$ is the Lagrange multiplier associated with the constraint that $|n| = 1$. The matrices $D = D(\nabla u)$ and $D_0 = D_0(\nabla u)$ are the symmetric and anti-symmetric parts of the velocity gradient tensor ∇u, respectively. Finally, $\tau_0 = \tau_0(n, u)$ is a stress tensor defined by

$$(\tau_0)_{ij} := \alpha_1 n_i n_j (Dn)\cdot n + \alpha_2 N_i n_j + \alpha_3 n_i N_j + \alpha_4 D_{ij} + \alpha_5 n_j (Dn)_i + \alpha_6 n_i (Dn)_j,$$

where $N := \partial_t n + (u\cdot\nabla)n - D_0 n$, and $\alpha_1, ..., \alpha_6$ are real constants known commonly as the *Leslie viscosities*. This is evidently a director field theory, in which a Navier-Stokes flow field u is coupled with the evolution of the unit vector field n. However, theories for the hydrodynamics of nematics that incorporate the tensor order parameter Q, such as the aforementioned model of Beris and Edwards [13] or the model of Qian and Sheng [71], have the advantage over director-field models that they can capture biaxial molecular configurations. We do not try to offer a comprehensive overview of nematic theories in this thesis, as this has been accomplished many times by more knowledgable authors. For a clear introduction to some of the prominent dynamic models of liquid crystal science, we refer the reader to consult either Sonnet and Virga [79] or Stewart [80].

In chapter 2 of this thesis, we shall perform a rigorous analysis of the so-called Beris-Edwards equations of nemato-hydrodynamics which have received attention recently in mathematics community. To be precise, we analyse a modified system in which the one-constant Landau-de Gennes energy $E^{(L)}_{\mathrm{LdG}}$ is replaced by the singular energy of Ball and Majumdar introduced in (1.10) above. Our reason for studying the modified equations is motivated by the observation that commonly-employed models for the dynamics of a Q-tensor field need not respect the eigenvalue inequalities (1.4). Indeed, we shall expound on this in greater detail in the following chapter.

Let us now present the form of the Beris-Edwards equations which is most prominent in the literature. For material-dependent constants $\Gamma, L, \vartheta, \kappa, \nu > 0$, the Beris-Edwards system

$(\widetilde{\text{BE}})$ is given by

$$\begin{cases} \dfrac{\partial Q}{\partial t} + (u\cdot\nabla)Q - S(Q,\nabla u) = \Gamma\left(L\Delta Q - a(\vartheta)Q + b\left(Q^2 - \dfrac{1}{3}\mathrm{tr}\left(Q^2\right)I\right) - c\,\mathrm{tr}\left(Q^2\right)Q\right), \\ \dfrac{\partial u}{\partial t} + (u\cdot\nabla)u + \nabla P = \nu\Delta u + \mathrm{Div}\left(\tau(Q) + \sigma(Q)\right), \\ \nabla\cdot u = 0, \end{cases}$$

where

$$S(Q,\nabla u) := (D_0(\nabla u) + \xi D)Q_1 - Q_1(D_0 - \xi D) - 2\xi\,\mathrm{tr}\left(Q\nabla u\right)Q_1, \tag{1.11}$$

with $Q_1 := Q + \frac{1}{3}I$, and $\xi \in \mathbb{R}$. The anti-symmetric part σ of the stress tensor appearing in the Navier-Stokes equations is given by

$$\sigma(Q) := Q\frac{\delta E^{(L)}_{\mathrm{LdG}}}{\delta Q} - \frac{\delta E^{(L)}_{\mathrm{LdG}}}{\delta Q}Q. \tag{1.12}$$

Finally, the symmetric part τ of the stress tensor has the form

$$\tau(Q) := -\xi Q_1\frac{\delta E^{(L)}_{\mathrm{LdG}}}{\delta Q} - \xi\frac{\delta E^{(L)}_{\mathrm{LdG}}}{\delta Q}Q_1 + 2\xi Q_1\mathrm{tr}\left(Q\frac{\delta E^{(L)}_{\mathrm{LdG}}}{\delta Q}\right) - L\,\mathrm{tr}\left(\nabla Q\odot\nabla Q\right), \tag{1.13}$$

where $\nabla Q\odot\nabla Q$ is the fourth-order tensor with components $(\nabla Q\odot\nabla Q)_{ijk\ell} := Q_{km,i}Q_{m\ell,j}$ and the trace is a contraction on the k and ℓ indices. In addition, Div denotes the differential operator

$$\left(\mathrm{Div}\left(\tau(Q) + \sigma(Q)\right)\right)_i := \frac{\partial}{\partial x_j}\left(\tau(Q)_{ij} + \sigma(Q)_{ij}\right) \quad \text{for } i = 1,2,3,$$

which takes a matrix-valued function to a vector-valued function. Moreover, we draw the reader's attention to the presence of the formal L^2-derivative of the one-constant Landau-de Gennes theory in the coupled system, namely

$$-\frac{\delta E^{(L)}_{\mathrm{LdG}}}{\delta Q} = L\Delta Q - a(\vartheta)Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}\left(Q^2\right)I\right) - c\,\mathrm{tr}\left(Q^2\right)Q, \tag{1.14}$$

as we argue in what is to come that it is more appropriate to replace (1.14) with the derivative of the singular energy E_{BM} of Ball and Majumdar, namely

$$-\frac{\delta E_{\mathrm{BM}}}{\delta Q} = L\Delta Q - \vartheta\left\langle\frac{\partial f}{\partial Q}(Q)\right\rangle + \kappa\,Q, \tag{1.15}$$

where the map $f : \mathrm{Sym}_0(3) \to \mathbb{R}\cup\{\infty\}$ was defined above in terms of the entropy minimisation problem, and the angular brackets $\langle\cdot\rangle$ signify that we take the *trace free* part of the matrix argument. We have more to say on this when providing the motivation for the study of the modified Beris-Edwards model in the next chapter.

In their book [13], Beris and Edwards advocate that the so-called *generalised bracket* formalism is an appropriate means by which to derive equations of evolution which model

the behaviour of systems with microstructure. It is by this approach that the authors derive a theory of dynamics for Q and u. For the convenience of the reader, we now perform a brief derivation of this model, known as the *non-inertial* theory. For a derivation of the *inertial* theory, we refer the reader to [13], chapter 11.

Derivation of the Beris-Edwards Equations

As perhaps indicated by the general title of their book [13], "*Thermodynamics of Flowing Systems with Internal Microstructure*", Beris and Edwards apply their bracket formalism to derive equations of motion for several distinct materials. Our presentation of their bracket formalism here, restricted to the case of nematic liquid crystals, is in many ways too brief; in particular, we have omitted a number of rather important arguments of Beris and Edwards designed to justify the use of the so-called *master equation*. We feel that a full and careful exposition would take us too far from our current path. Instead, we refer the reader to [13], chapters 1–7 for a full discussion of the *Poisson* and *dissipation* brackets, leading to a discussion of their appearance in the master equation itself. We emphasise that the following derivation is entirely formal.

We follow [13] (chapter 11, pp.546–549), in particular working with a symmetric 3×3 matrix with unit trace, as opposed to Q. We recover an equation for Q in the final steps of the derivation. Suppose, then, that we wish to determine an appropriate set of evolution equations to describe a nematic material filling a domain $\Omega \subseteq \mathbb{R}^3$. It is henceforth assumed that the state of the system can be characterised by the order parameters $(M(x,t), u(x,t)) \in \mathrm{Sym}_0(3) \times \mathbb{R}^3$ at any point in space and time, where M encodes the local degree of nematic alignment, and u represents the incompressible flow field of the centres of mass of the constituent nematic molecules. Furthermore, we suppose that the maps M and u evolve under an unknown law, whose representative equations are yet to be determined.

Before one is able to discuss the equations of evolution for M and u, it is necessary to specify what the authors call a *Hamiltonian* H that governs the 'energy' of the system, i.e. a functional of the maps $M(\cdot,t)$ and $u(\cdot,t)$ that tracks the global loss or gain of energy of the system in Ω over time. The authors suggest that

$$H[M(\cdot,t),u(\cdot,t)] := \int_\Omega \left(\frac{1}{2}|u(x,t)|^2 + \frac{L}{2}|\nabla M(x,t)|^2 + \frac{a(\vartheta)}{2}\mathrm{tr}\left(\overline{M}(x,t)^2\right) - \frac{b}{3}\mathrm{tr}\left(\overline{M}(x,t)^3\right) + \frac{c}{4}\left(\mathrm{tr}\left(\overline{M}(x,t)^2\right)\right)^2 \right) dx, \tag{1.16}$$

where $\overline{M} := M - \frac{1}{3}I$, is an appropriate choice for systems of nematic liquid crystals. At a glance, one sees that this so-called Hamiltonian is simply the one-constant Landau-de Gennes energy $E^{(L)}_{\mathrm{LdG}}[M] \equiv E^{(L)}_{\mathrm{LdG}}[Q]$ with an additional contribution from the kinetic energy of the flow field u.

Rather than considering individual trajectories $t \mapsto (M(\cdot,t), u(\cdot,t))$ evolving under the (as of yet, still unknown) law of evolution, Beris and Edwards advocate considering the following functional G of the dynamics,

$$G(M(\cdot,t), u(\cdot,t)) := \int_\Omega g(\nabla M(x,t), M(x,t), u(x,t))\, dx, \tag{1.17}$$

for a given smooth, integrable map $g : \mathbb{R}^{3\times3\times3} \times \mathrm{Sym}_0(3) \times \mathbb{R}^3 \to \mathbb{R}$. The fundamental postulate of their theory ([13], p.168) is that the so-called *master equation* governs the time evolution of any such functional G. This assumption can then be used, in turn, to determine a physically-meaningful set of coupled PDE for the maps Q and u. Let us now introduce the master equation.

Definition 1.4 (Master Equation for Nematic Systems)**.** Suppose that $g : \mathbb{R}^{3\times3\times3} \times \mathrm{Sym}_0(3) \times \mathbb{R}^3 \to \mathbb{R}$ is continuously differentiable. For associated functionals G of the form (1.17), the time evolution of the map $t \mapsto (M(\cdot,t), u(\cdot,t))$ is assumed to satisfy the *master equation*

$$\frac{dG}{dt} = \{G, H\} + [G, H], \tag{1.18}$$

where $\{\cdot,\cdot\}$ is a *Poisson bracket* defined by

$$\begin{aligned}
\{G,H\} := &-\int_\Omega u_i \left(\frac{\delta G}{\delta u_k} \left[\frac{\delta H}{\delta u_i}\right]_{,k} - \frac{\delta H}{\delta u_k}\left[\frac{\delta G}{\delta u_i}\right]_{,k}\right) dx \\
&-\int_\Omega M_{ij} \left(\frac{\delta G}{\delta u_k} \left[\frac{\delta H}{\delta M_{ij}}\right]_{,k} - \frac{\delta H}{\delta u_k}\left[\frac{\delta G}{\delta M_{ij}}\right]_{,k}\right) dx \\
&-\int_\Omega M_{ik} \left(\left[\frac{\delta G}{\delta u_j}\right]_{,k} \frac{\delta H}{\delta M_{ij}} - \left[\frac{\delta H}{\delta u_j}\right]_{,k}\frac{\delta G}{\delta M_{ij}}\right) dx \\
&-\int_\Omega M_{jk} \left(\left[\frac{\delta G}{\delta u_i}\right]_{,k} \frac{\delta H}{\delta M_{ij}} - \left[\frac{\delta H}{\delta u_i}\right]_{,k}\frac{\delta G}{\delta M_{ij}}\right) dx \\
&+2\int_\Omega M_{k\ell}M_{ij} \left(\left[\frac{\delta G}{\delta u_i}\right]_{,j} \frac{\delta H}{\delta M_{k\ell}} - \left[\frac{\delta H}{\delta u_i}\right]_{,j}\frac{\delta G}{\delta M_{k\ell}}\right) dx.
\end{aligned}$$

and $[\cdot,\cdot]$ is a so-called *dissipation bracket* defined by

$$\begin{aligned}
[G,H] := &-\int_\Omega R_{ijk\ell} \left[\frac{\delta G}{\delta u_j}\right]_{,i} \left[\frac{\delta H}{\delta u_\ell}\right]_{,k} dx \\
&-\int_\Omega P_{ijk\ell} \frac{\delta G}{\delta M_{ij}}\frac{\delta H}{\delta M_{k\ell}}\, dx - \int_\Omega L_{ijk\ell} \left(\left[\frac{\delta G}{\delta u_j}\right]_{,i} \frac{\delta H}{\delta M_{k\ell}} - \left[\frac{\delta H}{\delta u_j}\right]_{,i}\frac{\delta G}{\delta M_{k\ell}}\right) dx \\
&-\int_\Omega L_{ijkk}M_{\ell m} \left(\left[\frac{\delta G}{\delta u_j}\right]_{,i} \frac{\delta H}{\delta M_{\ell m}} - \left[\frac{\delta H}{\delta u_j}\right]_{,i}\frac{\delta G}{\delta M_{\ell m}}\right) dx.
\end{aligned}$$

The variations $\delta H/\delta M$ and $\delta H/\delta u$ are given by

$$\frac{\delta H}{\delta M_{ij}}(M,u) = \frac{1}{2}\left(\frac{\partial h}{\partial M_{ij}} + \frac{\partial h}{\partial M_{ji}}\right) - \frac{1}{3}\mathrm{tr}\left(\frac{\partial h}{\partial M}\right)\delta_{ij}$$

$$-\frac{1}{2}\left(\frac{\partial}{\partial x_k}\left[\frac{\partial h}{\partial M_{ij,k}}\right]+\frac{\partial}{\partial x_k}\left[\frac{\partial h}{\partial M_{ji,k}}\right]\right)+\frac{1}{3}\frac{\partial}{\partial x_k}\left[\frac{\partial h}{\partial M_{ii,k}}\right]\delta_{ij},$$

and

$$\frac{\delta H}{\delta u_i}(M,u)=u_i \qquad \text{subject to } \nabla\cdot u=0,$$

where $h=h(\nabla M(x,t),M(x,t),u(x,t))$ is the integrand of the Hamiltonian (1.16). The obvious notational modifcations are made when H is replaced by G. The rank-4 tensors R,P and L are defined component-wise by

$$\begin{aligned}2R_{ijk\ell}:=\beta_1&\left(M_{ik}M_{j\ell}+M_{i\ell}M_{jk}\right)+\beta_4\left(\delta_{ik}\delta_{j\ell}+\delta_{i\ell}\delta_{jk}\right)\\&+\beta_2\left(M_{ik}\delta_{j\ell}+M_{i\ell}\delta_{jk}+\delta_{ik}M_{j\ell}+\delta_{i\ell}M_{jk}\right)\\&+\beta_3\left(M_{im}M_{mk}\delta_{j\ell}+M_{im}M_{m\ell}\delta_{jk}+\delta_{ik}M_{jm}M_{m\ell}+\delta_{i\ell}M_{jm}M_{mk}\right)\\&+\beta_5\left(M_{im}M_{mk}M_{j\ell}+M_{im}M_{m\ell}M_{jk}+M_{ik}M_{jm}M_{m\ell}+M_{i\ell}M_{jm}M_{mk}\right)\\&+\beta_6\left(M_{im}M_{mk}M_{jn}M_{n\ell}+M_{im}M_{m\ell}M_{jn}M_{nk}\right),\end{aligned}$$

and

$$P_{ijk\ell}:=\frac{1}{2\beta_7}\left(\delta_{i\ell}\delta_{jk}+\delta_{j\ell}\delta_{ik}+bM_{ij}M_{k\ell}\right)$$

and also

$$L_{ijk\ell}:=\frac{1}{2}(\beta_8-1)\left(\delta_{i\ell}M_{jk}+\delta_{j\ell}M_{ik}+\delta_{ik}M_{j\ell}+\delta_{jk}M_{i\ell}\right),$$

for material-dependent constants $\beta_1,...,\beta_8$ in $\mathbb{R}$.

This framework may seem a little overwhelming at first sight, and one might wonder why such a choice of Poisson and dissipation brackets was made by the authors. This choice of brackets is consistent with the theory of Ericksen and Leslie, in the sense that the resulting tensor equations reduce to the general Ericksen-Leslie equations when Q is strictly of uniaxial form. See Beris and Edwards [13] (p.551) or Denniston, Orlandini and Yeomans [83] (appendix A) for the Ericksen-Leslie reduction of this tensor theory. As such, one can view the evolution equations of Beris and Edwards as a generalisation of the Ericksen-Leslie theory to the case of a tensor-valued order parameter. One attractive feature of this generalisation is that biaxial arrangements of uniaxial particles may be described by the resulting hydrodynamic theory.

Let us now extract a coupled system of PDE from the master equation (1.18). Despite the rather elaborate set-up, the evolution equations for M and u may be found rather simply by balancing terms on the LHS and RHS of (1.18). Firstly, one has formally by the chain rule that

$$\frac{dG}{dt}=\int_\Omega\left(\frac{\partial g}{\partial M_{ij}}\frac{\partial M_{ij}}{\partial t}+\frac{\partial g}{\partial u_i}\frac{\partial u_i}{\partial t}\right)dx.$$

By gathering those terms which have $\partial g/\partial M$ as a common factor, we infer that since g was chosen arbitrarily, M evolves under the system

$$\frac{\partial M}{\partial t} + (u\cdot\nabla)M = \frac{1}{\beta_7}\left(L\Delta M - a(\vartheta)\overline{M} + b\left(\overline{M}^2 - \frac{1}{3}\mathrm{tr}\left(\overline{M}^2\right)I\right) - c\,\mathrm{tr}\left(\overline{M}^2\right)\overline{M}\right)$$
$$+\widetilde{S}(M,\nabla u) + \frac{3}{\beta_7}\overline{M} : \left(L\Delta M - a(\vartheta)\overline{M} + b\left(\overline{M}^2 - \frac{1}{3}\mathrm{tr}\left(\overline{M}^2\right)I\right) - c\,\mathrm{tr}\left(\overline{M}^2\right)\overline{M}\right)\overline{M},$$

where $\widetilde{S}$ has the form

$$\widetilde{S}(M,\nabla u) := \frac{1}{2}(1+\beta_8)\left(M(\nabla u)^T + \nabla u M\right) - \frac{1}{2}(1-\beta_8)\left(M\nabla u + (\nabla u)^T M\right)$$
$$-2\beta_8\mathrm{tr}\left(M\nabla u\right)M.$$

In a similar way, by gathering terms which possess the common factor $\partial g/\partial u$, we may deduce that u evolves under the system

$$\frac{\partial u}{\partial t} + (u\cdot\nabla)u + \nabla P = \mathrm{Div}\,\widetilde{\tau}(M,\nabla u),$$

where

$$\widetilde{\tau}(Q)_{ij} := -L\,\mathrm{tr}\left(\frac{\partial M}{\partial x_i}\frac{\partial M}{\partial x_j}\right) + \frac{1}{2}R_{jik\ell}\left(\partial_j u_i + \partial_i u_j\right) + (1+\beta_8)M_{jk}\frac{\delta E^{(L)}_{\mathrm{LdG}}}{\delta Q_{ki}}(\overline{M})$$
$$+(\beta_8-1)M_{ik}\frac{\delta E^{(L)}_{\mathrm{LdG}}}{\delta Q_{kj}}(\overline{M}) - 2\beta_8\mathrm{tr}\left(M\frac{\delta E^{(L)}_{\mathrm{LdG}}}{\delta Q}(\overline{M})\right)M_{ij}.$$

Up until now, we have placed no conditions upon the free constants $\beta_1,...,\beta_8$ in the equations. We refer the reader to [13] p.549 for a discussion on appropriate coefficient relations.

Let us now transform the equations to express the evolution of the order parameter Q as opposed to M. We make choices of the free constants $\beta_1,...,\beta_8$ in agreement with Denniston, Orlandini and Yeomans [83], i.e. we set

$$\beta_4 := \nu, \quad \beta_7 := \frac{1}{\Gamma}, \quad \beta_8 := \xi \quad \text{and} \quad \beta_i = 0 \ \text{otherwise},$$

for $\nu,\Gamma>0$ and $\xi\in\mathbb{R}$. Noticing that spatial and temporal derivatives of M equal those of Q, some basic manipulations yield the following system, which we subsequently term (BE):

$$\begin{cases} \dfrac{\partial Q}{\partial t} + (u\cdot\nabla)Q - S(Q,\nabla u) = \Gamma\left(L\Delta Q - a(\vartheta)Q + b\left(Q^2 - \dfrac{1}{3}\mathrm{tr}\left(Q^2\right)I\right) - c\,\mathrm{tr}\left(Q^2\right)Q\right) \\ \qquad +3\Gamma Q : \left(L\Delta Q - a(\vartheta)Q + b\left(Q^2 - \dfrac{1}{3}\mathrm{tr}\left(Q^2\right)I\right) - c\,\mathrm{tr}\left(Q^2\right)Q\right)Q, \\ \dfrac{\partial u}{\partial t} + (u\cdot\nabla)u + \nabla P = \nu\Delta u + \mathrm{Div}\left(\tau(Q) + \sigma(Q)\right), \\ \nabla\cdot u = 0, \end{cases}$$

where S is defined in (1.11), σ is given as in (1.12) and τ has the form (1.13). One should be aware, however, that this form of the system does not agree with the system ($\widetilde{\text{BE}}$) introduced earlier in this chapter. In particular, the term

$$3\Gamma Q : \left(L\Delta Q - a(\vartheta)Q + b\left(Q^2 - \frac{1}{3}\text{tr}\left(Q^2\right) I \right) - c\,\text{tr}\left(Q^2\right) Q \right) Q \tag{1.19}$$

is missing from the final form of the evolution equations. One may quickly confirm that it is not possible to nullify this term by setting any constant to zero. All recent papers in the mathematical literature treat (BE) in the absence of the term (1.19): see articles [1, 35, 65, 66, 85]. It seems the omission of (1.19) from the Beris-Edwards equations originates from the paper of Denniston, Orlandini and Yeomans [83]. Despite this omission, the system ($\widetilde{\text{BE}}$) still possesses an energy dissipation law, which makes a rigorous construction of its weak solutions possible using energy estimates. We leave it to the reader to check that (BE) also has an energy dissipation law, which also makes it amenable to a rigorous mathematical analysis using similar techniques.

On the Beris-Edwards Model: Rigorous Results

The mathematical literature on the Beris-Edwards model is a nascent one. We present herein a very brief overview of what has been achieved in recent years.

In [66], Paicu and Zarnescu were able to establish the existence of global weak solutions of ($\widetilde{\text{BE}}$) in the case when $\xi = 0$, and the underlying spatial domain is the whole space $\mathbb{R}^d$ for $d = 2, 3$. In a subsequent publication [65], they were able to improve upon their previous results by constructing global weak solutions in the case when the modulus of $|\xi|$ is small. By employing techniques due to Frémond [38], Feireisl, Rocca, Schimperna and Zarnescu extended system ($\widetilde{\text{BE}}$) in [35] to include the effects of an evolving temperature field, also replacing the Landau-de Gennes energy by the singular energy (1.10) of Ball and Majumdar. The authors were able to construct global weak solutions on the torus $\mathbb{T}^d$ for $d = 2, 3$. More recently, Abels, Dolzmann and Liu [1] considered system ($\widetilde{\text{BE}}$) posed on a bounded domain $\Omega \subset \mathbb{R}^3$ subject to Dirichlet boundary conditions, with a modification allowing the viscosity $\nu = \nu(Q)$ in the Navier-Stokes equations to depend on the Q-tensor field. Let us remark that work still needs to be done to establish the existence of strong solutions of ($\widetilde{\text{BE}}$) on bounded domains which have physically-realistic boundary conditions, namely those which are either purely uniaxial or biaxial.

Our main contribution in this thesis with regards to the Beris-Edwards model (where $E^{(L)}_{\text{LdG}}$ is replaced by E_{BM} given in (1.15)), aside from establishing a global existence theory for the equations, is the proof of a maximum principle associated with its dynamics. This result allows us to obtain further results on higher regularity of solutions in two spatial

dimensions. We hope that our results of chapter 2, to appear in the publication WILKINSON [85], will be a welcome contribution to an understanding of this model.

1.4 Overview of this Thesis

In this thesis, we study two problems in the Q-tensor theory of nematic liquid crystals. The first problem in chapter 2 concerns the Beris-Edwards equations, and the second problem in chapter 3 involves the $L^2(\mathbb{R}^3)$-gradient flow of the Landau-de Gennes energy $E^{(L)}_{\mathrm{LdG}}$. Motivation for each problem is provided at the beginning of its respective chapter. For the convenience of the reader, we present statements of the main results proved in the following two chapters. First of all, we state the main results of chapter 2, *Dynamics and Eigenvalue Constraints*.

Theorem. Suppose $d = 2, 3$, and that the spatial domain on which we work is the torus $\mathbb{T}^d$. Let f denote the Ball-Majumdar potential given by

$$f(Q) := \begin{cases} \min\limits_{\rho \in \mathcal{A}_d(Q)} \displaystyle\int_{\mathbb{S}^{d-1}} \rho(\omega) \log \rho(\omega)\, d\omega & \text{when } \ -\frac{1}{d} < \lambda_i(Q) < 1 - \frac{1}{d}, \\ \infty & \text{otherwise,} \end{cases}$$

where

$$\mathcal{A}_d(Q) := \left\{ \rho : \mathbb{S}^{d-1} \to [0,1] \ : \ \int_{\mathbb{S}^{d-1}} \rho = 1 \ \text{ and } \ \int_{\mathbb{S}^{d-1}} \left(\omega \otimes \omega - \frac{1}{d} I \right) \rho(\omega)\, d\omega = Q \right\}.$$

Given $(Q_0, u_0) \in H^1 \times L^2_{\mathrm{div}}$ with the property that

$$f(Q_0) \in L^1 \qquad \text{(physical initial data)},$$

there exists a corresponding weak solution (Q, u) of the modified Beris-Edwards system

$$(\mathrm{S}) \begin{cases} \dfrac{\partial Q}{\partial t} + (u \cdot \nabla) Q - S(Q, \nabla u) = \Gamma \left(L \Delta Q - \vartheta \left\langle \dfrac{\partial f}{\partial Q}(Q) \right\rangle + \kappa\, Q \right) \\ \dfrac{\partial u}{\partial t} + (u \cdot \nabla) u + \nabla P = \nu \Delta u + \mathrm{Div}\big(\tau(Q) + \sigma(Q) \big), \\ \nabla \cdot u = 0, \end{cases}$$

which lies in the regularity class

$$(Q, u) \in L^\infty_{\mathrm{loc}}(0, \infty; H^1) \cap L^2_{\mathrm{loc}}(0, \infty; H^2) \times L^\infty_{\mathrm{loc}}(0, \infty; L^2_{\mathrm{div}}) \cap L^2_{\mathrm{loc}}(0, \infty; H^1_{\mathrm{div}}).$$

Moreover, the dynamics have the following 'range contraction effect' on initial data Q_0,

$$f(Q(\cdot, t)) \in L^\infty \quad \text{for almost every } \ t > 0.$$

In the case when $d = 2$ and initial data $(Q_0, u_0) \in H^{k+1} \times H^k_{\mathrm{div}}$ satisfy

$$f(Q_0) \in L^\infty \qquad \text{(strictly physical initial data)},$$

there exists a corresponding strong solution (Q, u) of system (S) in the regularity class

$$(Q, u) \in L^\infty_{\mathrm{loc}}(0, \infty; H^{k+1}) \cap L^2_{\mathrm{loc}}(0, \infty; H^{k+2}) \times L^\infty_{\mathrm{loc}}(0, \infty; H^k_{\mathrm{div}}) \cap L^2_{\mathrm{loc}}(0, \infty; H^{k+1}_{\mathrm{div}}).$$

We now state the main results of chapter 3, *Dynamic Statistical Scaling*.

Theorem. Let H denote the Banach space $L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$. For any Borel measure μ_0 on H we define the associated *two-point spatial correlation function* c_{μ_0} by

$$c_{\mu_0}(r, t) := \frac{\displaystyle\int_H \int_{\mathbb{R}^3} \mathrm{tr}\left(Q(x + r)Q(x)\right)\, dx d\mu_t(Q)}{\displaystyle\int_H \int_{\mathbb{R}^3} \mathrm{tr}\left(Q(x)^2\right)\, dx d\mu_t(Q)} \qquad \text{for } r \in \mathbb{R}^3 \text{ and } t \geq 0,$$

where $\{\mu_t\}_{t \geq 0}$ is a so-called *statistical solution* of the $L^2(\mathbb{R}^3)$-gradient flow of the one-constant quartic Landau-de Gennes energy,

$$\frac{\partial Q}{\partial t} = \Delta Q - a(\vartheta)Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}\left(Q^2\right) I\right) - c\,\mathrm{tr}\left(Q^2\right) Q.$$

Suppose $(a(\vartheta), b, c)$ belongs to the region $\mathcal{D}$, where

$$\mathcal{D} := \left\{(x, y, z) \in (0, \infty)^3 \,:\, y^2 > 27xz\right\}.$$

Then, for any $\delta > 0$, there exists $\eta = \eta(a(\vartheta), b, c, \delta)$ and an open dense subset of the set

$$\left\{R \in L^\infty(\mathbb{R}^3, \mathrm{Sym}_0(3)) \,:\, \operatorname*{ess\,sup}_{x \in \mathbb{R}^3} (1 + |x|)^{8+\delta} |R(x)| < \eta\right\}$$

such that the correlation function c_{μ_0} corresponding to any initial Borel measure supported therein exhibits the following asymptotic self-similar behaviour:

$$\left\| c_{\mu_0}(r, t) - e^{-\frac{|r|^2}{8t}} \right\|_{L^\infty(\mathbb{R}^3, dr)} = \mathcal{O}\left(t^{-\frac{1}{2}}\right) \quad \text{as} \quad t \to \infty.$$

Moreover, there exist initial measures μ_0 supported on 'large' initial data for which the associated correlation function exhibits the following qualitatively-different asymptotic behaviour,

$$\lim_{t \to \infty} \left\| c_{\mu_0}(r, t) - P\left(\frac{|r|}{t}\right) \right\|_{L^\infty(\mathbb{R}^3, dr)} = 0,$$

where P is a cubic polynomial.

We do not include a chapter on mathematical prerequisites; instead, we refer the reader to the following texts. For the basic properties of Sobolev spaces, we invite the reader to consult Adams [2] or Evans [32]. An introduction to dynamical systems for PDE can be found in either Henry [44] or Robinson [72]. A good reference for the analysis of evolution equations can be found in Evans [32] and Lions [57]. For a clear introduction to semigroup theory, see Pazy [68] or Belleni-Morante and McBride [12]. The notation we adopt is standard throughout. We introduce notation which is non-standard when necessary.

Chapter 2

Dynamics and Eigenvalue Constraints

Outline. In this chapter, we discuss both the modelling and analytical issues to which certain natural restrictions on the eigenvalues of the Q-tensor order parameter give rise. In particular, when orientations of nematic particles lie on the unit sphere $\mathbb{S}^2$, the eigenvalues of the Q-tensor $Q \in \mathrm{Sym}_0(3)$ should satisfy

$$-\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}$$

for $i = 1, 2, 3$.

We concern ourselves with the rigorous analysis of the Beris-Edwards model for the dynamics of nematic flow, into which a singular potential of Ball and Majumdar [7] is built. We establish the existence of weak and strong solutions of this system under various hypotheses. This potential penalises Q-tensor configurations that break the above constraint by assigning them an infinite energy cost. As a result, eigenvalues of solutions Q respect the above inequality pointwise in space and time. This yields an existence theory for the Beris-Edwards equations in which solutions are physically meaningful.

However, we consider our main contribution to be the proof of a certain maximum principle for this system, when this singular potential of Ball and Majumdar replaces the more commonly-employed quartic Landau-de Gennes potential.

The reader who is more eager to jump straight to the analysis may wish to start at section 2.3. Otherwise, background and motivation for the problem under study are provided in section 2.1.

The results of this chapter have been submitted for publication in Wilkinson [85].

2.1 Introduction

Suppose we are given a probability measure ϱ on the unit sphere $\mathbb{S}^2$ that possesses the reflection symmetry $\varrho(E) = \varrho(-E)$ for every measurable subset $E \subset \mathbb{S}^2$. As discussed in the previous chapter, this modelling assumption amounts to saying that the underlying nematic particles are supposed to possess head-to-tail symmetry. We recall that the *Q-tensor order parameter* Q associated with ϱ is the normalised matrix of second order moments, namely

$$Q = \int_{\mathbb{S}^2} \left(\omega \otimes \omega - \frac{1}{3} I \right) \, d\varrho(\omega).$$

From this definition, one may quickly deduce that Q is a traceless and symmetric 3×3 matrix with real components. By the spectral decomposition theorem, one may infer that

$$\int_{\mathbb{S}^2} \left(\omega \otimes \omega - \frac{1}{3} I \right) \, d\varrho(\omega) = \sum_{j=1}^{3} \lambda_j e_j \otimes e_j,$$

where each e_j is a unit-norm eigenvector of Q with corresponding eigenvalue λ_j. For a fixed choice of eigenvector e_i, it follows from the above line that the spectral identity

$$\int_{\mathbb{S}^2} \left((e_i \cdot \omega)^2 - \frac{1}{3} \right) \, d\varrho(\omega) = \lambda_i \tag{2.1}$$

holds for $i = 1, 2, 3$. This reveals that the eigenvalues of the order parameter Q can be expressed explicitly in terms of the underlying probability measure ϱ. In particular, this implies that *if* a given traceless and symmetric matrix Q is associated with a probability measure on $\mathbb{S}^2$, then its eigenvalues cannot be arbitrarily large in magnitude, but should in fact be constrained by the inequalities

$$-\frac{1}{3} \leq \lambda_i(Q) \leq \frac{2}{3}. \tag{2.2}$$

In addition, since the matrix Q is traceless, we also note that the sum of the eigenvalues of Q vanishes.

Let us now consider what inequality (2.2) indicates about underlying configurations of liquid crystal molecules when any one of the eigenvalues of Q lies at the end points of this interval. Suppose without loss of generality that $\lambda_1 = -1/3$. Using the fact that ϱ is a probability measure, one may deduce from the identity

$$\int_{\mathbb{S}^2} (e_1 \cdot \omega)^2 \, d\varrho(\omega) = 0$$

that the measure ϱ should be supported on the great circle in $\mathbb{S}^2$ which lies in the plane perpendicular to the direction e_1. Similarly, in the case that $\lambda_1 = 2/3$, one can deduce that ϱ is supported only on the two points e_1 and $-e_1$, i.e.

$$\varrho := \frac{1}{2} \left(\delta_{e_1} + \delta_{-e_1} \right).$$

Interpreting these observations in physical terms, it is evident that whenever one of the eigenvalues of Q assumes one of the endpoints $-1/3$ and $2/3$, such a Q-tensor captures the cases in which one can say *with certainty* that nematic particles lie either perpendicular or parallel to a given direction in $\mathbb{R}^3$, respectively.

In our work, Q describes liquid crystals at temperatures which forbid perfect crystallinity, and so such perfect orientational order will be excluded as a feature of any model we employ. In fact, for reasons that will become apparent in the coming section when we discuss the Maier-Saupe theory of nematics, such values of the order parameter correspond to *entropically inadmissible* underlying particle configurations at non-zero temperature.

We make the following definition with which we work in the sequel.

Definition 2.1. *Suppose $d = 2$ or 3. A matrix belonging to the set*

$$\mathrm{Sym}_0(d) := \left\{ A \in \mathbb{R}^{d\times d} \,:\, A^T = A \;\; \textit{and} \;\; \mathrm{tr}(A) = 0 \right\}$$

is said to be **physical** *if and only if its eigenvalues satisfy the strict inequality*

$$-\frac{1}{d} < \lambda_i(Q) < 1 - \frac{1}{d} \tag{2.3}$$

for $i = 1, ..., d$. Otherwise, a member of $\mathrm{Sym}_0(d)$ is said to be **unphysical**.

We are interested in analysing continuum theories of nematics which employ this tensor order parameter. It is a natural question to ask whether or not solutions (in whatever reasonable sense) of well-studied static or dynamic Q-tensor models respect the physical constraint (2.3) in general. For instance, with the models of the previous chapter in mind, we ask the following:

1. Within the context of static Landau-de Gennes theory,

$$E_{\mathrm{LdG}}[Q] := \int_\Omega \Big(w(\nabla Q(x), Q(x)) + f_{\mathrm{B}}(Q(x)) \Big)\, dx$$

   if we equip the domain Ω with boundary conditions $\overline{Q} : \partial\Omega \to \mathrm{Sym}_0(d)$ that respect inequality (2.3), i.e.

$$-\frac{1}{d} < \lambda_i\left(\overline{Q}(y)\right) < 1 - \frac{1}{d} \quad \text{for all} \quad y \in \partial\Omega,$$

   can we expect the same of global minimisers, in a suitable class $\mathcal{X} = \mathcal{X}(\overline{Q})$, pointwise in the interior of the domain?

2. In the setting of dynamics, if initial data Q_0 are endowed with physical eigenvalues, can we expect that solutions $Q = Q(x,t)$ have this property for positive time, i.e.

$$-\frac{1}{d} < \lambda_i\left(Q(x,t)\right) < 1 - \frac{1}{d} \quad \text{for almost every } \; x \in \Omega \;\text{ and }\; t > 0?$$

One can consider these questions to be important, as *if* one works with a Q-tensor model in which the order parameter is interpreted as the normalised matrix second order moments of some probability distribution on particle orientations, values of Q breaking the constraint (2.2) have no clear physical interpretation.

Our study of eigenvalue constraints on the Q-tensor will be in the context of dynamics, namely the dynamics generated by a modified Beris-Edwards Q-tensor Navier-Stokes system introduced in chapter 1. Our modification is motivated by the observation that, due to the influence of velocity gradients, it is unclear whether or not the model has the property that its solutions preserve the physical constraints on eigenvalues if its initial conditions do so. In order to justify our inclusion of the Ball-Majumdar singular potential as a feature of this model carefully, let us first consider the issue of eigenvalue constraints within the static Landau-de Gennes theory.

Remark 2.1. *Mathematical questions regarding constraints on order parameters are common in the liquid crystals literature. Perhaps the best-known example concerns dynamic director-field models, in particular the Ericksen-Leslie equations, whose order parameter is unit vector $n \in \mathbb{S}^2$. The Lagrange multiplier associated with the nonlinear algebraic constraint that $|n(x,t)| = 1$ almost everywhere presents analytical difficulties in the evolution equations. Consult* Lin and Liu [54] *for further details, especially for the Ginzburg-Landau relaxation of the unit modulus constraint.*

Issue I: Eigenvalues of Global Minimisers of the Landau-de Gennes Theory

Let $\Omega \subset \mathbb{R}^3$ be a bounded, smooth and simply-connected domain. For given positive constants $L, \alpha, b, c > 0$, a temperature parameter $\vartheta \in \mathbb{R}$ and a certain fixed temperature threshold $\vartheta_* \in \mathbb{R}$, we recall that the non-dimensional one-constant Landau-de Gennes energy $E^{(L)}_{\mathrm{LdG}}$ is given by

$$E^{(L)}_{\mathrm{LdG}}[Q] = \int_\Omega \left(\frac{L}{2}|\nabla Q|^2 + \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\left(\mathrm{tr}\left(Q^2\right)\right)^2 \right) dx,$$

where $a(\vartheta) := \alpha(\vartheta - \vartheta_*)$. Let us also equip the domain with smooth, uniaxial boundary conditions $\overline{Q}$ of the shape

$$\overline{Q} = s_+(\vartheta)\left(\overline{n} \otimes \overline{n} - \frac{1}{3}I\right) \quad \text{for} \quad \overline{n} \in C^\infty(\partial\Omega, \mathbb{S}^2), \tag{2.4}$$

where the temperature- and material-dependent constant $s_+(\vartheta)$ is defined to be

$$s_+(\vartheta) := \frac{b + \sqrt{b^2 - 24a(\vartheta)c}}{4c}.$$

This choice is made as the bulk density achieves its global minimum on $\partial\Omega$ for these given boundary conditions: consult the appendix of Majumdar and Zarnescu [61] for more

on this point. As it is of importance in what is to come, we note that a simple calculation reveals the eigenvalues of $\overline{Q}$ are physical if and only if the temperature parameter ϑ lies in the interval

$$\frac{b-2c}{3\alpha}+\vartheta_*<\vartheta<\frac{b^2}{24\alpha c}+\vartheta_*.$$

For a more detailed discussion of these issues, see Majumdar [59].

For a given fixed elastic constant $L>0$, consider minimising the energy functional $E^{(L)}_{\mathrm{LdG}}$ over the natural class $\mathcal{X}=\mathcal{X}(\overline{Q})$ of all $W^{1,2}(\Omega)$ maps whose trace on the boundary agrees with the given map $\overline{Q}$. Demonstrating the existence of global minimisers in $\mathcal{X}=\mathcal{X}(\overline{Q})$ is straightforward and can be achieved by an application of the direct method of the calculus of variations. Moreover, by elliptic regularity, one can show that global minimisers are C^∞ (even analytic) in the interior of the domain: see [61], proposition 13. With the knowledge that we are assured of the existence of global minimisers, let us now explore their qualitative properties.

It is helpful at this point to define some units. Let `J` denote the Joule, `m` denote the metre, and `K` denote the Kelvin. Following the discussion contained in the appendix of Nguyen and Zarnescu [63], we rewrite the non-dimensional theory $E^{(L)}_{\mathrm{LdG}}$ considered in this thesis to reveal the role of dimensional constants:

$$E^{(L)}_{\mathrm{LdG}}[Q]=\int_\Omega\left(\frac{\widehat{L}}{2\Lambda^2 k}|\nabla Q|^2+\frac{\widehat{\alpha}(\vartheta-\vartheta_*)}{2k}\mathrm{tr}\left(Q^2\right)-\frac{\widehat{b}}{3k}\mathrm{tr}\left(Q^3\right)+\frac{\widehat{c}}{2k}\left(\mathrm{tr}\left(Q^2\right)\right)^2\right)dx,$$

where $\Lambda>0$ has the unit of length (i.e. $[\Lambda]=\mathtt{m}$) and represents the typical dimensions of a nematic sample in the laboratory, $k=10^4$ with $[k]=\mathtt{Jm^{-3}}$, and the free constants $\widehat{L},\widehat{\alpha},\widehat{b}$ and $\widehat{c}$ are dimensional and depend on the particular nematic material under investigation. Thus, in line with our previously-established notation, we have

$$L=\frac{\widehat{L}}{\Lambda^2 k},\quad a=\frac{\widehat{\alpha}(\vartheta-\vartheta_*)}{k},\quad b=\frac{\widehat{b}}{k}\quad\text{and}\quad c=\frac{\widehat{c}}{k}.$$

By certain optical experiments, the constants $\widehat{L},\widehat{a},\widehat{b},\widehat{c}$ and ϑ_* for a given nematic compound can be measured in the laboratory: see, for instance, Coles [21] for more information. Below is a table with the recorded values for the liquid crystal materials MBBA (taken from Nguyen and Zarnescu [63]) and 5CB (taken from [21]).

Table 2.1: Landau-de Gennes Constants for Nematic Materials

Material	$\widehat{L}$ `[Jm^-1]`	$\widehat{\alpha}$ `[Jm^-3K^-1]`	$(\widehat{b},\widehat{c})$ `[Jm^-3]`	ϑ_* `[K]`
MBBA	0.61×10^{-11}	0.42×10^{3}	$(0.64,0.35)\times10^{4}$	318.15
5CB	6×10^{-12}	0.044×10^{6}	$(0.816,0.45)\times10^{6}$	307

Let us suppose that Λ is of the order of a micrometer, i.e. $\Lambda=10^{-4}$, which is an appropriate length scale for the study of nematic cells used in the display industry, for

instance. Let us also fix our attention on the data for MBBA above in table (2.1). Then, for temperatures such that $\vartheta - \vartheta_*$ is of the order to 10^1 Kelvins, one can show that a, b and c are of the order 1, but the elastic constant L is of the order 10^{-7}. It therefore makes good sense to ask about the qualitative properties global minimisers of the non-dimensional theory $E^{(L)}_{\mathrm{LdG}}$ for very small values of $L > 0$, and in particular what the distribution of their eigenvalues looks like.

Following the work of Majumdar and Zarnescu [61], we consider the mathematical problem of determining the limiting form of $Q^{(L)}$ as $L \to 0$, which we denote by $Q^{(0)}$ when a limit exists. Although this is a mathematical idealisation of the problem, it is a useful one to study. It allows one to think of global minimisers $Q^{(L)}$ for non-vanishing L as $Q^{(0)}$ (on which one can obtain good qualitative information, thanks to the work of Schoen and Uhlenbeck [76]) plus a perturbation which is small in some suitable norm. As such, one might say that these so-called 'limiting harmonic maps' $Q^{(0)}$ characterise the *essential* structure of global minimsers of $E^{(L)}_{\mathrm{LdG}}$ for small $L > 0$. The following result of [61] makes this reasoning precise.

Proposition 2.1. *There exist a sequence of elastic constants $L_j \to 0$, a sequence of associated global minimisers $Q^{(L_j)}$ of $E^{(L_j)}_{\mathrm{LdG}}$ in $\mathcal{X}(\overline{Q})$ and a 'limiting harmonic map' $Q^{(0)}$ of the form*

$$Q^{(0)} = s_+(\vartheta)\left(n^{(0)} \otimes n^{(0)} - \frac{1}{3}\right),$$

with the property that

$$\lim_{j\to\infty} \left\| Q^{(L_j)} - Q^{(0)} \right\|_{W^{1,2}(\Omega)} = 0.$$

Moreover, $n^{(0)}$ is a harmonic map which agrees with $\overline{n}$ on the boundary $\partial\Omega$, where $\overline{n}$ is as in (2.4).

Proof. See [61], lemma 3. □

This result reveals that global minimisers $Q^{(L)}$ look like a uniaxial harmonic map plus a possible biaxial perturbation which is small in the $\|\cdot\|_{W^{1,2}(\Omega)}$-norm. However, the authors are able to say more regarding closeness of $Q^{(L_j)}$ to $Q^{(0)}$ in a stronger topology, which is better for understanding the distribution of its eigenvalues.

Proposition 2.2. *Suppose $K \subset\subset \Omega$ is a subset which does not contain any of the (finite number of possible) singularities of $Q^{(0)}$. There exists a constant $C > 0$ independent of $j \geq 1$ such that*

$$\left| |Q^{(L_j)}(y)| - \sqrt{\frac{2}{3}} s_+(\vartheta) \right| < C\sqrt{L_j} \quad \text{for every} \quad y \in K.$$

Proof. See [61], proposition 7. □

This result indicates that, for sufficiently-small values of the elastic constant L, the magnitude of global minimisers $Q^{(L)}$ lies in a small neighbourhood of the value $\sqrt{2/3}s_+(\vartheta)$ on large subsets of the underlying spatial domain. To help us understand the relationship between the magnitude of the Q-tensor and its eigenvalues, we have the following simple lemma.

Lemma 2.3. *If $Q \in \mathrm{Sym}_0(d)$ is physical in the sense of definition, then $|Q|^2 < 1 - \frac{1}{d}$.*

Proof. This follows from an elementary calculation, which we leave to the reader. □

With this in mind, let us suppose for given non-dimensional constants α, b, c and ϑ_* we can find a temperature regime $\vartheta \leq \vartheta_0$ for which

$$s_+(\vartheta) > 1 + \varepsilon(\vartheta_0) \text{ whenever } \vartheta \leq \vartheta_*. \tag{2.5}$$

In particular, for the material MBBA, one can show that $s_+(\vartheta)$ is strictly greater than 1 whenever $\vartheta < 317.67$, otherwise said, for temperatures lower than 44.52°C: see Majumdar [59] for a careful discussion of this point. Under assumption (2.5), one may use the above results of Majumdar and Zarnescu to show that

$$|Q^{(L_j)}| > \sqrt{\frac{2}{3}} \quad \text{on the compact subset } K,$$

for all $j \geq J$ with $J > 0$ sufficiently large, and so by lemma 2.3 the eigenvalues exceed their physical bounds on this large subset K. This implies, in particular, that the Landau-de Gennes theory is not guaranteed to predict equilibrium configurations that can be interpreted in a physically meaningful way, especially at low temperatures. Given that physically-meaningful eigenvalues are essential to a good theory, it is desirable to have a theory into which this eigenvalue constraint is built. Before we address this point, let us briefly discuss one further shortcoming of the quartic Landau-de Gennes theory that suggests the construction of such a model is desirable.

Issue II: Ill-posedness of the General Landau-de Gennes Theory

Aside from the physical nature of eigenvalues of equilibrium configurations, there is yet another analytical issue with the Landau-de Gennes theory. Let us switch our attention to the more general four elastic constant theory,

$$E_{4-\mathrm{LdG}}[Q] := \int_\Omega \left(w(\nabla Q, Q) + \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\mathrm{tr}\left(Q^2\right)^2 \right) dx,$$

where

$$w(\nabla Q, Q) := L_1 Q_{ij,k} Q_{ij,k} + L_2 Q_{ik,j} Q_{ij,k} + L_3 Q_{ij,j} Q_{ik,k} + L_4 Q_{k\ell} Q_{ij,k} Q_{ij,\ell},$$

together with appropriate conditions on the so-called elastic constants L_i: see the lecture notes of Ball [5]. We recall that this particular choice of elastic energy density is important as it reduces to the full Oseen-Frank theory in the case where Q is of uniaxial form. The following observation of Ball and Majumdar [8] demonstrates that, in the presence of the cubic bulk term $-b\,\mathrm{tr}(Q^3)$ when $L_4 \neq 0$, the Landau-de Gennes energy is unbounded from below on natural spaces of candidate minimisers.

Proposition 2.4. *Suppose $L_4 \neq 0$ and $b > 0$. For any suitably-smooth boundary conditions $\overline{Q}$, there exists a sequence of maps $\{Q_j\}_{j=1}^{\infty}$ in the admissible set*

$$\mathcal{X}(\overline{Q}) := \left\{ Q \in W^{1,2}(\Omega) \,:\, \mathrm{Tr}\, Q = \overline{Q} \ \text{ in } \ L^2(\partial\Omega) \right\}$$

for which

$$E_{4-\mathrm{LdG}}[Q_j] < -j \quad \text{when} \quad j = 1, 2, 3, \ldots.$$

Proof. See [7], proposition 7 for a sketch of this result. □

It is immediate from this observation that the problem of minimising $E_{4-\mathrm{LdG}}$ over the rather natural set of candidates $\mathcal{X}(\overline{Q})$ is not well posed. Not only this, but these more structurally-complex gradient terms are specific to the tensor theory of nematic order. Thus, if one wishes to retain the richness of structure that these additional gradient terms offer, it is desirable to construct a theory which is indeed well posed whenever $L_4 \neq 0$.

A Resolution

Recognising these limitations of the quartic Landau-de Gennes theory, and motivated by the work of Fatkullin and Slastikov [33, 34] and Katriel, Kventsel, Luckhurst and Sluckin [49], Ball and Majumdar turned their efforts in [7] to the construction of a qualitatively-similar theory into which the eigenvalue restriction (2.3) on global minimisers is built. Moreover, as we shall soon see, this newly-constructed theory is well posed in natural settings in the presence of a non-zero elastic constant L_4. The authors achieved this by constructing a singular map $f : \mathrm{Sym}_0(d) \to \mathbb{R} \cup \{\infty\}$ (which has its genesis in Maier-Saupe theory) that blows up as the eigenvalues of its argument approach the endpoints of the interval (2.3).

An understanding of this map is central to our study of the Beris-Edwards dynamic model in section 2.3 below. We now briefly consider its construction and main properties, in order to justify its inclusion in our model.

2.2 The Ball-Majumdar Singular Potential f

For clarity, let us fix our attention to the case when $Q \in \mathrm{Sym}_0(3)$. Recall from the discussion at the beginning of this chapter that Q-tensors possessing eigenvalues equal to $-1/3$ or $2/3$ were said to be "entropically inadmissible" within the context of liquid crystals modelled at finite temperatures, as the corresponding probability measures described crystalline molecular configurations. To justify the use of this terminology, let us consider the following. For a given $Q \in \mathrm{Sym}_0(d)$ satisfying (2.3), we investigate the associated minimisation problem

$$\inf_{\rho \in \mathcal{A}(Q)} \int_{\mathbb{S}^2} \rho(\omega) \log \rho(\omega)\, d\omega,$$

where

$$\mathcal{A}(Q) := \left\{ \rho : \mathbb{S}^2 \to [0,1] \ : \ \int_{\mathbb{S}^2} \rho = 1 \ \text{ and } \ \int_{\mathbb{S}^2} \left(\omega \otimes \omega - \frac{1}{3} I \right) \rho(\omega)\, d\omega = Q \right\}.$$

It was demonstrated in Ball and Majumdar [7] that this minimisation problem has a unique minimiser ρ^* in the class $\mathcal{A}(Q)$ given explicitly by

$$\rho^*(\omega) := \frac{1}{Z(\mu_1, \mu_2, \mu_3)} \exp\left(\sum_{i=1}^{3} \mu_i \omega_i^2 \right),$$

where the so-called partition function $Z = Z(\mu_1, \mu_2, \mu_3)$ is given by

$$Z(\mu_1, \mu_2, \mu_3) := \int_{\mathbb{S}^2} \exp\left(\sum_{i=1}^{3} \mu_i \omega_i^2 \right) d\omega,$$

and the constants μ_1, μ_2, μ_3 are Lagrange multipliers associated with the constraint that ρ^* have Q as its normalised matrix of second moments. By uniqueness of minimisers, this construction yields a map from the set of all elements of $\mathrm{Sym}_0(3)$ satisfying (2.3) into the real numbers. An important property of this map is contained in the following proposition.

Proposition 2.5. *The map*

$$Q \mapsto \min_{\rho \in \mathcal{A}(Q)} \int_{\mathbb{S}^2} \rho(\omega) \log \rho(\omega)\, d\omega$$

blows up logarithmically as $\lambda_i(Q) \to -1/3$ from above.

Proof. See [7], proposition 2 for details. □

This observation regarding the behaviour of the entropy map motivates the following definition of a singular map $f : \mathrm{Sym}_0(d) \to \mathbb{R} \cup \{\infty\}$ which one can generalise from the 3-dimensional setting (as it was set out in Ball and Majumdar [7]) to the d-dimensional

setting ($d = 2, 3$). See the work of Fatkullin and Slastikov [33, 34] for an investigation of the case when $d = 2$. In what follows, we define $f : \mathrm{Sym}_0(d) \to \mathbb{R} \cup \{\infty\}$ to be

$$f(Q) := \begin{cases} \min\limits_{\rho \in \mathcal{A}_d(Q)} \displaystyle\int_{\mathbb{S}^{d-1}} \rho(\omega) \log \rho(\omega)\, d\omega & \text{if } -\frac{1}{d} < \lambda_i(Q) < 1 - \frac{1}{d}, \\ \infty & \text{otherwise,} \end{cases}$$

where

$$\mathcal{A}_d(Q) := \left\{ \rho : \mathbb{S}^{d-1} \to [0,1] \,:\, \int_{\mathbb{S}^{d-1}} \rho = 1 \text{ and } \int_{\mathbb{S}^{d-1}} \left(\omega \otimes \omega - \frac{1}{d} I \right) \rho(\omega)\, d\omega = Q \right\}.$$

We denote the associated effective domain by $\mathsf{D}(f) := \{Q \in \mathrm{Sym}_0(d) : f(Q) < \infty\}$, i.e. $\mathsf{D}(f)$ is the subset of all Q-tensors whose eigenvalues are physical. This map has a number of useful analytical properties, which we record here for later use.

Proposition 2.6. *The Ball-Majumdar potential f has the following properties:*

(P0) *The map f is an isotropic function of Q, i.e. $f(\mathsf{R}Q\mathsf{R}^T) = f(Q)$ for all $\mathsf{R} \in \mathrm{O}(d)$.*

(P1) *The map f is smooth on its effective domain, i.e. $f \in C^\infty(\mathsf{D}(f))$;*

(P2) *It is bounded from below, i.e. there exists $f_0 > 0$ such that $-f_0 \leq f(Q)$ for all $Q \in \mathrm{Sym}_0(d)$;*

(P3) *It exhibits logarithmic blow-up as $Q \to \partial\mathsf{D}(f)$ from the interior;*

(P4) *The map f is strictly convex on $\mathsf{D}(f)$, which is itself a convex subset of $\mathrm{Sym}_0(d)$.*

Proof. We store the demonstration of these properties in the appendix 2.11 at the end of this chapter. □

Within the context of theories of nematic liquid crystals, this entropy term is present in the spatially-homogeneous Maier-Saupe theory, whose representative integral functional is given by

$$N \cdot I_{\mathrm{MS}}[\rho] := \vartheta \int_{\mathbb{S}^{d-1}} \rho(\omega) \log \rho(\omega)\, d\omega + \frac{\kappa}{2} \int_{\mathbb{S}^{d-1}} \int_{\mathbb{S}^{d-1}} \left(\frac{1}{d} - (\alpha \cdot \omega)^2 \right) \rho(\alpha)\rho(\omega)\, d\alpha d\omega,$$

where $N \in \mathbb{N}$ denotes the number of particles in the considered system. We make the simple remark that spatial homogeneity of the probability density does not necessarily imply that the macroscopic line field is itself constant in space. Now, if $Q(\rho)$ denotes the normalised matrix of second order moments of ρ, a quick calculation reveals that

$$I_{\mathrm{MS}}[\rho] = \vartheta \int_{\mathbb{S}^{d-1}} \rho(\omega) \log \rho(\omega)\, d\omega - \frac{\kappa}{2} |Q(\rho)|^2,$$

which indicates there is a natural link between Maier-Saupe and Q-tensor theory. This link was explored by Ball and Majumdar by considering a new bulk potential

$$f_{\mathrm{BM}}(Q) := \vartheta\, f(Q) - \frac{\kappa}{2} |Q|^2 \tag{2.6}$$

as an alternative to the usual quartic Landau-de Gennes potential f_{LdG},

$$f_{\mathrm{LdG}}(Q) := \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\mathrm{tr}\left(Q^2\right)^2.$$

The rather nice fact is that f_{BM} has close connections with the quartic polynomial f_{LdG}. For example, using elementary methods from asymptotic analysis, one can show that

$$f_{\mathrm{BM}}(Q) = \vartheta \log 4\pi + \left(\frac{15\vartheta}{4} - \frac{\kappa}{2}\right)\mathrm{tr}\left(Q^2\right) - \frac{225\vartheta}{42}\mathrm{tr}\left(Q^3\right) + \frac{225\vartheta}{112}\mathrm{tr}\left(Q^2\right)^2 + ...,$$

and so up to a constant, the singular map f_{BM} is well approximated by f_{LdG} in the interior of its effective domain for suitably small magnitude of Q: see the lecture notes of Ball [5] for details. Moreover, both maps are C^∞ on their effective domains and, importantly, both predict a first-order isotropic-to-nematic phase transition: we refer the reader to [7], section 4 for a sketch of this fact.

Recognising the qualitative similarities of the two maps f_{BM} and f_{LdG}, the authors replace the study of E_{LdG} with the following theory:

$$E[Q] := \int_\Omega \left(w(\nabla Q, Q) + \vartheta\, f(Q) - \frac{\kappa}{2}|Q|^2\right) dx,$$

where $\vartheta > 0$ and $\kappa > 0$. The authors establish the following result regarding the qualitative properties of H^1-global minimisers.

Proposition 2.7. *Suppose $L_2 = L_3 = L_4 = 0$, and $d = 3$. Suppose further that the smooth map $\overline{Q} : \partial\Omega \to \mathrm{Sym}_0(3)$ satisfies*

$$-\frac{1}{3} + \varepsilon \leq \lambda_i(Q(y)) \leq \frac{2}{3} - \varepsilon \qquad i = 1, 2, 3,$$

for $\varepsilon > 0$ sufficiently small and all $y \in \partial\Omega$. Then there exists $\varepsilon' > 0$ such that global minimisers of E in the class

$$\mathcal{X}(\overline{Q}) := \left\{Q \in H^1(\Omega, \mathsf{D}(f)) \,:\, \mathrm{Tr}Q = \overline{Q} \ \text{ in } \ L^2(\partial\Omega)\right\} \tag{2.7}$$

satisfy

$$-\frac{1}{3} + \varepsilon' \leq \lambda_i(Q(x)) \leq \frac{2}{3} - \varepsilon' \qquad i = 1, 2, 3,$$

for all $x \in \Omega$.

Proof. See [8], theorem 4. □

Thus, global minimisers are guaranteed to be physically meaningful if the boundary datum itself is so. In addition, this new theory is well posed in the presence of a non-zero L_4. In particular, the authors also demonstrate the following existence result which one should compare with proposition 2.4 above.

Proposition 2.8. *Suppose the elastic constants L_1, L_2, L_3, L_4 satisfy the inequalities*

$$L_3 - \frac{1}{3}|L_4| > 0, \qquad -\left(L_3 - \frac{1}{3}|L_4|\right) < L_2 < 2\left(L_3 - \frac{1}{3}|L_4|\right)$$

and

$$L_1 + \frac{L_2}{10} + \frac{3}{5}\left(L_3 - \frac{1}{3}|L_4|\right) > 0.$$

For any smooth boundary data $\overline{Q} : \partial\Omega \to \mathsf{D}(f)$, there exists a global minimiser of E in $\mathcal{X}(\overline{Q})$ defined above in (2.7).

Thus, having constructed the singular map f and established a number of its salient properties, the authors establish a variational theory into which the restriction (2.3) is built and which is also well posed in the presence of a non-zero L_4 elastic constant.

However, the main topic of this chapter will be dynamics. The map

$$f(Q) := \begin{cases} \min\limits_{\rho \in \mathcal{A}_d(Q)} \displaystyle\int_{\mathbb{S}^{d-1}} \rho(\omega) \log \rho(\omega)\, d\omega & \text{if } -\frac{1}{d} < \lambda_i(Q) < 1 - \frac{1}{d}, \\ \infty & \text{otherwise,} \end{cases}$$

is certainly not restricted to a study of statics of nematics. Indeed, properties **(P0)** to **(P4)** quoted above allow it also to be employed within the context of dynamical models. Of particular use are those techniques from convex analysis: the texts of Brezis [17] and Barbu [9] provide stimulating introdutions to the role of convexity in dynamics. Let us now consider the issue of preservation of the constraint (2.3) in the context of dynamics.

Eigenvalues and Dynamics

We fix our attention here on three spatial dimensions, where $Q \in \mathrm{Sym}_0(3)$. In this direction, let us consider a simple model of the dynamics of the Q-tensor, namely the $L^2(\mathbb{R}^3)$-gradient flow of the one-elastic constant Landau-de Gennes theory, which takes the shape

$$\frac{\partial Q}{\partial t} = L\,\Delta Q - a(\vartheta)Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}(Q^2)I\right) - c\,\mathrm{tr}(Q^2)Q.$$

One can show that this equation generates a strongly-continuous semigroup $\{S(t)\}_{t\geq 0}$ on the Banach space $H := L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$: see chapter 3 for a treatment of this model. Suppose further that $Q_0(x) \in \mathsf{D}(f)$ almost everywhere. We want to investigate whether or not the dynamics has the property that $Q(x,t) \in \mathsf{D}(f)$ for $x \in \mathbb{R}^3$ and $t > 0$. In order to see how this might be the case, we consider the related ODE problem

$$\begin{cases} \dfrac{dQ}{dt} = -a(\vartheta)Q + b\left(Q^2 - \dfrac{1}{3}\mathrm{tr}(Q^2)I\right) - c\,\mathrm{tr}(Q^2)Q, \\ Q(0) = \overline{Q} \in \mathsf{D}(f). \end{cases}$$

Since there is no explicit spatial dependence, we can diagonalise this system by the *same* element $\mathsf{R} \in \mathrm{O}(3)$, which yields the following system satisfied by the two distinct eigenvalues of Q:

$$\begin{cases} \dfrac{d\lambda}{dt} = -a(\vartheta)\lambda + \dfrac{b}{3}\left(\lambda^2 - 2\lambda\mu - 2\mu^2\right) - 2\left(\lambda^2 + \lambda\mu + \mu^2\right)\lambda, \\ \dfrac{d\mu}{dt} = -a(\vartheta)\mu - \dfrac{b}{3}\left(2\lambda^2 + 2\lambda\mu - \mu^2\right) - 2\left(\lambda^2 + \lambda\mu + \mu^2\right)\mu, \\ \lambda(0) = \overline{\lambda}, \mu(0) = \overline{\mu} \quad \text{with} \quad -\dfrac{1}{3} < \overline{\lambda}, \overline{\mu} < \dfrac{2}{3}. \end{cases}$$

Let $\{e^{t\Delta}\}_{t\geq 0}$ denote the heat semigroup and $\{U(t)\}_{t\in\mathbb{R}}$ denote the flow generated on $\mathrm{Sym}_0(3)$ by the ODE system for Q above. By the Trotter product formula (see, for instance, Pazy [68]. Section 3.4), one may represent the action of $S(t)$ on given initial data $Q_0 \in H$ by

$$S(t)Q_0 = \lim_{N\to\infty}\left(e^{\frac{t}{N}\Delta}U\left(\frac{t}{N}\right)\right)^N Q_0,$$

i.e. one can view the profile $S(t)Q_0$ as having been generated by successive applications of the heat semiflow and the ODE flow to the initial datum Q_0 over the time interval $[0,T]$. One benefit of such an explicit representation of the dynamics is that one can use it to understand how the semiflow $S(t)$ evolves the eigenvalues of Q_0. According to Iyer, Xu and Zarnescu [48], one can show the following.

Proposition 2.9. *Suppose $|a| < b^2/3c$. Let the eigenvalue maps of $Q_0 \in H^k(\mathbb{R}^3)$ $(k \geq 3/2)$ satisfy*

$$-\frac{s_+(\vartheta)}{3} \leq \lambda_i(Q_0(x)) \leq \frac{s_+(\vartheta)}{2},$$

where $s_+(\vartheta)$ was defined above in (2.1). Then, for $t > 0$,

$$-\frac{s_+(\vartheta)}{3} \leq \lambda_i(Q(x,t)) \leq \frac{s_+(\vartheta)}{2}.$$

Proof. This follows from the fact that the heat equation preserves the convex hull of the range of its initial data, and that an application of the maximum principle is applicable to the Frobenius norm of solutions of the ODE. □

One might say that this result simply follows from the good structure of the gradient flow of $E^{(L)}_{\mathrm{LdG}}$. The question of the preservation of the eigenvalue constraint (2.3) becomes much harder when one works with more physical, structurally complex evolution equations. Even if we introduce the effect of an externally-imposed tensor field U to the above gradient flow model, depending on its fluctuations in magnitude over small intervals of time, it may not be the case that the semiflow corresponding to the evolution equation

$$\frac{\partial Q}{\partial t} = L\,\Delta Q + U(t)Q - a(\vartheta)Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}(Q^2)I\right) - c\,\mathrm{tr}(Q^2)Q$$

preserves the initial bounds on the eigenvalues of Q_0. This question becomes pertinent if U is replaced by ∇u, where u evolves under the incompressible Navier-Stokes equations.

In all that follows in this chapter, we work with a modified Beris-Edwards model, whose original form ($\widetilde{\text{BE}}$) was introduced earlier in the introduction. This coupled system is more structurally complex than the gradient flow model, and it is for this reason we decide to incorporate the Ball-Majumdar singular potential and study the properties of its dynamics. With our preliminary discussion over, let us now introduce the problem under study in this chapter.

2.3 The Modified Beris-Edwards Model

In what follows, the spatial dimension d will be either 2 or 3 and we employ the Einstein summation convention over repeated indices i, j, k, ℓ, m and n with range in $\{1, ..., d\}$ throughout. Once again, the angular brackets $\langle A \rangle := A - d^{-1}\text{tr}(A)I$ signify that we take the trace-free part of the given matrix $A \in \mathbb{R}^{d\times d}$. For strictly positive constants

$$\Lambda, \Gamma, L, \vartheta, \kappa \quad \text{and} \quad \nu,$$

we search for spatially-periodic maps $Q : \mathbb{R}^d \times (0, \infty) \to \text{Sym}_0(d)$ and $u : \mathbb{R}^d \times (0, \infty) \to \mathbb{R}^d$ which satisfy the coupled system

$$\text{(S)} \begin{cases} \dfrac{\partial Q}{\partial t}(x,t) + (u(x,t)\cdot\nabla)\, Q(x,t) - S(Q(x,t), \nabla u(x,t)) = -\Gamma \dfrac{\delta E}{\delta Q}(Q(x,t)), \\ \dfrac{\partial u}{\partial t}(x,t) + (u(x,t)\cdot\nabla)\, u(x,t) = \nu\Delta u(x,t) - \nabla P(x,t) + \text{Div}\ (\tau(x,t) + \sigma(x,t))\,, \\ \nabla \cdot u(x,t) = 0, \end{cases}$$

in the distributional sense. We define the precise notion of distributional solution of system (S) in the section to come. Solutions are subject to the periodicity conditions

$$Q\,(x + \Lambda\pi e_i, t) = Q(x,t) \quad \text{and} \quad u(x + \Lambda\pi e_i, t) = u(x,t),$$

where $\{e_i\}_{i=1}^d$ is the canonical orthonormal basis of $\mathbb{R}^d$. Moreover, solutions evolve from given initial spatially $\Lambda\pi$-periodic data

$$Q_0 : \mathbb{R}^d \to \text{Sym}_0(d) \qquad \text{and} \qquad u_0 : \mathbb{R}^d \to \mathbb{R}^d \ \text{ with } \ \nabla \cdot u_0 = 0,$$

to which they converge in an appropriate topology (strong-in-norm or weakly, for instance) as t tends to 0 from above. We denote by I^d the fundamental cell $[-\Lambda\pi/2, \Lambda\pi/2]^d$. The energy E, which incorporates the Ball-Majumdar singular potential, is defined for suitable maps Q to be

$$E[Q] := \int_{I^d} \left(\frac{L}{2}|\nabla Q|^2 + f_{\text{BM}}(Q) \right) dx \equiv \int_{I^d} \left(\frac{L}{2}|\nabla Q|^2 + \vartheta f(Q) - \frac{\kappa}{2}|Q|^2 \right) dx,$$

where f_{BM} was the bulk energy density introduced in (2.6). The term S expresses to what extent the flow u locally rotates and dilates the order parameter Q, and is given by

$$S(Q, \nabla u) := (D_0 + \xi D)\, Q_1 - Q_1\, (D_0 - \xi D) - 2\xi Q_1 \mathrm{tr}\, (Q \nabla u)\,,$$

where $Q_1 := Q + (1/d)I$ and $\xi \in \mathbb{R}$ is a rotational parameter whose value will be of significance in the course of our analysis. The tensors D_0 and D defined by

$$D_0 := \frac{1}{2}\left((\nabla u) - (\nabla u)^T\right) \qquad \text{and} \qquad D := \frac{1}{2}\left((\nabla u) + (\nabla u)^T\right)$$

are the anti-symmetric and symmetric parts of the velocity gradient tensor ∇u, respectively. We denote the symmetric part of the stress tensor appearing in the Navier-Stokes equations by τ, which is given component-wise by

$$\begin{aligned}\tau_{ij} :=& \xi \left(Q_{ik} + \frac{1}{d}\delta_{ik}\right) \frac{\delta E}{\delta Q_{kj}}(Q) + \xi \frac{\delta E}{\delta Q_{ik}}(Q) \left(Q_{kj} + \frac{1}{d}\delta_{kj}\right) \\ & - 2\xi \left(Q_{ij} + \frac{1}{d}\delta_{ij}\right) \mathrm{tr}\left(Q \frac{\delta E}{\delta Q}(Q)\right) - L\, \mathrm{tr}\left(\frac{\partial Q}{\partial x_i}\frac{\partial Q}{\partial x_j}\right)\end{aligned}$$

and the anti-symmetric part by σ, where

$$\sigma_{ij} := -Q_{ik}\frac{\delta E}{\delta Q_{kj}}(Q) + \frac{\delta E}{\delta Q_{ik}}(Q) Q_{kj}.$$

The quantity $(\delta E/\delta Q)(Q)$ can be interpreted as the formal L^2 Gâteaux derivative (or L^2 subdifferential) of E evaluated at Q, namely

$$-\frac{\delta E}{\delta Q}(Q) = L\Delta Q - \vartheta \left\langle \frac{\partial f}{\partial Q}(Q) \right\rangle + \kappa\, Q.$$

We make the remark that the results of this chapter hold not only for the Ball-Majumdar potential f, but for *any* map that belongs to the non-empty class of all singular maps on $\mathrm{Sym}_0(d)$ satisfying properties **(P0)** to **(P4)** above.

Remark 2.2. *As we have already mentioned, one can view the Beris-Edwards hydrodynamic theory of nematics as a generalisation of that of Ericksen and Leslie to a* tensor-valued *order parameter. For comments related to the connection between the Beris-Edwards and Ericksen-Leslie models, especially with regard to the stress tensors appearing in the Navier-Stokes contribution to the systems, see Appendix A of* Denniston, Orlandini and Yeomans *[25].*

Remark 2.3. *We make the important remark that the system* (S) *is more commonly studied in the literature when the energy E is simply the quartic Landau-de Gennes energy functional,*

$$E^{(L)}_{\mathrm{LdG}}[Q] = \int_{I^d} \left(\frac{L}{2}|\nabla Q|^2 + a(\vartheta)\mathrm{tr}\,(Q^2) - \frac{b}{3}\mathrm{tr}\,(Q^3) + \frac{c}{4}\left(\mathrm{tr}\,(Q^2)\right)^2\right) dx;$$

see, for example, Paicu and Zarnescu [66, 65] *or* Denniston, Orlandini and Yeomans [26]. *As discussed in the previous section, these two energies can be considered as qualitatively-similar, in the sense that* f_{LdG} *and* f_{BM} *are both smooth on their effective domains, possess the same symmetries and also both predict a first-order isotropic-nematic phase transition. We argue that these qualitative similarities between the quartic Landau-de Gennes theory and the singular Ball-Majumdar theory make our modification of the Beris-Edwards model in this work a justifiable one.*

Regularisation of f

Let us recall the definition of the singular map $f : \mathrm{Sym}_0(d) \to \mathbb{R} \cup \{\infty\}$,

$$f(Q) := \begin{cases} \min\limits_{\rho \in \mathcal{A}_d(Q)} \displaystyle\int_{\mathbb{S}^{d-1}} \rho(\omega) \log \rho(\omega)\, d\omega & \text{if } -\tfrac{1}{d} < \lambda_i(Q) < 1 - \tfrac{1}{d}, \\ \infty & \text{otherwise,} \end{cases}$$

where $\mathcal{A}_d(Q)$ is the class of all probability densities ρ which have $Q + (1/d)I$ as their matrix of second-order moments. The effective domain $\mathsf{D}(f)$ was simply defined to be the set of all Q-tensors Q for which $f(Q) < \infty$, and is characterised by the fact that all its elements have eigenvalues strictly between $-1/d$ and $1 - 1/d$.

When building weak solutions to the system (S), it is convenient for us not to have to worry about forcing the range of approximants to lie in $\mathsf{D}(f)$ at every stage of the construction. For this reason, we regularise f using the well-known Yosida-Moreau regularisation of convex analysis (see Showalter [78], Chapter IV, Proposition 1.8), thereby extending the effective domain of f to all of $\mathrm{Sym}_0(d)$. In particular, for $J \in \{1, 2, 3, ...\}$ we define $\widetilde{f}_J$ to be

$$\widetilde{f}_J(Q) := \min_{A \in \mathrm{Sym}_0(d)} \left(J|A - Q|^2 + f(A) \right).$$

The map $\widetilde{f}_J$ is not guaranteed to be smooth, even if f is C^∞ on its effective domain, as the following example shows.

Example 2.10. Consider the convex map $g : \mathbb{R} \to \{0, \infty\}$ defined by

$$g(x) := \begin{cases} 0 & \text{for } -1 < x < 1, \\ \infty & \text{otherwise,} \end{cases}$$

which is C^∞ in $\mathsf{D}(g) = (-1, 1)$. Using the notation introduced above, it is straightforward to show that

$$\widetilde{g}_J(x) = \begin{cases} J(x+1)^2 & \text{for } -\infty < x \leq -1, \\ 0 & \text{for } -1 < x < 1, \\ J(x-1)^2 & \text{for } 1 \leq x < \infty, \end{cases}$$

for each $J = 1, 2, 3, ...$ One may quickly check that $\widetilde{g}_J \in C^1(\mathbb{R})$, but fails to be $C^2(\mathbb{R})$.

In this work, we requre a suitable regularisation of f to be $C^2(\mathbb{R}^{d\times d})$, in order that its Hessian exists in the classical sense. Thus, for fixed J and any $K \in \{1, 2, 3, ...\}$ we define $\widetilde{f}_{J,K}$ to be

$$\widetilde{f}_{J,K}(Q) := K^{d^2} \int_{\mathbb{R}^{d\times d}} \widetilde{f_J}(K(Q-R))\Phi(R)\, dR,$$

where $\Phi \in C_c^\infty(\mathbb{R}^{d\times d}, \mathbb{R}_+)$ is of unit mass, i.e. $\int_{\mathbb{R}^{d\times d}} \Phi(R)\, dR = 1$. Finally, we extract the diagonal subsequence $\widetilde{f}_{N,N}$ and define the regularisation of the Ball-Majumdar to be

$$f_N(Q) := \widetilde{f}_{N,N}(Q) = N^{d^2} \int_{\mathbb{R}^{d\times d}} \widetilde{f_N}(N(Q-R))\Phi(R)\, dR.$$

This choice of regularisation is convenient as the map f_N inherits many of the important properties of f, and also has good convergence properties to its limit f. For future use, we quote without proof the following properties of the mollified potential, to which we refer frequently during the rest of the chapter.

Proposition 2.11. *For each $N \geq 1$, the regularisation f_N of the Ball-Majumdar potential has the following properties:*

(M0) *The map f_N is an isotropic function of Q ;*

(M1) *The map f_N is both C^∞ and convex on $\mathbb{R}^{d\times d}$;*

(M2) *It is bounded from below, i.e. $-f_0 \leq f_N(X)$ for all $X \in \mathbb{R}^{d\times d}$ and for all $N \geq 1$, where $f_0 > 0$ is the same constant appearing in* **(P2)***;*

(M3) *$f_N \leq f_{N+1} \leq f$ on $\mathbb{R}^{d\times d}$ for $N \geq 1$;*

(M4) *$f_N \to f$ in $L^\infty_{\mathrm{loc}}(\mathsf{D}(f))$ as $N \to \infty$, and f_N is uniformly divergent on $\mathrm{Sym}_0(d) \setminus \mathsf{D}(f)$ as $N \to \infty$;*

(M5) *$\dfrac{\partial f_N}{\partial Q} \to \dfrac{\partial f}{\partial Q}$ in $L^\infty_{\mathrm{loc}}(\mathsf{D}(f))$ as $N \to \infty$;*

(M6) *Its classical derivative satisfies*

$$c_N^1|X| - c_N^2 \leq \left|\left\langle \frac{\partial f_N}{\partial Q}(X)\right\rangle\right| \leq C_N^1|X| + C_N^2$$

for all $X \in \mathbb{R}^{d\times d}$ and positive constants c_N^i and C_N^i which depend on the mollification parameter $N \geq 1$;

(M7) *The higher derivatives of f_N satisfy the following bound:*

$$\left|\left\langle \frac{\partial^k f_N}{\partial Q^k}(X)\right\rangle\right| \leq C_{N,k}^1|X|^2 + C_{N,k}^2 \quad \text{for} \quad k \geq 2.$$

Although many properties of f are inherited by f_N, there is one important property in particular that is lost, namely that $f_N(Q) \in L^1$ no longer implies that $Q \in L^\infty$, as this property is removed by the Yosida-Moreau regularisation. We show how this information can be carefully recovered in the limit in due course.

2.4 Statement of Main Results

The main result of this chapter is the proof of a certain a maximum principle for the map $f(Q)$ evolving under (S), the notion of dynamics suitably interpreted. However, before we give precise statements of the main results of this chapter, we make some important definitions. In section 2.1 we stated what it meant for a given matrix $Q \in \mathrm{Sym}_0(d)$ to be physical; now we define two important senses in which a *map* into $\mathrm{Sym}_0(d)$ can be considered as physical.

Definition 2.2. *A measurable map Q from a spatial domain Ω into $\mathrm{Sym}_0(d)$ is said to be* ***physical*** *if and only if*

$$-\frac{1}{d} < \lambda_i(Q(x)) < 1 - \frac{1}{d} \quad i = 1, ..., d,$$

for almost every $x \in \Omega$.

We contrast this with the following stronger property of being *strictly physical*, which is particularly useful when it comes to constructing solutions of (S) which enjoy good regularity properties.

Definition 2.3. *A measurable map Q from a spatial domain Ω into $\mathrm{Sym}_0(d)$ is said to be* ***strictly physical*** *if and only if there exists $\delta > 0$ sufficiently small such that*

$$-\frac{1}{d} + \delta \leq \lambda_i(Q(x)) \leq 1 - \frac{1}{d} - \delta \quad i = 1, ..., d,$$

for almost every $x \in \Omega$.

An important observation is that one may express these notions in terms of the summability of the map $f(Q)$. In particular, it follows directly from the definition of the singular potential that $f(Q) \in L^1$ implies that Q is physical. However, one may show that a map Q is strictly physical if and only if $f(Q) \in L^\infty$, i.e. strict physicality of Q is characterised by the membership of $f(Q)$ in L^∞. In what follows, we shall no longer refer to the eigenvalues of a Q-tensor field, instead concerning ourselves with the summability of the map $f(Q)$.

Under various restrictions on the regularity of initial data (Q_0, u_0) and also on the distribution of eigenvalues of Q_0, we aim to construct suitable solutions of the system (S). Let us now set out precisely the various notions of solution we employ in the sequel.

Definition 2.4. *The pair (Q, u) is said to be a* **global weak solution** *of the Beris-Edwards system* (S) *subject to initial data $(Q_0, u_0) \in H^1 \times L^2_{\mathrm{div}}$ if and only if*

$$Q \in L^\infty_{\mathrm{loc}}(0, \infty; H^1) \cap L^2_{\mathrm{loc}}(0, \infty; H^2) \quad \textit{and} \quad u \in L^\infty_{\mathrm{loc}}(0, \infty; L^2_{\mathrm{div}}) \cap L^2_{\mathrm{loc}}(0, \infty; H^1_{\mathrm{div}})$$

satisfy the integral equalities

$$\begin{cases} \displaystyle\int_0^\infty \int_{I^d} \left(-Q : \partial_t \chi + (u \cdot \nabla) Q - S(Q, \nabla u) + \Gamma \frac{\delta E}{\delta Q}(Q) \right) : \chi \, dx dt = 0, \\ \displaystyle\int_0^\infty \int_{I^d} \Big(- u_i \cdot \partial_t \omega_i + (u \cdot \nabla) u_i \omega_i + \nu \nabla u_i \cdot \nabla \omega_i + (\tau(Q)_{ij} + \sigma(Q)_{ij}) \, \partial_j \omega_i \Big) \, dx dt = 0, \end{cases}$$

for all $\chi \in C_c^\infty(I^d \times (0,\infty); \mathrm{Sym}_0(d))$ *and divergence-free* $\omega \in C_c^\infty(I^d \times (0,\infty); \mathbb{R}^d)$. *Moreover, the maps* Q *and* u *should be compatible with the initial data in the sense that*

$$\lim_{t \to 0} \int_{I^d} (Q(x,t) - Q_0(x)) : \chi(x) \, dx = 0$$

and

$$\lim_{t \to 0} \int_{I^d} (u(x,t) - u_0(x)) \cdot \omega(x) \, dx = 0$$

for all $\chi \in H^1$ *and* $\omega \in L^2_{\mathrm{div}}$.

We also work with the following stronger notion of solution of (S). In what follows, a single dot above a map denotes its distributional time derivative.

Definition 2.5. *Suppose* $k \geq 1$. *The pair* (Q, u) *is said to be a* **global strong solution** *of the Beris-Edwards system* (S) *subject to initial data* $(Q_0, u_0) \in H^{k+1} \times H^k_{\mathrm{div}}$ *if and only if* $Q \in L^\infty_{\mathrm{loc}}(0,\infty; H^{k+1}) \cap L^2_{\mathrm{loc}}(0,\infty; H^{k+2})$ *and* $u \in L^\infty_{\mathrm{loc}}(0,\infty; H^k_{\mathrm{div}}) \cap L^2_{\mathrm{loc}}(0,\infty; H^{k+1}_{\mathrm{div}})$ *satisfy the equations*

$$\begin{cases} \dot{Q} + (u \cdot \nabla) Q - S(Q, \nabla u) = \Gamma \left(L \Delta Q - \vartheta \left\langle \dfrac{\partial f}{\partial Q}(Q) \right\rangle + \kappa \, Q \right), \\ \dot{u} + (u \cdot \nabla) u = \nu \Delta u + \mathrm{Div} \, (\tau(Q) + \sigma(Q)) \end{cases}$$

in $L^2_{\mathrm{loc}}(0,\infty; L^2)$ *and* $L^2_{\mathrm{loc}}(0,\infty; L^2_{\mathrm{div}})$, *respectively. Moreover, the maps* Q *and* u *should be compatible with the initial data in the sense that*

$$Q \in C([0,T]; H^{k+1}) \qquad \text{and} \qquad u \in C([0,T]; H^k_{\mathrm{div}})$$

with $Q(\cdot, 0) = Q_0$ *and* $u(\cdot, 0) = u_0$.

Finally, we shall call a solution of (S) **classical** if and only if for given initial data (Q_0, u_0) there exists a unique smooth solution on $\mathbb{R}^d \times (0,\infty)$.

With all of these definitions laid out, let us now present the main results of this chapter. Importantly, using a maximum principle argument outlined below in section 2.6, we establish the following theorem.

Theorem 2.12 (Dimension $d = 2, 3$; Co-rotational regime $\xi = 0$)**.** *For initial data* $(Q_0, u_0) \in H^1 \times L^2_{\mathrm{div}}$ *with the property that*

$$f(Q_0) \in L^1 \quad \text{(physical initial data)},$$

there exists a corresponding global weak solution (Q, u) *of system* (S).

Moreover, the map Q *is also strictly physical for positive time, i.e.*

$$f(Q(\cdot, t)) \in L^\infty \quad \text{for all } t > 0.$$

This result establishes an existence theory for the equations (S) in which solutions Q can be interpreted in a physically-meaningful way. However, the property of being strictly physical is more than just aesthetic: one needs the fact that the range of solutions Q belongs to a compact subset of $\mathsf{D}(f)$ for $t \geq 0$ to construct solutions of (S) with better regularity properties. In order to achieve this, we impose stricter conditions on initial data Q_0, namely that their range should be contained in a compact subset of $\mathsf{D}(f)$, and that (Q_0, u_0) should lie in the class of more regular maps $H^2 \times H^1_{\mathrm{div}}$.

Theorem 2.13 (Dimension $d = 2$; Co-rotational regime $\xi = 0$)**.** *For initial data* $(Q_0, u_0) \in H^2 \times H^1_{\mathrm{div}}$ *with the property that*

$$f(Q_0) \in L^\infty \quad \text{(strictly physical initial data)},$$

there exists a corresponding global strong solution (Q, u) *of system* (S) *with* $f(Q(\cdot, t)) \in L^\infty$ *for* $t \geq 0$.

A bootstrap argument leads us to

Corollary 2.14 (Dimension $d = 2$; Co-rotational regime $\xi = 0$)**.** *Suppose* $k \geq 1$. *For initial data* $(Q_0, u_0) \in H^{k+1} \times H^k_{\mathrm{div}}$ *such that*

$$f(Q_0) \in L^\infty \quad \text{(strictly physical initial data)},$$

there exists a global strong solution (Q, u) *of* (S) *with* $Q \in L^\infty_{\mathrm{loc}}(0, \infty; H^{k+1}) \cap L^2_{\mathrm{loc}}(0, \infty; H^{k+2})$ *and* $u \in L^\infty_{\mathrm{loc}}(0, \infty; H^k_{\mathrm{div}}) \cap L^2_{\mathrm{loc}}(0, \infty; H^{k+1}_{\mathrm{div}})$.

The assumption that $\xi = 0$ is somewhat strong, as it simplifies the analysis of the coupled system significantly. In the last section of this chapter, we pass comment on the case when $\xi \in \mathbb{R} \setminus \{0\}$, where we can only establish the local existence of weak solutions using the energy method.

2.5 Energy Dissipation of the Beris-Edwards Equations

As is customary, we procede in a formal manner when treating the energy structure of the equations in order to obtain useful *a priori* estimates associated with solutions of (S). However, in section 2.7 we design an approximation scheme in which approximate solutions Q^β and u^β satisfy a system that posseses the same energy structure and so the following

preliminary formal computations are appropriate. In what follows, the index β in Q^β and u^β should be considered as a *label*, not as a power. When powers of the matrix Q^β are taken, a distinction will be drawn clearly.

Moreover, we replace the Ball-Majumdar potential f in the following formal argument with a map $f_* : \mathrm{Sym}_0(d) \to [-f_0, \infty)$ that satisfies properties **(M0)** to **(M7)** above, which one should think of as f_N for some N. We adopt this practice in order to avoid writing the dependence of approximate solutions on the smoothness parameter N explicitly in the following calculation, as we believe it would obscure the essential argument. We do, however, make this dependence explicit later in our construction. As mentioned above, we lose uniform spatial L^∞ information on maps Q^β in space and time as we are no longer assured that they have the property $Q^\beta(x,t) \in \mathsf{D}(f)$ almost everywhere. It is our aim to recover such information on solutions as we pass to limits whilst recovering f from f_*.

An Energy Identity for the System (S)

Firstly, considering the evolution equation for the Q-tensor field,

$$\frac{\partial Q}{\partial t} + (u\cdot\nabla)Q - S(Q,\nabla u) = \Gamma\left(L\Delta Q - \vartheta\left\langle \frac{\partial f_*}{\partial Q}(Q)\right\rangle + \kappa\, Q\right)$$

taking L^2 inner products throughout against $-(\delta E/\delta Q)(Q)$, where

$$-\frac{\delta E}{\delta Q}(Q) = L\Delta Q - \vartheta\left\langle \frac{\partial f_*}{\partial Q}(Q)\right\rangle + \kappa\, Q,$$

one finds after integrating by parts that

$$\begin{aligned}
&\frac{d}{dt}\left(\frac{L}{2}\|\nabla Q\|_2^2 + \vartheta\int_{I^d} f_*(Q) - \frac{\kappa}{2}\|Q\|_2^2\right) + \Gamma\left\|L\Delta Q - \vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle + \kappa\, Q\right\|_2^2 \\
&= \underbrace{L\int_{I^d}(u\cdot\nabla)Q : \Delta Q\, dx}_{\mathcal{T}_1^+} + \underbrace{\int_{I^d}(D_0Q - QD_0) : \left(\vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle - \kappa\, Q\right)\, dx}_{\mathcal{I}} \\
&\quad - \underbrace{L\int_{I^d}(D_0Q - QD_0) : \Delta Q\, dx}_{\mathcal{T}_2^+} - \underbrace{L\xi\int_{I^d}\left(D_1\left(Q+\frac{1}{d}I\right) + \left(Q+\frac{1}{d}I\right)D_1\right) : \Delta Q\, dx}_{\mathcal{T}_3^+} \\
&\quad + \underbrace{2L\xi\int_{I^d}\mathrm{tr}\,(Q\nabla u)\left(Q+\frac{1}{d}I\right) : \Delta Q\, dx}_{\mathcal{T}_4^+} \\
&\quad + \underbrace{\xi\int_{I^d}\left(D_1\left(Q+\frac{1}{d}I\right) + \left(Q+\frac{1}{d}I\right)D_1\right) : \left(\vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle - \kappa\, Q\right)\, dx}_{\mathcal{T}_5^+} \\
&\quad - \underbrace{2\xi\int_{I^d}\left(Q+\frac{1}{d}I\right) : \left(\vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle - \kappa\, Q\right)\mathrm{tr}\,(Q\nabla u)\, dx}_{\mathcal{T}_6^+}.
\end{aligned} \tag{2.8}$$

Secondly, considering the evolution of the velocity profile

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u - \nu\Delta u + \nabla P = \mathrm{Div}\,(\tau + \sigma)$$

and this time taking inner products in L^2_{div} throughout the equation against u, one obtains in a similar way

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\left(\|u\|_2^2\right) + \nu\|\nabla u\|_2^2 \\
= \;& \underbrace{L\int_{I^d} \partial_i Q_{j\ell}\partial_k Q_{\ell j}\partial_k u_i\,dx}_{\mathcal{T}_1^-} \underbrace{- L\int_{I^d}(Q\Delta Q - \Delta Q\,Q) : \nabla u\,dx}_{\mathcal{T}_2^-} \\
&+ \underbrace{L\xi\int_{I^d}\left(\left(Q+\frac{1}{d}I\right)\Delta Q + \Delta Q\left(Q+\frac{1}{d}I\right)\right) : \nabla u\,dx}_{\mathcal{T}_3^-} \\
&\underbrace{- 2L\xi\int_{I^d}\mathrm{tr}\,(Q\Delta Q)\left(Q-\frac{1}{d}I\right) : \nabla u\,dx}_{\mathcal{T}_4^-} \\
&\underbrace{- \xi\int_{I^d}\left(\left(Q+\frac{1}{d}I\right)\left(\vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle - \kappa\,Q\right) + \left(\vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle - \kappa\,Q\right)\left(Q+\frac{1}{d}I\right)\right) : \nabla u\,dx}_{\mathcal{T}_5^-} \\
&+ \underbrace{2\xi\int_{I^d}\mathrm{tr}\left[Q\left(\vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle - \kappa\,Q\right)\right]\left(Q+\frac{1}{d}I\right) : \nabla u\,dx}_{\mathcal{T}_6^-} \\
&+ \underbrace{\int_{I^d}\left(Q\left(\vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle - \kappa\,Q\right) - \left(\vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle - \kappa\,Q\right)Q\right) : \nabla u\,dx.}_{\mathcal{J}} \qquad (2.9)
\end{aligned}$$

Let us write $\mathcal{E}_* : H^1 \times L^2_{\mathrm{div}} \to \mathbb{R}\cup\{\infty\}$ to denote the functional

$$\mathcal{E}_*(Q,u) := \frac{L}{2}\|\nabla Q\|_2^2 + \vartheta\int_{I^d} f_*(Q)\,dx - \frac{\kappa}{2}\|Q\|_2^2 + \frac{1}{2}\|u\|_2^2.$$

By adding the contributions of (2.8) and (2.9) together and noting the cancellations $\mathcal{T}_j^+ + \mathcal{T}_j^- = 0$ for $j = 1, ..., 6$ together with the null terms $\mathcal{I} = \mathcal{J} = 0$, one discovers

$$\frac{d\mathcal{E}_*}{dt} = -\Gamma\left\|L\Delta Q - \vartheta\left\langle\frac{\partial f_*}{\partial Q}(Q)\right\rangle + \kappa\,Q\right\|_2^2 - \nu\|\nabla u\|_2^2, \qquad (2.10)$$

which implies that the functional $\mathcal{E}_*$ is non-increasing along solution trajectories $(Q(t), u(t))$ in $H^1 \times L^2_{\mathrm{div}}$.

At this point, we have paid a price for the cancellations of highest derivative terms (like $\mathcal{T}_1^+$ and $\mathcal{T}_1^-$ in the Q- and u-equations respectively, for example) which would otherwise complicate our subsequent analysis: the functional $\mathcal{E}_*$ is not of one sign due to the negative

contribution of the 2-norm of the tensor field. This could cause a problem in the sequel if we attempt to use $\mathcal{E}_*$ to obtain bounds on Q and u and their distributional gradients in natural function spaces which are uniform in approximation parameters.

This issue, however, is remedied as follows. Suppose now that the smooth maps $Q = Q^\beta$ and $u = u^\beta$ depend on an approximation parameter $\beta \in \{1, 2, 3, ...\}$, but that the initial data $Q_0 \in H^1$ and $u_0 \in L^2_{\text{div}}$ are independent of β. Equality (2.10) above implies the simple inequality

$$\frac{d}{dt}\big(\mathcal{E}_*(Q^\beta(t), u^\beta(t))\big) \leq 0,$$

from which we deduce by integration in time,

$$\begin{aligned} &\frac{L}{2}\|\nabla Q^\beta(\cdot,t)\|_2^2 + \vartheta\int_{I^d} f_*(Q^\beta(x,t))\,dx - \frac{\kappa}{2}\|Q^\beta(\cdot,t)\|_2^2 + \frac{1}{2}\|u^\beta(\cdot,t)\|_2^2 \\ \leq\ &\frac{L}{2}\|\nabla Q_0\|_2^2 + \vartheta\int_{I^d} f_*(Q_0(x))\,dx - \frac{\kappa}{2}\|Q_0\|_2^2 + \|u_0\|_2^2. \end{aligned} \tag{2.11}$$

Now, noting that f_* satisfies the property **(M2)**, which implies that

$$-\vartheta\,(\Lambda\pi)^d\,f_0 \leq \vartheta\int_{I^d} f_*(Q^\beta(x,t))\,dx,$$

and *if* we make in addition the crucial assumption that

$$\sup_t \|Q^\beta(\cdot,t)\|_2 \leq c_0, \tag{2.12}$$

where $c_0 > 0$ is some constant independent of β, we may deduce from (2.11) using such bounds that

$$\sup_t\left(\frac{L}{2}\|\nabla Q^\beta(\cdot,t)\|_2^2 + \frac{1}{2}\|u^\beta(\cdot,t)\|_2^2\right) \leq C_0,$$

where

$$C_0 := \frac{L}{2}\|\nabla Q_0\|_2^2 + \frac{1}{2}\|u_0\|_2^2 + \vartheta\int_{I^d}\underbrace{(f_0 + f_*(Q_0(x))}_{\geq 0}\,dx + \frac{\kappa}{2}c_0^2 \geq 0.$$

Thus, the existence of the functional $\mathcal{E}_*$, along with the additional stipulation that $\{Q^\beta\}_{\beta=1}^\infty$ be uniformly bounded in $L^\infty_t L^2_x$, allows us to infer that

$$\{Q^\beta\}_{\beta=1}^\infty \quad \text{is uniformly bounded in} \quad L^\infty_t H^1_x$$

and

$$\{u^\beta\}_{\beta=1}^\infty \quad \text{is uniformly bounded in} \quad L^\infty_t L^2_{\text{div}}.$$

We can use these uniform bounds to glean yet more information from the identity (2.10). Performing an expansion of the right-hand side, one finds

$$\frac{d}{dt}\big(\mathcal{E}_*(Q^\beta(t), u^\beta(t))\big) + \Gamma L^2\|\Delta Q^\beta\|_2^2 + \Gamma\vartheta^2\left\|\left\langle\frac{\partial f_*}{\partial Q}(Q^\beta)\right\rangle\right\|_2^2 + \Gamma\kappa\|Q^\beta\|_2^2$$

$$= -\nu\|\nabla u^\beta\|_2^2 + 2\Gamma L\kappa\|\nabla Q^\beta\|_2^2 + 2\Gamma L\vartheta\int_{I^d}\Delta Q^\beta : \left\langle\frac{\partial f_*}{\partial Q}(Q^\beta)\right\rangle dx$$
$$+ 2\Gamma\vartheta\kappa\int_{I^d}\left\langle\frac{\partial f_*}{\partial Q}(Q^\beta)\right\rangle : Q^\beta\, dx. \tag{2.13}$$

Now, a straightforward integration by parts reveals

$$\int_{I^d}\Delta Q^\beta : \frac{\partial f_*}{\partial Q}(Q^\beta)\, dx = -\sum_{m=1}^{d}\int_{I^d}\partial_m Q_{ij}^\beta\frac{\partial^2 f_*(Q^\beta)}{\partial Q_{ji}\partial Q_{\ell k}}\partial_m Q_{k\ell}^\beta\, dx.$$

Since the map f_* is convex, its Hessian is a positive definite form: see, for instance, Rockafellar ([73] chapter 4, theorem 4.5). Thus, convexity of f implies that

$$2\Gamma L\vartheta\int_{I^d}\Delta Q^\beta : \frac{\partial f_*}{\partial Q}(Q^\beta)\, dx \leq 0.$$

By Young's inequality, one may also obtain the simple estimate

$$2\Gamma\vartheta\kappa\int_{I^d}\left\langle\frac{\partial f_*}{\partial Q}(Q^\beta)\right\rangle : Q^\beta\, dx \leq \frac{\Gamma\vartheta^2}{2}\left\|\left\langle\frac{\partial f_*}{\partial Q}(Q^\beta)\right\rangle\right\|_2^2 + 2\Gamma\kappa^2\|Q^\beta\|_2^2.$$

Using these observations, integrating in time across equality (2.13) yields the following improved bounds on approximants, again under assumption (2.12):

$$\{Q^\beta\}_{\beta=1}^\infty \quad \text{is uniformly bounded in} \quad L_t^\infty H_x^1 \quad \text{and} \quad L_t^2 H_x^2,$$

$$\{u^\beta\}_{\beta=1}^\infty \quad \text{is uniformly bounded in} \quad L_t^\infty L_{\text{div}}^2 \quad \text{and} \quad L_t^2 H_{\text{div}}^1,$$

and

$$\left\{\left\langle\frac{\partial f_*}{\partial Q}(Q^\beta)\right\rangle\right\}_{\beta=1}^\infty \quad \text{is uniformly bounded in} \quad L_t^2 L_x^2.$$

Thus, the moral of this section is that if we can establish the energy identity (2.10) rigorously, along with $L_t^\infty L_x^2$-bounds on $\{Q^\beta\}_{\beta=1}^\infty$ and the convexity inequality

$$2\Gamma L\vartheta\int_{I^d}\Delta Q^\beta : \frac{\partial f_*}{\partial Q}(Q^\beta)\, dx \leq 0,$$

we are immediately in the familiar setting in which we aim to employ topological arguments, such as Banach-Alaoglu and Aubin-Lions compactness, to identify candidate solutions for a limiting system (S).

Remark 2.4. *One should note that, despite the apparent complexity of the system* (S)*, it has a rather simple energy law. One important observation is that no term which is premultiplied by the parameter ξ contributes towards the energy dissipation law* (2.10)*. As the value parameter ξ is crucial when it comes to proving a certain maximum principle for the quantity $f(Q)$, it may prove to be of importance to understand this feature of system* (S)*.*

2.6 A Formal Maximum Principle for $f(Q)$

Let us now explain heuristically the reason the dynamics generated by the Beris-Edwards equations has the following instantaneous *range contraction effect* on initial data:

$$f(Q_0) \in L^1 \Longrightarrow f(Q(\cdot,t)) \in L^\infty \text{ for } t > 0.$$

In other words, for any positive time $t > 0$ the range of weak solutions $Q(\cdot,t)$ is contained essentially in some t-dependent compact, convex subset of $\mathsf{D}(f)$. We obtain this result by a maximum principle argument applied to the map $f(Q)$, in particular by constructing a function $\omega : (0,\infty) \to \mathbb{R}_+$ (that necessarily blows up as the origin is approached) which dominates $f(Q)$, i.e.

$$f(Q(\cdot,t)) \leq \omega(t) \quad \text{for} \quad t > 0.$$

Since the set $\{Q \in \mathrm{Sym}_0(d) \,:\, f(Q) \leq \omega(t)\}$ is a closed subset of $\mathsf{D}(f)$, it follows any Q belonging to this set satisfies $|Q| \leq \alpha(t) < \sqrt{1-1/d}$ for an appropriate bound α.

For simplicity of presentation, we once again replace the Ball-Majumdar potential f with f_* in what follows, which one should think of as f_N for some $N \geq 1$. We establish the maximum principle argument at the level of smooth approximate solutions Q^β, as weak solutions Q lie in the regularity class $L^\infty_t H^1_x \cap L^2_t H^2_x$ and are not even known to be distributionally-differentiable in time. As such, weak solutions possess neither enough spatial nor temporal regularity for a classical maximum principle argument to be valid. The main idea is to establish that approximate maps $f_*(Q^\beta)$ are strictly physical in the sense of definition 2.3, and then to carry this information through to weak solutions. With this strategy in mind, we now present the formal calculation.

For reasons related to lack of uniform control on approximants $\nabla u^\beta(\cdot,t)$ in L^∞, we set $\xi = 0$; we discuss this point in more detail later. We start from the evolution equation for Q^β,

$$\frac{\partial Q^\beta}{\partial t} + (u^\beta \cdot \nabla)Q^\beta - S(Q^\beta, \nabla u^\beta) = \Gamma\left(L\Delta Q^\beta - \vartheta\left\langle \frac{\partial f_*}{\partial Q}(Q^\beta)\right\rangle + \kappa\, Q^\beta\right)$$

supplemented with mollified initial datum $Q_{0,\beta}$. By taking matrix product throughout the above equation by

$$\left\langle \frac{\partial f_*}{\partial Q}(Q^\beta)\right\rangle = \frac{\partial f_*}{\partial Q}(Q^\beta) - \frac{1}{d}\mathrm{tr}\left[\frac{\partial f_*}{\partial Q}(Q^\beta)\right] I,$$

and using the fact that f_* is an isotropic function by property **(M0)**, whence

$$f_*(Q) = \widetilde{f}_*\left(\mathrm{tr}(Q^2), \mathrm{tr}(Q^3)\right)$$

for some smooth map $\widetilde{f}_* : \mathbb{R}^2 \to \mathbb{R}$, one may deduce that

$$\left(\frac{\partial}{\partial t} + \mathcal{L}_\beta\right) f_*(Q^\beta) = -\Gamma L\, \partial_m Q^\beta_{ij} \frac{\partial^2 f_*}{\partial Q_{ij}\partial Q_{k\ell}} \partial_m Q^\beta_{k\ell} - \Gamma\vartheta \left|\frac{\partial f_*}{\partial Q}(Q^\beta)\right|^2 + \Gamma\kappa\, Q^\beta : \frac{\partial f_*}{\partial Q}(Q^\beta),$$

where $\mathcal{L}_\beta := u^\beta \cdot \nabla - \Gamma L\,\Delta$, since

$$\operatorname{tr}\left(S(Q^\beta, \nabla u^\beta)Q^k\right) = 0 \quad \text{for all} \quad k \geq 1.$$

By the convexity property **(M1)** of f_*, one may infer that $f_*(Q^\beta)$ satisfies the parabolic inequality

$$\left(\frac{\partial}{\partial t} + \mathcal{L}_\beta\right) f_*(Q^\beta) \leq \frac{\Gamma\kappa^2}{2\vartheta}|Q^\beta|^2$$

subject to the initial condition $f_*(Q(\cdot,0)) = f_*(Q_{0,\beta})$. By considering the following auxiliary initial-value problem for $g = g^\beta$,

$$\begin{cases} \left(\dfrac{\partial}{\partial t} + \mathcal{L}_\beta\right) g = \dfrac{\Gamma\kappa^2}{2\vartheta}|Q^\beta|^2 \\ \\ g(\cdot,0) = f_*(Q_{0,\beta}) \end{cases}$$

one may infer by comparing $f_*(Q)$ with g that the classical maximum principle implies

$$f_*(Q^\beta(x,t)) \leq g^\beta(x,t) \quad \text{on} \quad I^d \times (0,T].$$

Thus, if one can control the comparison function $g^\beta(\cdot,t)$ in L^∞ uniformly in β for $t > 0$ *and* in a manner which is independent of the regularisation of the singular potential, one has hope of showing that

$$f(Q(x,t)) \leq \omega(t) \quad \text{on} \quad I^d \times (0,T]$$

once we pass to limits and approximation parameters are removed. Although this argument is somewhat rough, it contains the spirit of the proof contained in Stage III of section 2.7 to follow.

2.7 Existence of Strictly Physical Weak Solutions

In this section, we provide a proof of Theorem 2.12, namely the existence of global weak solutions of (S) and the fact that the dynamics instantaneously contracts the range of the initial data in the case when $\xi = 0$. We emphasise, however, that the comparison principle for $f(Q)$ is currently out of reach in the non-corotational case, i.e. when $\xi \neq 0$.

The plan runs as follows. We perform three levels of regularisation in our construction of weak solutions:

1. (Parameter $\eta > 0$) Mollification of the initial data $Q_0 \in H^1$, yielding $Q_{0,\eta} \in C^\infty$;
2. (Parameter $N \geq 1$) Regularisation of the singular potential f in the manner of section 2.3, yielding f_N;

3. (Parameter $M \geq 1$) Projection of the Navier-Stokes equations onto an appropriate M-dimensional subspace of L^2_{div}.

We establish the maximum principle argument at the highest level of smoothness, namely when the approximate solutions depend on all three parameters M, N and η. We subsequently remove dependence of approximate solutions on η, N and M (in this order), whilst ensuring that information obtained in the maximum principle argument can be carried all the way through to weak solutions.

Let us begin the construction, and thereby the proof of theorem 2.12.

Stage I: Existence of Smooth Approximants

Let us now set out the basic objects which we use to build weak solutions. Suppose initial data $(Q_0, u_0) \in H^1 \times L^2_{\text{div}}$ are given. For any $\eta > 0$ and $\zeta \in C^\infty_c(\mathbb{R}^d, \mathbb{R}_+)$ of unit mass, we define the standard η-mollification of the initial datum Q_0 to be $Q_{0,\eta}$, namely

$$Q_{0,\eta}(x) := \frac{1}{\eta^d} \int_{\mathbb{R}^d} \zeta\left(\frac{x-y}{\eta}\right) Q_0(y)\, dy.$$

By standard theory (Evans [32], Appendix C) we know that $Q_0 \in C^\infty$ and $\|Q_{0,\eta}\|_{H^1(I^d)} \to \|Q_0\|_{H^1(I^d)}$ as $\eta \to 0$. We make the obvious remark at this point that although $f(Q_0) \in L^1$, it may not be the case that $f(Q_{0,\eta}) \in L^1$; however, we have designed our approximation scheme in such a way that we need only consider $f_N(Q_{0,\eta})$ (which does lie in L^1 by **(M1)**) before passing to $f_N(Q_0)$ as $\eta \to 0$.

It is well known (Temam [82], Section 2.2) that the periodic Stokes eigenvalue problem on $\mathbb{R}^d$

$$\begin{cases} -\nu\Delta\phi + \nabla P = \mu\phi \quad \text{on} \quad \mathbb{R}^d, \\ \nabla \cdot \phi = 0, \\ \phi(x + \Lambda\pi e_i) = \phi(x) \quad \text{for all} \quad x \in \mathbb{R}^d \quad \text{and} \quad i = 1, ..., d, \end{cases}$$

has a countable set of solutions $\{\phi_{j,k} : j = 1, ..., d,\ k \in \mathbb{Z}^d\}$ given explicitly by

$$\phi_{j,k}(x) := \left(e_j - \frac{k_j}{|k|^2} k\right) e^{\frac{2\sqrt{-1}k\cdot x}{\Lambda}} \quad \text{for } j = 1, ..., d \text{ and } k \in \mathbb{Z}^d,$$

with corresponding eigenvalues $\mu_{j,k} := 4|k|^2\Lambda^2$, where $\{e_j\}_{j=1}^d$ denotes the canonical orthonormal basis of $\mathbb{R}^d$. Moreover, this countable set forms an orthonormal basis for L^2_{div}. For convenience, we enumerate this countable sequence by $\{\phi_1, \phi_2, \phi_3, ...\}$ with corresponding eigenvalues $\{\mu_1, \mu_2, \mu_3, ...\}$. For each $M \geq 1$, we define the orthogonal projection operator $\mathbb{P}_M : L^2_{\text{div}} \to \text{span}_{\mathbb{C}}\{\phi_m\}_{m=1}^M$ by

$$\mathbb{P}_M u := \sum_{m=1}^{M} (u, \phi_m)\, \phi_m \quad \text{for any} \quad u \in L^2_{\text{div}}.$$

Finally, we also consider the orthonormal basis of periodic L^2-functions associated with the eigenvalue problem for the negative Laplacian on $\mathbb{R}^d$, namely

$$\begin{cases} -\Delta\varphi = \lambda\varphi \quad \text{on} \quad \mathbb{R}^d, \\ \varphi(x + \Lambda\pi e_i) = \varphi(x) \quad \text{for all} \quad x \in \mathbb{R}^d \quad \text{and} \quad i = 1, ..., d, \end{cases}$$

whose countable set of solutions may enumerated as $\{\varphi_k\}_{k=1}^{\infty}$ with corresponding eigenvalues $\{\lambda_k\}_{k=1}^{\infty}$.

It will also be convenient to denote the regularised free energy by E_N for each $N = 1, 2, 3, ...$, namely

$$E_N(Q) := \int_{I^d} \left(\frac{L}{2}|\nabla Q|^2 + \vartheta\, f_N(Q) - \frac{\kappa}{2}\,|Q|^2 \right) dx.$$

Finally, since we work with three regularisation parameters, namely M, N and η, we denote the corresponding approximate solutions of (S) by

$$\left(Q^{M,N,\eta}, u^{M,N,\eta}\right), \quad \left(Q^{M,N}, u^{M,N}\right) \quad \text{and} \quad \left(Q^{M}, u^{M}\right),$$

where the superscripts are *labels*, as opposed to powers. With all of this set out, let us now consider the following.

Proposition 2.15. *Let $M, N \geq 1$ and $\eta > 0$ be given and fixed. For initial data $u_0 \in L^2_{\text{div}}$ and physical $Q_0 \in H^1$ (i.e. $f(Q_0) \in L^1$), there exist $T = T(Q_0, u_0) > 0$ and smooth maps $Q^{M,N,\eta}$ and $u^{M,N,\eta}$ satisfying the system*

$$\begin{cases} \dfrac{\partial Q^{M,N,\eta}}{\partial t} + (u^{M,N,\eta} \cdot \nabla)Q^{M,N,\eta} - S(Q^{M,N,\eta}, \nabla u^{M,N,\eta}) = -\Gamma \dfrac{\delta E_N}{\delta Q}(Q^{M,N,\eta}), \\ \dfrac{\partial u^{M,N,\eta}}{\partial t} + \mathbb{P}_M \left[(u^{M,N,\eta} \cdot \nabla)u^{M,N,\eta}\right] = \nu\Delta u^{M,N,\eta} + \mathbb{P}_M \left[\text{Div}\left(\tau(Q^{M,N,\eta}) + \sigma(Q^{M,N,\eta})\right)\right], \end{cases}$$

pointwise in $\text{Sym}_0(d)$ and $\mathbb{R}^d$ respectively for all $x \in \mathbb{R}^d$ and $t \in [0, T]$. Moreover, $Q^{M,N,\eta}(\cdot, 0) = Q_{0,\eta}$ and $u^{M,N,\eta}(\cdot, 0) = \mathbb{P}_M u_0$.

Proof. The basic idea of the proof (a Schauder and Banach fixed point argument) is taken from the work of Lin and Liu ([55], Theorem 2.1), in which a modified Ericksen-Leslie system is studied, as opposed to the Beris-Edwards model.

The essence of the argument is as follows. We begin with a convex subset K of a complete metric space comprised of approximate velocity fields. Any member w of K can be used to generate a solution $Q = Q_w$ of the equation

$$\frac{\partial Q}{\partial t} + (w \cdot \nabla)\, Q - S(Q, \nabla w) = -\Gamma \frac{\delta E_N}{\delta Q}(Q).$$

In turn, the map Q_w can be used to generate a solution $u = u_w$ of the equation

$$\frac{\partial u}{\partial t} + \mathbb{P}_M \left[(u \cdot \nabla u)\right] - \nabla P = \nu\Delta u + \mathbb{P}_M \left[\text{Div}\left(\tau(Q_w) + \sigma(Q_w)\right)\right],$$

which belongs to the same convex set K. We then show that the operator $\mathcal{S} : K \to K$ defined by $\mathcal{S}w := u_w$ satisfies the hypotheses of the Schauder fixed point theorem, from which we deduce the existence of at least one pair (Q, u) which satisfies an approximate coupled system with the same energy structure as (S).

The proof runs from *Step I* to *Step IV* below.

Step I. For sufficiently small $T > 0$ (which is to be determined in the course of the contraction argument below), choose an initial collection of co-ordinate maps $d = (d_1, ..., d_M) \in C([0,T]; \mathbb{C}^M)$ belonging to the closed convex subset K,

$$K := \left\{ b \in C([0,T]; \mathbb{C}^M) \,:\, |b(t)|_{\mathbb{C}^M} \leq 1 + 2\|\mathbb{P}_M u_0\|_2 \quad \text{for} \quad 0 \leq t \leq T \right\}.$$

Since K is a closed topological subspace of $C([0,T]; \mathbb{C}^M)$ when equipped with the uniform (metric) subspace topology, we know it to be a complete metric space. Consider the parabolic initial-value problem parameterised by $w := \sum_{k=1}^M d_k \phi_k$,

$$(\mathrm{P}_w) \begin{cases} \dfrac{\partial Q}{\partial t} + (w \cdot \nabla) Q - S(Q, \nabla w) = \Gamma \left(L\Delta Q - \vartheta \left\langle \dfrac{\partial f_N}{\partial Q}(Q) \right\rangle + \kappa\, Q \right) \\ Q(\cdot, 0) = Q_{0,\eta}. \end{cases}$$

We construct a unique strong solution of this problem in the following way. For any given positive integer $R \geq 1$, suppose we are given co-ordinate maps $q^R = (q_1^R, ..., q_R^R) \in C([0,T]; \mathrm{Sym}_0(d)^R)$, where $\mathrm{Sym}_0(d)^R$ is simply the R-fold cartesian product of $\mathrm{Sym}_0(d)$ with itself. We now define a map $\mathcal{T}_R q^R : C([0,T]; \mathrm{Sym}_0(d)^R) \to C([0,T]; \mathrm{Sym}_0(d)^R)$ pointwise in time by

$$(\mathcal{T}_R q^R)_j(t) := q_j^R(0) + \Gamma\left(L\lambda_j + \kappa\right) \int_0^t q_j^R(s)\, ds + \int_0^t F_j(q^R(s), s)\, ds$$

for $j = 1, ..., R$, where

$$F(q^R(t), t) := -\sum_{r=1}^R \int_{I^d} q_r^R(t)(w(y,t) \cdot \nabla)\varphi_r(y)\varphi_j(y)\, dy$$

$$+\frac{1}{2}\sum_{r=1}^R \int_{I^d} \left(D_0(w(y,t)) : q_r^R(t) - q_r^R(t) : D_0(w(y,t)) \right) \varphi_r(y)\varphi_j(y)\, dy$$

$$-\Gamma\vartheta \int_{I^d} \left\langle \frac{\partial f_N}{\partial Q}(Q^R(y,t)) \right\rangle \varphi_j(y)\, dy.$$

and $q_j^R(0) := (Q_{0,\eta}, \varphi_j)$. Since $F = F(q,t)$ is merely continuous and not Lipschitz in its q argument, Peano's theorem (Hartman [43], Theorem 2.1) secures us the existence of a local-in-time solution to the ODE

$$\frac{dq^R}{dt}(t) = \Gamma(L\lambda_j + \kappa) q^R(t) + F(q^R(t), t) \quad \text{on} \quad (0,T). \tag{2.14}$$

Defining approximate tensor fields Q^R to be

$$Q^R(x,t) := \sum_{r=1}^{R} q_r^R(t)\varphi_r(x),$$

one can show that the ODE (2.14) implies that Q^R satisfies the equality

$$\frac{\partial Q^R}{\partial t} + \mathbb{P}_R\left[(w\cdot\nabla)Q^R - S(Q^R,\nabla w)\right] = \Gamma\left(L\Delta Q^R - \vartheta\mathbb{P}_R\left[\left\langle\frac{\partial f_N}{\partial Q}(Q^R)\right\rangle\right] + \kappa\, Q^R\right) \tag{2.15}$$

pointwise in $\mathrm{Sym}_0(d)$ for all $x \in I^d$ and $t \in (0,T)$. This construction holds for any $R \in \{1,2,3,...\}$, and thus we have constructed a sequence $\{Q^R\}_{R=1}^{\infty}$ of smooth approximants to problem (P_w). By smoothness of the initial datum $Q_{0,\eta}$ and property **(M7)** of the regularised potential f_N, namely that its derivatives grow no faster than quadratically at infinity, one can show that

$$\{Q^R\}_{R=1}^{\infty} \quad \text{and} \quad \left\{\frac{\partial Q^R}{\partial t}\right\}_{R=1}^{\infty} \quad \text{are uniformly bounded in} \quad L^\infty(0,T;H^k)$$

for any $k \geq 0$. By the Banach-Alaoglu, Aubin-Lions and Rellich-Kondrashov compactness theorems (see Lions [57]), we infer the existence of a map $Q \in L^2(0,T;H^k)$ such that

$$Q^R \longrightarrow Q \quad \text{and} \quad \frac{\partial Q^R}{\partial t} \longrightarrow \dot{Q} \quad \text{in} \quad L^2(0,T;H^k),$$

where $\dot{Q}$ denotes the distributional time derivative of Q. Note at this point, as we only know w to be continuous in time, we cannot infer that Q is classically-differentiable in time as a map into the Hilbert spaces H^k for $k \geq 1$. Thus, passing to the limit $R \to \infty$ in equation (2.15) we deduce that the map Q satisfies

$$\dot{Q} + (w\cdot\nabla)Q - S(Q,\nabla w) = \Gamma\left(L\Delta Q - \vartheta\left\langle\frac{\partial f_N}{\partial Q}(Q)\right\rangle + \kappa\, Q\right) \tag{2.16}$$

in $L^2(0,T;H^k)$ for all $k \geq 0$.

For the purposes of achieving our fixed point argument, it is important for us to know that the solution Q just constructed is unique. Since f_N is smooth and convex by property **(M1)**, we know by standard results in convex analysis (Barbu [9], Theorem 2.8) that the subdifferential of f_N on $\mathbb{R}^{d\times d}$ (which coincides with its classical derivative) satisfies

$$\left(\frac{\partial f_N}{\partial Q}(X) - \frac{\partial f_N}{\partial Q}(Y)\right) : (X-Y) \geq 0 \tag{2.17}$$

for all $X, Y \in \mathbb{R}^{d\times d}$. Supposing, then, that there exist two strong solutions Q and $\overline{Q}$ satisfying (2.16) for the given initial datum $Q_{0,\eta}$, one may show using (2.17) that

$$\frac{d}{dt}\|Q(\cdot,t) - \overline{Q}(\cdot,t)\|_2^2 \leq C\|Q(\cdot,t) - \overline{Q}(\cdot,t)\|_2^2$$

whence Gronwall's inequality allows us to deduce $Q(\cdot,t) = \overline{Q}(\cdot,t)$ in L^2, and so strong solutions of (2.16) are indeed unique for the given initial datum. Let us henceforth denote the unique solution of (2.16) by $\widetilde{Q_w}$ to emphasise its dependence on the divergence-free vector field w.

We now use this solution $\widetilde{Q_w}$ to generate a solution of the approximate Navier-Stokes equations. For a newly-chosen $b \in K$ consider now the element $\mathcal{T}b$ built using the solution $\widetilde{Q_w}$ and the initial datum $u_0 \in L^2_{\mathrm{div}}$, defined componentwise by

$$\begin{aligned}(\mathcal{T}b)_m(t) := \quad & (u_0,\phi_m)_{H_0} - \nu\mu_m \int_0^t b_m(s)\,ds - \alpha_{jkm}\int_0^t b_j(s)b_k(s)\,ds \\ & - \int_0^t \int_{I^d} \Big(\tau_{ik}(\widetilde{Q_w}(y,s)) + \sigma_{ik}(\widetilde{Q_w}(y,s))\Big)\,\partial_k\phi_{m,i}(y)\,dyds\end{aligned}$$

for $0 \leq t \leq T$ and $m = 1,...,M$. The constants α_{jkm} are given by

$$\alpha_{jkm} := \int_{I^d} \phi_{k,i}\partial_i\phi_{j,\ell}\phi_{m,\ell},$$

each of which is finite since $\phi_j \in C^\infty_{\mathrm{per}}(\mathbb{R}^d,\mathbb{C}^d)$ for $j \geq 1$. One may check that $\mathcal{T}b$ is an element of $K \subset C([0,T];\mathbb{C}^M)$ and that as an operator $\mathcal{T}: K \to K$ is continuous with respect to the uniform topology. Furthermore, one may show that $\mathcal{T}: K \to K$ is a contractive operator, assuming that we adjust $T > 0$ to be as small as is required. Thus, following an application of the Banach fixed point theorem (Bollobás [15], Chapter 7, Theorem 1) we deduce the existence of a unique continuous map $b^* = b^*_w \in K$ satisfying

$$\begin{aligned}b^*_m(t) := \quad & (u_0,\phi_m)_{H_0} - \nu\mu_m \int_0^t b^*_m(s)\,ds - \alpha_{jkm}\int_0^t b^*_j(s)b^*_k(s)\,ds \\ & - \int_0^t \int_{I^d} \Big(\tau_{ik}(\widetilde{Q_w}(y,s)) + \sigma_{ik}(\widetilde{Q_w}(y,s))\Big)\,\partial_k\phi_{m,i}(y)\,dyds,\end{aligned}$$

for $m = 1,...,M$ and $t \in [0,T]$. By the fundamental theorem of calculus, we infer that $b^* \in C^1((0,T);\mathbb{C}^M)$ and that the system of ordinary differential equations

$$\begin{aligned}& \frac{db^*_m}{dt}(t) + \alpha_{jkm}b^*_j(t)b^*_k(t) \\ = \quad & -\nu\mu_m b^*_m(t) + \int_{I^d}\Big(\tau_{ik}(\widetilde{Q_w}(\cdot,t)) + \sigma_{ik}(\widetilde{Q_w}(\cdot,t))\Big)\,\partial_k\phi_{m,i}\end{aligned}$$

is satisfied by $b^*(t)$ for $0 < t < T$.

Step II. As the map b^* generated by Banach's fixed point theorem in the previous step is unique, it is clear that we have constructed an operator $\mathcal{S}$ from K into K given by $\mathcal{S}d := b^*$ for all $d \in K$. It is at this point we require uniqueness of Q_w in *Step I*, in order to prevent the operator $\mathcal{S}$ from being multivalued. We now show that there exists $c = c^{M,N,\eta} \in K$ (depending on the dimension M of Galerkin space, the degree of regularisation of f_N and the initial datum $Q_{0,\eta}$) such that $\mathcal{S}c = c$ in $C([0,T];\mathbb{C}^M)$.

Following a lengthy calculation, one may demonstrate that $\mathcal{S} : K \to K$ is continuous with respect to the uniform topology, and yet another lengthy calculation reveals that the family $\mathcal{S}(K) \subset K$ is also equicontinuous. By the Arzelà-Ascoli theorem (Dudley [29], Theorem 2.4.7), it follows that $\mathcal{S}(K)$ is a compact topological subspace of K. In turn, the Schauder fixed point theorem (Bollobás [15], Chapter 15, Theorem 7) confirms to us the existence of an element $c = c^{M,N,\eta} \in K$ satisfying $\mathcal{S}c = c$.

Step III. If we denote by $u^{M,N,\eta}$ the finite-dimensional divergence free velocity field given by $u^{M,N,\eta} := \sum_k c_k^{M,N,\eta}\phi_k$ and by $Q^{M,N,\eta}$ the solution of the above problem (P_w) parameterised by $w \equiv u^{M,N,\eta}$, by following the construction outlined in the first step one quickly sees that *Step II* implies that the coupled system

$$\begin{cases} \dot{Q} + (u^{M,N,\eta} \cdot \nabla)Q^{M,N,\eta} - S(Q^{M,N,\eta}, \nabla u^{M,N,\eta}) = -\Gamma \dfrac{\delta E_N}{\delta Q}(Q^{M,N,\eta}), \\ \dfrac{dc_m}{dt} + \alpha_{jkm}c_j c_k = -\nu\mu_m c_m + \displaystyle\int_{I^d} \left(\tau_{ik}(Q^{M,N,\eta}) - \sigma_{ik}(Q^{M,N,\eta})\right) \partial_k \phi_{m,i} \\ \nabla \cdot u^{M,N,\eta} = 0, \end{cases}$$

is satisfied by $Q^{M,N,\eta}$ and $u^{M,N,\eta}$. Now, since $\{\phi_j\}_{j=1}^{\infty}$ constitutes an orthonormal family for L^2_{div}, we make the observation that

$$\frac{dc_m}{dt} = \frac{dc_k}{dt}\delta_{km} = \frac{dc_k}{dt}(\phi_k, \phi_m) = \left(\frac{dc_k}{dt}\phi_k, \phi_m\right) = \int_{I^d} \frac{\partial u^{M,N,\eta}}{\partial t} \cdot \phi_m.$$

Similar observations hold for the other terms of the ODE system for $c = c^{M,N,\eta}$, keeping in mind that each ϕ_j is an eigenfunction of the Stokes operator on $\mathbb{R}^d$ subject to periodicity conditions. Thus, the system of ordinary differential equations for the evolution of the co-ordinates c is equivalent to the equality

$$\frac{\partial u^{M,N,\eta}}{\partial t} + \mathbb{P}_M\left[(u^{M,N,\eta} \cdot \nabla)u^{M,N,\eta}\right] = \nu\Delta u^{M,N,\eta} + \mathbb{P}_M\left[\mathrm{Div}\left(\tau(Q^{M,N,\eta}) + \sigma(Q^{M,N,\eta})\right)\right],$$

which holds in L^2_{div} for $t \in (0, T)$.

Step IV. We now wish to show that strong solutions of the $Q^{M,N,\eta}$-equation (2.16) are classical. By considering the auxiliary problem

$$\begin{cases} \dfrac{\partial R}{\partial t} + (u^{M,N,\eta} \cdot \nabla)R - S(R, \nabla u^{M,N,\eta}) = \Gamma\left(L\Delta R - \vartheta\left\langle \dfrac{\partial f_N}{\partial Q}(R)\right\rangle + \kappa R\right), \\ R(\cdot, 0) = Q_{0,\eta}, \end{cases}$$

and using the fact that $u^{M,N,\eta}$ is known to be $C^1((0,T); C^{\infty}_{\mathrm{per}}(\mathbb{R}^d))$ (whereas w was only known to be in $C([0,T]; \mathbb{C}^M)$ in *Step I* of the construction), we can once again, by standard methods, construct a classical solution to this problem. Once again, by the previous

uniqueness argument we deduce that $R^{M,N,\eta} = Q^{M,N,\eta}$, whence $Q^{M,N,\eta}$ is indeed a classical solution of the approximate system.

The proof is now complete. □

Stage II: Relaxing Regularity on Initial Data

In order that our classical maximum principle argument may be applied in Stage III below, it is crucial that we regularise the initial Q-tensor field Q_0 to construct approximate maps which are smooth and thus suitable for the purposes of applying this technique. It is necessary to remove smoothness of initial data at this stage before progressing to remove the regularisation on the singular potential f, so that we need not worry about the possible lack of integrability of $f(Q_{0,\eta})$.

We now demonstrate the following.

Proposition 2.16. *For each fixed $M, N \in \{1, 2, 3, ...\}$, there exist maps $Q^{M,N} \in L^\infty_t H^1_x \cap L^2_t H^2_x$ and $u^{M,N} \in C([0,T]; \mathbb{P}_M L^2_{\mathrm{div}})$ such that the following convergence results hold (up to a subsequence, $\{\eta_j\}_{j=1}^\infty$ with $\eta_k \to 0$):*

$$Q^{M,N,\eta} \longrightarrow Q^{M,N} \quad \text{in} \quad L^2(0,T;H^2),$$

and

$$u^{M,N,\eta} \longrightarrow u^{M,N} \quad \text{uniformly on} \quad I^d \times [0,T].$$

Moreover, these limit points satisfy the system

$$\begin{cases} \dot{Q}^{M,N} + (u^{M,N} \cdot \nabla) Q^{M,N} - S(Q^{M,N}, \nabla u^{M,N}) = -\Gamma \dfrac{\partial E_N}{\partial Q}(Q^{M,N}) \\ \dot{u}^{M,N} + \mathbb{P}_M \left[(u^{M,N} \cdot \nabla) u^{M,N} \right] = \nu \, \Delta u^{M,N} + \mathbb{P}_M \left[\mathrm{Div} \left(\tau(Q^{M,N}) + \sigma(Q^{M,N}) \right) \right] \end{cases}$$

in the strong sense in $L^2_t L^2_x$ and $L^2(0,T;\mathbb{P}_M L^2_{\mathrm{div}})$, respectively.

Proof. With the formal manipulations of the system (S) of section 2.5 in mind, as $Q^{M,N,\eta}$ and $u^{M,N,\eta}$ are smooth in space and time, one can show that the approximate coupled system at level-(M,N,η) has the energy law

$$\frac{d\mathcal{E}^{M,N,\eta}}{dt} + \left\| L\Delta Q^{M,N,\eta} - \vartheta \left\langle \frac{\partial f_N}{\partial Q}(Q^{M,N,\eta}) \right\rangle + \kappa \, Q^{M,N,\eta} \right\|_2^2 + \nu \|\nabla u^{M,N,\eta}\|_2^2 = 0, \quad (2.18)$$

where

$$\mathcal{E}^{M,N,\eta}(t) := \frac{1}{2}\|u^{M,N,\eta}(\cdot,t)\|_2^2 + \frac{L}{2}\|\nabla Q^{M,N,\eta}(\cdot,t)\|_2^2 + \vartheta \int_{I^d} f_N(Q^{M,N,\eta}(z,t))\, dz - \frac{\kappa}{2}\|Q^{M,N,\eta}(\cdot,t)\|_2^2.$$

As we employ f_N instead of the full potential f at this level of regularity, we need not worry about the range of the approximants $Q^{M,N,\eta}$. As such, by the convexity property **(M1)** of the mollified potential f_N, we have the useful sign condition

$$\int_{I^d} \Delta Q^{M,N,\eta}(z,t) : \frac{\partial f_N}{\partial Q}(Q^{M,N,\eta}(z,t))\, dz \leq 0.$$

To obtain bounds on the approximate maps $Q^{M,N,\eta}$ and $u^{M,N,\eta}$ which are independent of $\eta > 0$ for any fixed M and N, we fix our attention on the evolution equation for $Q^{M,N,\eta}$. Recall from our discussion in section 2.5 that we need to verify that

$$\left\{Q^{M,N,\eta}\right\}_{\eta>0} \text{ is uniformly bounded in } \eta \text{ in } L^2_t L^2_x$$

in order to obtain uniform bounds on approximants $Q^{M,N,\eta}$ and $u^{M,N,\eta}$ in higher Sobolev spaces. In this direction, by multiplying throughout by

$$\vartheta \left\langle \frac{\partial f_N}{\partial Q}(Q^{M,N,\eta}) \right\rangle + \kappa\, Q^{M,N,\eta}$$

and integrating over space, by the convexity property **(M1)** of f_N we may derive the inequality

$$\frac{d}{dt}\left(\frac{\kappa}{2}\|Q^{M,N,\eta}\|_2^2 + \vartheta \int_{I^d} f_N(Q^{M,N,\eta})\, dz\right) + \Gamma L \|\nabla Q^{M,N,\eta}\|_2^2 \leq \Gamma \kappa^2 \|Q^{M,N,\eta}\|_2^2.$$

By property **(M2)** of f_N, namely that it is bounded below on $\mathrm{Sym}_0(d)$, integration in time over the interval $[0,T]$ yields

$$\begin{aligned}\frac{\kappa}{2}\|Q^{M,N,\eta}(\cdot,t)\|_2^2 + \vartheta \int_{I^d} f_N(Q^{M,N,\eta}(z,t))\, dz \leq e^{2\Gamma\kappa t}\left(\frac{\kappa}{2}\|Q_{0,\eta}\|_2^2 + \vartheta \int_{I^d} f_N(Q_{0,\eta})\, dz\right) \\ + \vartheta(\pi\Lambda)^d f_0\left(e^{2\Gamma\kappa t} - 1\right).\end{aligned}$$

The boundedness property **(M2)** of the regularised potential allows us to infer that

$$-\vartheta(\Lambda\pi)^d f_0 \leq \vartheta \int_{I^d} f_N(Q^{M,N,\eta}(z,t))\, dz,$$

and since $Q_{0,\eta} \to Q_0$ pointwise almost everywhere, by the dominated convergence theorem we may deduce that

$$\lim_{\eta\to 0} \int_{I^d} f_N(Q_{0,\eta})\, dz = \int_{I^d} f_N(Q_0)\, dz,$$

since $f_N(Q_{0,\eta})$ is dominated by the constant $\max_{Q\in K} f_N(Q)$ for a suitably large compact subset $K \supset \mathsf{D}(f)$ containing the effective domain of f whenever $\eta \leq 1$, say. It follows from these observations, along with continuity of the mollification operator on $L^2(I^d)$, that there exists $\overline{\eta} = \overline{\eta}(N) > 0$ such that

$$\frac{\kappa}{2}\|Q^{M,N,\eta}(\cdot,t)\|_2^2 \leq e^{2\Gamma\kappa T}\left(\|Q_0\|_2^2 + \vartheta + \vartheta \int_{I^d}(f_0 + f_N(Q_0))\right)$$

for all $0 < \eta \leq \overline{\eta}$, whence $\{Q^{M,N,\eta}\}_{\eta \leq \overline{\eta}}$ is indeed a uniformly bounded sequence in $L^\infty_t L^2_x$ for any fixed M and N. Moreover, it is at this point we can extend the time of existence $T > 0$ that was constrained in the course of the previous contraction argument to be as large as desired.

As outlined previously in section 2.5, one can use this information on $Q^{M,N,\eta}$ to find an explicitly-computable constant $C = C(Q_0, u_0, f, T, \Gamma, L, \kappa, \vartheta) > 0$ such that

$$\|Q^{M,N,\eta}(\cdot,t)\|^2_{H^1} + \|u^{M,N,\eta}(\cdot,t)\|^2_2 \leq C(Q_0, u_0, f, T, \Gamma, L, \kappa, \vartheta); \tag{2.19}$$

for all $t \in [0,T]$, which in turn yields the L^2-in time estimates

$$\begin{aligned}\int_0^T \|Q^{M,N,\eta}(\cdot,s)\|^2_{H^2}\, ds + \int_0^T \left\| \left\langle \frac{\partial f_N}{\partial Q}(Q^{M,N,\eta}(\cdot,s)) \right\rangle \right\|^2_2 ds \\ + \int_0^T \|u^{M,N,\eta}(\cdot,s)\|^2_{H^1_{\mathrm{div}}}\, ds \leq C(Q_0, u_0, f, T, \Gamma, L, \kappa, \vartheta).\end{aligned} \tag{2.20}$$

We also record the bound

$$\int_{I^d} \left(f_0 + f_N(Q^{M,N,\eta}(z,t))\right)\, dz \leq C(Q_0, u_0, f, T, \Gamma, L, \kappa, \vartheta) \tag{2.21}$$

which holds for all $t \in [0,T]$, and is crucial when it comes to recovering spatial L^∞ information on approximants when $N \to \infty$, i.e. when we recover the singular potential f from its regularisation f_N.

We may also, at this level of regularity, extract better uniform bounds on the approximate velocity fields from the bound (2.19). Firstly, by using orthonormality in L^2_{div} of the family of eigenfunctions of the Stokes operator $\{\phi_j\}_{j=1}^\infty$, the L^2-norm of $u^{M,N,\eta}(\cdot,t)$ is realised as

$$\|u^{M,N,\eta}(\cdot,t)\|^2_2 = \sum_{j=1}^M |c_j^{M,N,\eta}(t)|^2,$$

where $u^{M,N,\eta} = \sum_{m=1}^M c_m^{M,N,\eta}\phi_j$, a quantity whose supremum in time we know to be uniformly bounded in $\eta \leq \overline{\eta}$. Using the above uniform bounds (2.19) and (2.20) together with the equality

$$\frac{\partial Q^{M,N,\eta}}{\partial t} = -\left(u^{M,N,\eta}\cdot\nabla\right) Q^{M,N,\eta} + S(Q^{M,N,\eta}, \nabla u^{M,N,\eta}) - \Gamma \frac{\delta E_N}{\delta Q}(Q^{M,N,\eta}),$$

we are able to infer that

$$\left\{\frac{\partial Q^{M,N,\eta}}{\partial t}\right\}_{\eta \leq \overline{\eta}} \text{ is uniformly bounded in } L^2_t L^2_x.$$

Moreover, since we take the M-dimensional projection of the forcing term in the Navier-Stokes equations, using the fact that $\{Q^{M,N,\eta}\}_{\eta \leq \overline{\eta}}$ is uniformly bounded in $L^\infty_t H^1_x$ by (2.20), appealing to the equality

$$\frac{\partial u^{M,N,\eta}}{\partial t} = \nu\Delta u^{M,N,\eta} - \mathbb{P}_M\left[\left(u^{M,N,\eta}\cdot\nabla\right)u^{M,N,\eta} - \mathrm{Div}\left(\tau(Q^{M,N,\eta}) + \sigma(Q^{M,N,\eta})\right)\right],$$

we may infer that

$$\left\{\frac{\partial u^{M,N,\eta}}{\partial t}\right\}_{\eta\leq\overline{\eta}} \text{ is uniformly bounded in } L^\infty_t L^2_{\text{div}},$$

or equivalently,

$$\left\{\sum_{m=1}^{M}\left|\frac{dc_m^{M,N,\eta}}{dt}(t)\right|^2\right\}_{\eta\leq\overline{\eta}} \text{ is uniformly bounded in } L^\infty(0,T). \tag{2.22}$$

By the Banach-Alaoglu and Aubin-Lions compactness theorems, we may infer the existence of maps $Q^{M,N} \in L^\infty_t H^1_x \cap L^2_t H^2_x$ and $u^{M,N} \in L^\infty_t L^2_{\text{div}} \cap L^2_t H^1_{\text{div}}$ and relabeled subsequences such that

$$Q^{M,N,\eta} \text{ tends to } Q^{M,N} \text{ weakly in } L^2_t H^2_x \text{ and strongly in } L^2_t H^1_x \tag{2.23}$$

and

$$u^{M,N,\eta} \text{ tends to } u^{M,N} \text{ weakly in } L^2_t H^1_{\text{div}} \text{ and strongly in } L^2_t L^2_{\text{div}}.$$

At this point it will prove useful, for the purposes of achieving the maximum principle argument in the section to come, to strengthen the notion of convergence of approximate velocity fields. In fact, we have the following result by virtue of the previous uniform bound (2.22).

Lemma 2.17. *There exists a relabeled subsequence of $\{u^{M,N,\eta}\}_{\eta\leq\overline{\eta}}$ such that $u^{M,N,\eta}$ converges to $u^{M,N}$ uniformly in space and time.*

Proof. This follows from the Arzelá-Ascoli compactness lemma applied to the co-ordinate maps of $u^{M,N,\eta}$. Indeed, since the sequence $\{u^{M,N,\eta}\}_{\eta\leq\overline{\eta}}$ is uniformly bounded in $L^\infty_t L^2_{\text{div}}$ by (2.19) and since the co-ordinate maps are C^1 functions in time by the construction of proposition 2.15 in stage I, it follows that the sequence of co-ordinate maps $\{c^{M,N,\eta}\}_{\eta\leq\overline{\eta}}$ constitutes a bounded set in the space $C([0,T];\mathbb{C}^M)$. Moreover, by making use of the simple identity

$$c^{M,N,\eta}(t) = (u_0,\phi_j)e_j + \int_0^t \frac{dc^{M,N,\eta}}{dt}(s)\,dx \quad \text{for} \quad t\in[0,T]$$

and considering the difference of the maps $c^{M,N,\eta}(t)$ and $c^{M,N,\eta}(t+\tau)$ for any $\tau > 0$, it quickly follows that

$$\left|c^{M,N,\eta}(t) - c^{M,N,\eta}(t+\tau)\right| \leq \sqrt{\tau}\left(\int_0^T \left|\frac{dc^{M,N,\eta}}{dt}(s)\right|^2 ds\right)^{\frac{1}{2}},$$

and so by (2.22) we may infer that the sequence $\{c^{M,N,\eta}\}_{\eta\leq\overline{\eta}}$ also constitutes an equi-continuous family of maps in $C([0,T];\mathbb{C}^M)$. In turn, by the Arzelá-Ascoli lemma (see

Bollobás [15] Chapter 6, Theorem 4), it follows that $c^{M,N,\eta}$ converges to some $c^{M,N}$, from which we can deduce that $\sum_{m=1}^{M} c_m^{M,N}\phi_m$ is indeed equal to the limit point $u^{M,N} \in C([0,T];\mathbb{P}_M L^2_{\mathrm{div}})$ previously provided by Banach-Alaoglu compactness. □

Returning to the proof of proposition 2.16, we are now ready to pass to a limiting system as $\eta \to 0$. By property **(M6)** of the regularised potential, we have that

$$\left|\left\langle \frac{\partial f_N}{\partial Q}(Q^{M,N,\eta}(x,t))\right\rangle\right| \leq C_N^1 \left|Q^{M,N,\eta}(x,t)\right| + C_N^2,$$

and therefore by the dominated convergence theorem,

$$\left\langle \frac{\partial f_N}{\partial Q}(Q^{M,N,\eta})\right\rangle \longrightarrow \left\langle \frac{\partial f_N}{\partial Q}(Q^{M,N})\right\rangle \quad \text{in} \quad L^2_t L^2_x.$$

From this point onwards, it is straightforward to show that the limiting equations

$$\begin{cases} \dot{Q}^{M,N} + (u^{M,N}\cdot\nabla)Q^{M,N} - S(Q^{M,N},\nabla u^{M,N}) = -\Gamma\dfrac{\partial E_N}{\partial Q}(Q^{M,N}) \\ \dot{u}^{M,N} + \mathbb{P}_M\left[(u^{M,N}\cdot\nabla)u^{M,N}\right] = \nu\,\Delta u^{M,N} + \mathbb{P}_M\left[\mathrm{Div}\left(\tau(Q^{M,N}) + \sigma(Q^{M,N})\right)\right] \end{cases}$$

hold in the strong sense as claimed. □

Before we lift the regularisation on the Ball-Majumdar potential f, we make the following useful observations. Since the distributional time derivatives $\dot{Q}^{M,N}$ and $\dot{u}^{M,N}$ lie in $L^2_t L^2_x$ and $L^2_t L^2_{\mathrm{div}}$ respectively, we may infer that $Q^{M,N} \in C([0,T];H^1)$, $u^{M,N} \in C([0,T];L^2_{\mathrm{div}})$ and further that $Q^{M,N}(\cdot,0) = Q_0$ and $u^{M,N}(\cdot,t) = \mathbb{P}_M u_0$: see, for instance, Robinson ([72], Corollary 7.3). Now, since the $L^2_t L^2_x$- and $L^2_t L^2_{\mathrm{div}}$-norms are lower semi-continuous with respect to weak convergence (see Lieb and Loss [53], Theorem 2.11), the uniform estimates (2.19), (2.20) and (2.21), have the limiting forms

$$\|Q^{M,N}(\cdot,t)\|^2_{H^1} + \|u^{M,N}(\cdot,t)\|^2_2 \leq C(Q_0,u_0,f,T,\Gamma,L,\kappa,\vartheta) \text{ for all } t\in[0,T], \tag{2.24}$$

and also

$$\begin{aligned}\int_0^T \|Q^{M,N}(\cdot,s)\|^2_{H^2}\,ds + \int_0^T \left\|\left\langle \frac{\partial f_N}{\partial Q}(Q^{M,N}(\cdot,s))\right\rangle\right\|^2_2 ds \\ + \int_0^T \|u^{M,N}(\cdot,s)\|^2_{H^1_{\mathrm{div}}}\,ds \leq C(Q_0,u_0,f,T,\Gamma,L,\kappa,\vartheta),\end{aligned} \tag{2.25}$$

as $\eta \to 0$. Moreover, as it will prove important when we come to demonstrate physicality of weak solutions, in particular the preliminary step that

$$Q^M(x,t) \in \mathsf{D}(f) \quad \text{almost everywhere},$$

we also take note of the fact that

$$\int_{I^d} \left(f_0 + f_N(Q^{M,N}(z,t))\right)\,dz \leq C(Q_0,u_0,f,T,\Gamma,L,\kappa,\vartheta)$$

for all $t\in[0,T]$.

Remarks on Passing to the Limit $N \to \infty$

Before we pass to a limiting equation which limit points of the sequences $\{Q^{M,N}\}_{N=1}^{\infty}$ and $\{u^{M,N}\}_{N=1}^{\infty}$ satisfy, let us discuss a number of important observations. From the point of view of obtaining compactness results for the sequences $\{Q^{M,N}\}_{N=1}^{\infty}$ and $\{u^{M,N}\}_{N=1}^{\infty}$, the methods of this stage do not differ from the last, thanks to the uniform estimates (2.24) and (2.25). As such, we quickly deduce the existence of $Q^M \in L^{\infty}_t H^1_x \cap L^2_t H^2_x$ and $u^M \in L^{\infty}_t L^2_{\mathrm{div}} \cap L^2_t H^1_{\mathrm{div}}$ such that

$$Q^{M,N} \text{ tends to } Q^M \text{ weakly in } L^2_t H^2_x \text{ and strongly in } L^2_t H^1_x \tag{2.26}$$

and

$$u^{M,N} \text{ tends to } u^M \text{ weakly in } L^2_t H^1_{\mathrm{div}} \text{ and strongly in } L^2_t L^2_{\mathrm{div}}. \tag{2.27}$$

The main point to be checked at this stage is that it is possible to coerce the range of the approximants $Q^{M,N}$ to lie *essentially* in the set $\mathsf{D}(f)$ in the limit as $N \to \infty$, as otherwise $f(Q^M)$ and $\langle (\partial f/\partial Q)(Q^M) \rangle$ have no hope of being integrable. We achieve this by using the convergence properties **(M4)** and **(M5)** of f_N to f, the energy estimate (2.25) and the monotone convergence theorem. In fact, we have the following:

Proposition 2.18. *The approximate tensor field Q^M satisfies*

$$\int_{I^d} f(Q^M(z,t))\, dz < \infty$$

for $t \geq 0$. In particular, $Q^M(x,t) \in \mathsf{D}(f)$ almost everywhere.

Proof. Let us fix $\overline{N} \geq 1$ and suppose that N is taken to be such that $N \geq \overline{N}$. Since we know $Q^{M,N} \to Q^M$ in $L^2_t H^1_x$, it follows by the smoothness property **(M1)** of $f_{\overline{N}}$ that $f_{\overline{N}}(Q^{M,N}(x,t)) \to f_{\overline{N}}(Q^M(x,t))$ for almost every x and t as $N \to \infty$. Recalling that we have the uniform bound (2.25),

$$\int_{I^d} \left(f_0 + f_{\overline{N}}(Q^{M,N}(z,t))\right)\, dz \leq C(Q_0, u_0, f, T, \Gamma, L, \kappa, \vartheta) \text{ for all } n \geq \overline{N},$$

by Fatou's lemma and the monotonicity property **(M3)** we may deduce that

$$\int_{I^d} f_{\overline{N}}(Q^M(z,t))\, dz \leq C(Q_0, u_0, f, T, \Gamma, L, \kappa, \vartheta)$$

for $t \geq 0$ and any chosen $\overline{N} \geq 1$. An application of the monotone convergence theorem, together with property **(M3)** of the regularised potential yields that $f(Q^M(\cdot,t)) \in L^1$, and so by definition of the map f, it follows that $Q^M(x,t) \in \mathsf{D}(f)$ almost everywhere. □

It is immediate from this result together with lemma 2.3 that

$$|Q^M(x,t)| \leq \sqrt{1 - \frac{1}{d}} \quad \text{almost everywhere in space and time,}$$

from which we record the useful fact that $\{Q^M\}_{M=1}^{\infty}$ is uniformly bounded in $L_t^\infty L_x^\infty$.

To facilitate the passage to weak solutions at level M as $N \to \infty$, we pause at this point in order to demonstrate that the approximate tensor fields Q^M are in fact strictly physical for positive time $t > 0$.

Stage III: Approximants Q^M are Strictly Physical

It is in this stage we establish rigorously the maximum principle argument outlined in section 2.6. Let us begin at the level of regularity of Stage I, namely $Q^{M,N,\eta}$ and $u^{M,N,\eta}$ are smooth maps (proposition 2.15). Considering the evolution equation for the approximate tensor field,

$$\frac{\partial Q^{M,N,\eta}}{\partial t} + (u^{M,N,\eta} \cdot \nabla) Q^{M,N,\eta} - S(Q^{M,N,\eta}, \nabla u^{M,N,\eta}) = -\Gamma \frac{\delta E_M}{\delta Q}(Q^{M,N,\eta})$$

and multiplying throughout by $\langle (\partial f_N \partial Q)(Q^{M,N,\eta}) \rangle$, by the reasoning outlined in section 2.5 we deduce that $f_N(Q^{M,N,\eta})$ satisfies the parabolic inequality

$$\left(\frac{\partial}{\partial t} + u^{M,N,\eta} \cdot \nabla - \Gamma L \, \Delta \right) f_N(Q^{M,N,\eta}) \leq \frac{\Gamma \kappa^2}{2\vartheta} \left| Q^{M,N,\eta} \right|^2 .$$

Moreover, since f_N is smooth by property **(M1)**, it follows by smoothness of $Q^{M,N,\eta}$ that $f_N(Q^{M,N,\eta}(x,0)) = f_N(Q_{0,\eta}(x))$ on I^d. Such an inequality suggests that a comparison principle argument would be appropriate to control the quantity $f_N(Q^{M,N,\eta})$. In fact, we are able to prove the following:

$$\begin{gathered} \text{It is possible to control } f_N(Q^{M,N,\eta}) \text{ uniformly in } M \text{ in } L^\infty \\ \text{in the limit as } \eta \to 0 \text{ and } N \to \infty. \end{gathered}$$

If we can then ensure pointwise convergence of Q^M to the limit Q in the effective domain $\mathsf{D}(f)$ (which is the case if we establish strong convergence in, say, $L_t^2 L_x^2$), it will follow that $f(Q) \in L^\infty$ from which we infer that the limit Q is strictly physical (according to definition 2.3).

In order to achieve this, let us consider now the comparison maps $G = G^{M,N,\eta}$ and $H = H^{M,N,\eta}$, where G solves the homogeneous problem

$$(\mathrm{P})^1_{(M,N,\eta)} \begin{cases} \dfrac{\partial G}{\partial t} + (u^{M,N,\eta} \cdot \nabla) G - \Gamma L \, \Delta G = 0, \\ G(\cdot, 0) = f_N(Q_{0,\eta}) - \fint_{I^d} f_N(Q_{0,\eta}) \, dz \end{cases}$$

supplemented with *mean zero* initial data, and H solves the inhomogeneous problem

$$(\mathrm{P})^2_{(M,N,\eta)} \begin{cases} \dfrac{\partial H}{\partial t} + (u^{M,N,\eta} \cdot \nabla) H - \Gamma L \, \Delta H = \dfrac{\Gamma \kappa^2}{2\vartheta} \left| Q^{M,N,\eta} \right|^2, \\ H(\cdot, 0) = \fint_{I^d} f_N(Q_{0,\eta}) \, dz \end{cases}$$

with constant initial data. Since $Q_{0,\eta} \in C^\infty$ and $Q^{M,N,\eta}$ and $u^{M,N,\eta}$ are smooth, it follows by a standard construction in parabolic theory (see Evans [32], Section 7.1) that both problems above have unique smooth solutions.

Let us define $K^{M,N,\eta}$ to be the difference $f_N(Q^{M,N,\eta}) - G^{M,N,\eta} - H^{M,N,\eta}$, which is clearly a smooth map in space and time. One can quickly show that $K^{M,N,\eta}$ satisfies

$$\left(\frac{\partial}{\partial t} + u^{M,N,\eta} \cdot \nabla - \Gamma L \Delta\right) K^{M,N,\eta} \leq 0$$

with $K^{M,N,\eta}(x,0) = 0$ for all $x \in I^d$. By the classical parabolic maximum principle (see, for instance, Pucci and Serrin [70]), we find that this inequality implies that $K^{M,N,\eta} \leq 0$ on $I^d \times [0,T]$, whence

$$f_N(Q^{M,N,\eta}(x,t)) \leq G^{M,N,\eta}(x,t) + H^{M,N,\eta}(x,t) \quad \text{on} \quad I^d \times [0,T].$$

Suppose, then, that $Q^{M,N,\eta}(x,t)$ tends to $Q^M(x,t)$ almost everywhere. If we can obtain bounds on $G^{M,N,\eta}(\cdot,t)$ and $H^{M,N,\eta}(\cdot,t)$ in L^∞ for time $t > 0$ which are *independent of* M in the limit as $\eta \to 0$ and $N \to \infty$, we can infer by property **(M4)** of f_N that the approximants Q^M are strictly physical, since

$$f(Q^M(x,t)) \leq \lim_{N\to\infty} \lim_{\eta \to 0} f_N(Q^{M,N,\eta}(x,t)) \leq \lim_{N\to\infty} \lim_{\eta \to 0} \left(G^{M,N,\eta}(x,t) + H^{M,N,\eta}(x,t)\right) \leq \omega(t),$$

where $\omega(t)$ is independent of M for $t > 0$. Finally, if $Q^M \to Q$ almost everywhere in space and time, it will follow that

$$f(Q(x,t)) = \lim_{M\to\infty} f(Q^M(x,t)) \leq \omega(t),$$

from which we infer that the limit Q is strictly physical. We now perform an analysis of the comparison functions $G^{M,N,\eta}$ and $H^{M,N,\eta}$.

Analysis of the Comparison Function $G^{M,N,\eta}$

Although we know that the maps $f_N(Q_{0,\eta})$ lie in L^2 by property **(M6)**, we only know $f(Q_0)$ to be in L^1. Thus, to gain control on $G^{M,N,\eta}$ in the limit as $\eta \to 0$ and $N \to \infty$, we require the following $L^1 \to L^\infty$ estimate for spatially-periodic solutions of advection-diffusion equations due originally to Constantin et al. [23] but taken from Iyer [47], which we state without proof.

Lemma 2.19. *Let w be a smooth, spatially-periodic divergence-free velocity field, and suppose $\gamma > 0$. If g evolves under the advection-diffusion equation associated with w on $\mathbb{R}^d$, namely*

$$\begin{cases} \dfrac{\partial g}{\partial t} + (w \cdot \nabla) g - \Gamma L \Delta g = 0, \\ g(\cdot, 0) = g_0 \in L^1, \end{cases}$$

subject to mean-zero initial data, i.e. $\int_{I^d} g_0 = 0$*, then there exists a positive constant* $C = C(\gamma)$ *which is independent of* w *such that*

$$\|g(\cdot,t)\|_\infty \leq Ct^{-\frac{d}{2}-\gamma}\|g_0\|_1$$

for $t > 0$*.*

Remark 2.5. *The above* $L^1 \to L^\infty$ *estimate for solutions* g *of advection-diffusion equations was established in [23] in the general context of profiles* g *evolving on smooth, compact Riemannian manifolds. Moreover, in the case when dimension* $d = 3$*, one may take* $\gamma = 0$*, although this is unimportant for us in the context of obtaining a uniform bound on the comparison map* $G = G^{M,N,\eta}$ *for time* $t > 0$*.*

We use the result of this lemma directly. Setting $w = u^{M,N,\eta}$ and $g_0 = f_N(Q_{0,\eta}) - \fint_{I^d} f_N(Q_{0,\eta})\,dz$, we find that

$$\left|G^{M,N,\eta}(x,t)\right| \leq Ct^{-\frac{d}{2}-\gamma}\left\|f_N(Q_{0,\eta}) - \fint_{I^d} f_N(Q_{0,\eta})\,dz\right\|_1$$

for all $x \in I^d$ and $t > 0$. Using the fact that $f_N(Q_{0,\eta}) \to f_N(Q_0)$ in L^1 as $\eta \to 0$, we have

$$\left|G^{M,N,\eta}(x,t)\right| \leq Ct^{-\frac{d}{2}-\gamma}\left(1 + \|f_N(Q_0)\|_1\right),$$

for sufficiently-small $\eta > 0$. Finally, by property **(M3)** of the regularised potential, namely that f_N is bounded pointwise on $\mathsf{D}(f)$ by f, we can find a constant $C = C(\gamma, Q_0)$ such that

$$\left|G^{M,N,\eta}(x,t)\right| \leq Ct^{-\frac{d}{2}-\gamma} \quad \text{for} \quad t > 0. \tag{2.28}$$

Therefore, in one step, we have found a bound on $G^{M,N,\eta}(\cdot,t)$ in L^∞ which is independent of all approximation parameters, *including* M. Let us now treat the other comparison function H satisfying $(\mathrm{P})^2_{(M,N,\eta)}$, whose analysis is a little more involved.

The Comparison Function $H^{M,N,\eta}$

To treat those comparison maps which satisfy $(\mathrm{P})^2_{(M,N,\eta)}$, we must compare them sequentially with solutions of the following two problems:

$$(\mathrm{P})_{(M,N)}\begin{cases} \dfrac{\partial H^{M,N}}{\partial t} + (u^{M,N}\cdot\nabla)H^{M,N} - \Gamma L\,\Delta H^{M,N} = \dfrac{\Gamma\kappa^2}{2\vartheta}\left|Q^{M,N}\right|^2, \\ H^{M,N}(\cdot,0) = \fint_{I^d} f_N(Q_0)\,dz \end{cases}$$

and also

$$(\mathrm{P})_{(M)}\begin{cases} \dfrac{\partial H^{M}}{\partial t} + (u^{M}\cdot\nabla)H^{M} - \Gamma L\,\Delta H^{M} = \dfrac{\Gamma\kappa^2}{2\vartheta}\left|Q^{M}\right|^2, \\ H^{M}(\cdot,0) = \fint_{I^d} f(Q_0)\,dz. \end{cases}$$

By the regularity results of the previous stage, it follows by a standard construction that $(\mathrm{P})_{(M,N)}$ has a unique strong solution, and $(\mathrm{P})_{(M)}$ possess a unique strong solution $H^{M,N} \in L^2_t H^4_x$ with $\dot{H}^{M,N} \in L^2(0,T;H^2_x)$. We now establish the connection between these three initial-value problems.

Proposition 2.20. *Solutions of* $(\mathrm{P})_{(M,N,\eta)}$ *and* $(\mathrm{P})_{(M,N)}$ *have the following convergence properties:*

$$\lim_{\eta\to 0} \|H^{M,N,\eta}(\cdot,t) - H^{M,N}(\cdot,t)\|_2 = 0 \tag{2.29}$$

and

$$\lim_{N\to\infty} \|H^{M,N}(\cdot,t) - H^{M}(\cdot,t)\|_2 = 0 \tag{2.30}$$

for all $t \in [0,T]$.

Proof. Let us consider the first case (2.29). If we denote the difference $H^{M,N,\eta} - H^{M,N}$ by $\overline{H}^{M,N,\eta}$, one may verify that it satisfies the equality

$$\begin{aligned} &\frac{\partial \overline{H}^{M,N,\eta}}{\partial t} + \left(u^{M,N}\cdot\nabla\right)\overline{H}^{M,N,\eta} - \Gamma L\,\Delta \overline{H}^{M,N,\eta} \\ &= \frac{\Gamma\kappa^2}{2\vartheta}\left(\left|Q^{M,N,\eta}\right|^2 - \left|Q^{M,N}\right|^2\right) - \left(\left(u^{M,N,\eta} - u^{M,N}\right)\cdot\nabla\right) H^{M,N,\eta} \end{aligned}$$

Taking spatial inner products in L^2 with $\overline{H}^{M,N,\eta}$ itself, one may use the fact that $\{H^{M,N,\eta}\}_{\eta>0}$ is a uniformly bounded sequence in $L^\infty_t L^2_x$ for fixed M and N to reveal the estimate

$$\begin{aligned} \frac{d}{dt}\|\overline{H}^{M,N,\eta}(\cdot,t)\|_2^2 &\le C\|\overline{H}^{M,N,\eta}(\cdot,t)\|_2^2 \\ +C\Big(\|Q^{M,N,\eta}(\cdot,t) - Q^{M,N}(\cdot,t)\|_4^2 &+ \|u^{M,N,\eta} - u^{M,N}\|_{\infty,\infty}\|\nabla H^{M,N}(\cdot,t)\|_2\Big), \end{aligned}$$

for a constant $C > 0$ independent of $\eta > 0$, where $\|\cdot\|_{\infty,\infty}$ denotes a supremum taken both in space and time. An application of Gronwall's inequality yields

$$\begin{aligned} \|\overline{H}^{M,N,\eta}(\cdot,t)\|_2^2 &\le e^{CT}\left|\fint_{I^d} f_N(Q_{0,\eta}(z))\,dz - \fint_{I^d} f_N(Q_0(z))\,dz\right| \\ +Ce^{CT}\Big(\int_0^T \|Q^{M,N,\eta} - Q^{M,N}\|_4^2\,ds &+ \|u^{M,N,\eta} - u^{M,N}\|_{\infty,\infty}\int_0^T \|\nabla H^{M,N}\|_2\,ds\Big) \end{aligned}$$

from which we deduce by (2.23) and lemma 2.17 that $H^{M,N,\eta}(\cdot,t)$ tends to $H^{M,N}(\cdot,t)$ in L^2 for $t \in [0,T]$. In particular, this provides pointwise convergence almost everywhere up to a subsequence.

The case of (2.30) follows in a similar manner, and so we omit the proof. □

At this point, we can say the following. Since $f_N(Q^{M,N,\eta}) \le G^{M,N,\eta} + H^{M,N,\eta}$, using property **(M4)** of the regularised potential and the fact that $Q^{M,N,\eta} \overset{\eta\to\infty}{\longrightarrow} Q^{M,N} \overset{N\to\infty}{\longrightarrow} Q^{M}$

pointwise almost everywhere by the respective strong convergence results in $L^2_t H^1_x$, we may deduce from the previous estimate (2.28) that

$$f_N(Q^{M,N,\eta}(x,t)) \leq Ct^{-\frac{d}{2}-\gamma} + H^{M,N,\eta}(x,t),$$

whence

$$f(Q^M(x,t)) = \lim_{N\to\infty}\lim_{\eta\to 0} f_N(Q^{M,N,\eta}(x,t)) \leq Ct^{-\frac{d}{2}-\gamma} + H^M(x,t)$$

almost everywhere. Therefore, if we can find a bound on $H^M(\cdot,t)$ in L^∞ which is independent of M, we will have demonstrated our earlier claim that $f(Q^M(\cdot,t))$ may be controlled in L^∞ uniformly in M for $t>0$.

Uniform Bounds in L^∞ on H^M

Let us recall that H^M is defined to be the solution of the problem

$$(\mathrm{P})_{(M)} \begin{cases} \dfrac{\partial H^M}{\partial t} + (u^M\cdot\nabla)H^M - \Gamma L\,\Delta H^M = \dfrac{\Gamma\kappa^2}{2\vartheta}\left|Q^M\right|^2, \\ H^M(\cdot,0) = \fint_{I^d} f(Q_0)\,dz. \end{cases}$$

Let us firstly consider the case where $d=2$. Since we know that $Q^M \in L^2_t H^2_x \cap L^\infty_t L^\infty_x$, it follows that the forcing term $|Q^M|^2$ also belongs to $L^2_t H^2_x$. Also, since $\dot{Q}^M \in L^2_t L^2_x$, it follows that the distributional time derivative of $|Q^M|^2$ lies in $L^2_t L^2_x$. Thus, since $u^M \in C([0,T];\mathbb{P}_M L^2_{\mathrm{div}})$ with $\dot{u}^M \in L^2(0,T;\mathbb{P}_M L^2_{\mathrm{div}})$, it follows that one may construct a strong solution $H^M \in C^1((0,T);H^1)$ of $(\mathrm{P})_{(M)}$ that is unique for the given initial datum.

We remark that since $\ddot{H}^M \in L^2_t L^2_x$, it follows that $H^M \in C^1((0,T);H^1)$, and so by standard embedding results in dimension two that $H^M \in C^1((0,T);L^p)$ for all $1\leq p<\infty$. This level of regularity on H^M allows us to make the following argument. For any $p>2$, taking inner products with $|H^M|^{p-2}H_M$ we find

$$\frac{1}{p}\frac{d}{dt}\|H^M(\cdot,t)\|_p^p \leq \frac{1}{p}\left(\frac{\Gamma\kappa^2}{2\vartheta}\right)^p \|Q^M(\cdot,t)\|_{2p}^{2p} + \left(1-\frac{1}{p}\right)\|H^M(\cdot,t)\|_p^p,$$

and so using the fact that $Q^M(x,t)\in\mathsf{D}(f)$ almost everywhere (and so $|Q^M(x,t)|\leq\sqrt{1-1/d}$ by lemma 2.3), we deduce by passing to the limit $p\to\infty$ that

$$\|H^M(\cdot,t)\|_\infty \leq \left|\int_{I^d} f(Q_0)\,dz\right| e^T + \frac{\Gamma\kappa^2}{2\vartheta}e^T, \tag{2.31}$$

and so the sequence $\{H^M\}_{M=1}^\infty$ is uniformly bounded in $L^\infty_t L^\infty_x$ as claimed, when the dimension $d=2$.

In the case where $d=3$, we need to be a little more careful. Although we know Q^M to lie in $L^2_t H^2_x$, we only know the forcing term $|Q^M|^2$ to lie in $L^2_t H^1_x$ (actually, it lies in $L^{\frac{4}{3}}_t H^2_x$

by Ladyzhenskaya's inequality). As a result, the unique strong solution H^M of $(\mathrm{P})_{(\mathrm{M})}$ lies in $L^2_t H^3_x$, while $\dot{H}^M \in L^2_t H^2_x$ and $\ddot{H}^M \in L^2_t L^2_x$. We establish the following lemma, whose proof is skipped.

Lemma 2.21. *For almost every $t \in [0,T]$, we have*

$$\|H^M(\cdot,t)\|_p^p = \|H^M(\cdot,0)\|_p^p + p\int_0^t \int_{I^d} \dot{H}^M(y,s)\left|H^M(y,s)\right|^{p-1}\,dyds$$

for all $2 \le p < \infty$. Thus, the map $t \mapsto \|H^M(\cdot,t)\|_p$ is differentiable almost everywhere, and

$$\frac{1}{p}\frac{d}{dt}\|H^M(\cdot,t)\|_p^p = \int_{I^d} \dot{H}^M(y,s)\left|H^M(y,s)\right|^{p-1}\,dy.$$

Thus, using the result of this lemma we find that the estimate (2.31) holds in the case $d = 3$ also.

Piecing together the remarks of this stage, we conclude that

$$f(Q^M(x,t)) \le Ct^{-\frac{d}{2}-\gamma} + \left|\int_{I^d} f(Q_0)\,dz\right| e^T + \frac{\Gamma\kappa^2}{2\vartheta}e^T, \tag{2.32}$$

almost everywhere, whence $Q^M(\cdot,t)$ is strictly physical for $t > 0$. This property will automatically be inherited by weak solutions Q if we can show $Q^M \to Q$ almost everywhere in space and time, as then

$$f(Q(x,t)) = \lim_{M\to\infty} f(Q^M(x,t)) \le Ct^{-\frac{d}{2}-\gamma} + \left|\int_{I^d} f(Q_0)\,dz\right| e^T + \frac{\Gamma\kappa^2}{2\vartheta}e^T$$

almost everywhere, whence Q is indeed strictly physical.

Remark 2.6. *In the case $\xi \neq 0$, the parabolic inequality for $f_N(Q^{M,N,\eta})$ becomes*

$$\left(\frac{\partial}{\partial t} + u^{M,N,\eta}\cdot\nabla - \Gamma L\,\Delta\right) f_N(Q^{M,N,\eta}) \le C\left(|\xi||\nabla u^{M,N,\eta}|^2 + |Q^{M,N,\eta}|^2\right).$$

In order to carry out the program described above for the co-rotational case, we would require bounds on $\nabla u^{M,N,\eta}$ in L^∞ in both space and time which are independent of all approximation parameters. This cannot be achieved in our framework since we do not know if weak solutions u have the property that $\nabla u \in L^\infty_t L^\infty_{\mathrm{div}}$.

Stage IV: Passing to Weak Solutions as $M \to \infty$

Let us now resume the construction of weak solutions as we left it at the end of stage II. In order to pass to the limit as $N \to \infty$, we need to concern ourselves with the term

$$\frac{\partial f_N}{\partial Q}(Q^{M,N}).$$

Since we know by estimate (2.32) that for every $\delta > 0$ there exists a compact subset $K_\delta \subset \mathsf{D}(f) \subset \mathrm{Sym}_0(d)$ given by

$$K_\delta := \left\{ X \in \mathrm{Sym}_0(d) \,:\, f(X) \leq C\delta^{-\frac{d}{2}-\gamma} + \left| \int_{I^d} f(Q_0)\, dz \right| e^T + \frac{\Gamma\kappa}{2\vartheta} e^T \right\}$$

such that $Q^M(x,t) \in K_\delta$ for almost every $x \in I^d$ and $t \in [\delta, T]$, we can show by the dominated convergence theorem that

$$\lim_{N\to\infty} \int_0^T \int_{I^d} \frac{\partial f_N}{\partial Q}(Q^{M,N}) : \chi \, dxdt = \int_0^T \int_{I^d} \frac{\partial f}{\partial Q}(Q^M) : \chi \, dxdt$$

for all $\chi \in C_c^1((0,T); C^\infty_{\mathrm{per}})$. Finally, using the convergence results (2.26) and (2.27), we can show that the limit points (Q^M, u^M) satisfy

$$\int_0^T \int_{I^d} \left(-Q^M : \partial_t \chi + \left(u^M \cdot \nabla\right) Q^M : \chi + S(Q^M, \nabla u^M) : \chi + \Gamma \frac{\delta E}{\delta Q}(Q^M) : \chi \right) dxdt = 0$$

and

$$\int_0^T \int_{I^d} \Big(- u^M \cdot \partial_t \omega + \mathbb{P}_M \left[\left(u^M \cdot \nabla\right) u^M \right] \cdot \omega - \nu \Delta u^M \cdot \omega \\ - \mathbb{P}_M \left[\mathrm{Div}\left(\tau(Q^M) + \sigma(Q^M) \right) \right] \cdot \omega \Big) dxdt = 0$$

for all $\chi \in C_c^1(0,T; C^\infty_{\mathrm{per}})$ and $\omega \in C_c^1(0,T; C^\infty_{\mathrm{div}})$.

Once again, by the lower-semicontinuity of L^p-norms with respect to weak convergence, we deduce from (2.24) and (2.25) that Q^M and u^M are uniformly bounded in the usual spaces. In particular, we may deduce the existence of a map $Q \in L^2_t H^2_x$ to which Q_M tends strongly in $L^2_t H^1_x$, whence pointwise almost everywhere, following extraction of a suitable subsequence. This allows us to infer that

$$f(Q(x,t)) \leq Ct^{-\frac{d}{2}-\gamma} + \left| \int_{I^d} f(Q_0)\, dz \right| e^T + \frac{\Gamma\kappa^2}{2\vartheta} e^T,$$

from which we deduce that Q is strictly physical for $t > 0$. Finally, by using the facts that $Q^M \to Q$ in $L^2_t H^1_x$, $u^M \to u$ in $L^2_t L^2_{\mathrm{div}}$ and both Q^M and Q are strictly physical, one may show that

$$\int_0^T \int_{I^d} \left(-Q : \partial_t \chi + (u \cdot \nabla) Q : \chi - S(Q, \nabla u) : \chi + \Gamma \frac{\delta E}{\delta Q}(Q) : \chi \right) dxdt = 0$$

for all $\chi \in C_c^\infty(I^d \times (0,T))$, and also

$$\int_0^T \int_{I^d} \left(- u \cdot \partial_t \omega + (u \cdot \nabla) u \cdot \omega + \nu \nabla u : \nabla \omega + (\tau(Q) + \sigma(Q)) : \nabla \omega \right) dxdt = 0$$

holds for all divergence-free $\omega \in C_c^\infty(I^d \times (0,T))$. Thus, this completes the construction and so theorem 2.12 is proved.

2.8 Existence of Global Strong Solutions in Dimension 2

In this section, we demonstrate that the notion of solution of system (S) can be strengthened when we place higher regularity conditions on the initial data (Q_0, u_0) and stipulate that Q_0 be *strictly* physical, as opposed to merely physical.

Theorem 2.22 (Dimension $d = 2$; Co-rotational regime $\xi = 0$)**.** *For initial data* $(Q_0, u_0) \in H^2 \times H^1_{\mathrm{div}}$ *with the property that*

$$f(Q_0) \in L^\infty \quad \text{(strictly physical initial data)},$$

there exists a corresponding strong solution (Q, u) *of system* (S) *with* $f(Q(\cdot, t)) \in L^\infty$ *for* $t \geq 0$.

We shall not run through the construction in full, but instead highlight the main modifications in the previous construction of global weak solutions. The reason we cannot carry through the analysis of this section to the case of three spatial dimensions is due to the fact Ladyzhenskaya's inequality reads

$$\|Q\|_4 \leq C\|Q\|_2^{\frac{1}{4}}\|\nabla Q\|_2^{\frac{3}{4}}$$

in dimension three, whereas

$$\|Q\|_4 \leq C\|Q\|_2^{\frac{1}{2}}\|\nabla Q\|_2^{\frac{1}{2}}$$

in dimension two: see, for instance, Robinson ([72], Section 9.3).

Let us begin at the (M, N)-level of regularity, namely at the point of having demonstrated the existence of maps $Q^{M,N}$ and $u^{M,N}$ which satisfy

$$\begin{cases} \dot{Q}^{M,N} + (u^M \cdot \nabla)Q^{M,N} - S(Q^{M,N}, \nabla u^{M,N}) = -\Gamma \dfrac{\delta E_N}{\delta Q}(Q^{M,N}), \\ \dot{u}^{M,N} + \mathbb{P}_M\left[(u^M \cdot \nabla)u^M\right] = \nu\Delta u^M + \mathbb{P}_M\left[\mathrm{Div}\left(\tau(Q^{M,N}) + \sigma(Q^{M,N})\right)\right], \end{cases}$$

in the strong sense. We would like to pass to a strong solution of the limiting (Q^M, u^M) system as $N \to \infty$ as opposed to a weak solution. This can be achieved by demonstrating

$$\lim_{N\to\infty} \int_0^T \int_{I^d} \left\langle \frac{\partial f_N}{\partial Q}(Q^{M,N}) \right\rangle : \chi \, dxdt = \int_0^T \int_{I^d} \left\langle \frac{\partial f}{\partial Q}(Q^M) \right\rangle : \chi \, dxdt \tag{2.33}$$

for all $\chi \in L^2_t L^2_x$. In order to establish this result, we modify the maximum principle technique previously demonstrated by constructing different comparison functions, thanks to the improved properties of Q_0, namely that $Q_0 \in H^2$ with $f(Q_0) \in L^\infty$. In particular, we have the following.

Proposition 2.23. *For given initial data* $(Q_0, u_0) \in H^2 \times H^1_{\mathrm{div}}$ *such that*

$$Q_0 \text{ is strictly physical, i.e. } f(Q_0) \in L^\infty,$$

there exists a compact subset $K = K(Q_0) \subset \mathsf{D}(f)$*, depending only on the initial datum* Q_0 *and time of existence* $T > 0$*, such that* $Q^M(x,t) \in K$ *for all* $x \in I^d$ *and* $t \in [0,T]$*.*

Proof. We remark that, up until this point in the construction of strong solutions of (S), we have the same regularity and convergence properties of approximate maps at our disposal as in the proof of the previous theorem. We now consider the following modified comparison functions $G = G^{M,N,\eta}$ and $H = H^{M,N,\eta}$ which are solutions to the problems

$$\begin{cases} \dfrac{\partial G}{\partial t} + (u^{M,N,\eta} \cdot \nabla) G - \Gamma L \, \Delta G = 0, \\ G(\cdot, 0) = f(Q_{0,\eta}), \end{cases}$$

and

$$\begin{cases} \dfrac{\partial H}{\partial t} + (u^{M,N,\eta} \cdot \nabla) H - \Gamma L \, \Delta H = \dfrac{\Gamma \kappa^2}{2\vartheta} \left| Q^{M,N,\eta} \right|^2, \\ H(\cdot, 0) = 0. \end{cases}$$

Firstly, basic energy estimates reveal that the classically-smooth function $G = G^{M,N,\eta}$ satisfies

$$\| G^{M,N,\eta}(\cdot, t) \|_\infty \leq \| f(Q_{0,\eta}) \|_\infty$$

for $t \geq 0$. Now, since we know that $\max_{x \in I^d} |Q_{0,\eta}(x)| \leq \max_{x \in I^d} |Q_0(z)|$ as $Q_0 \in H^2$ and is therefore continuous, it follows that

$$\| G^{M,N,\eta}(\cdot, t) \|_\infty \leq \max_{X \in \mathrm{range}(Q_0)} f(X) \tag{2.34}$$

and so once again that comparison map $G^{M,N,\eta}$ is uniformly bounded in L^∞ in all approximation parameters. Note, however, in contrast with inequality (2.28) derived in the proof of proposition 2.7, the comparison map $G^{M,N,\eta}$ is dominated by a function in L^∞ that does not blow up as the origin is approached.

Similarly, by comparing the map $H^{M,N,\eta}$ with other suitable comparison maps $H^{M,N}$ and H^M (constructed using the pairs $(Q^{M,N}, u^{M,N})$ and (Q^M, u^M), respectively) in the manner of proposition 2.20, one may show that $\lim_{N \to \infty} \lim_{\eta \to 0} H^{M,N,\eta}(x,t) = H^M(x,t)$ everywhere in space and time, where H^M is the unique strong solution of the problem

$$\begin{cases} \dfrac{\partial H^M}{\partial t} + \left(u^M \cdot \nabla \right) H^M - \Gamma L \Delta H^M = \dfrac{\Gamma \kappa^2}{2\vartheta} \left| Q^M \right|^2, \\ H^M(\cdot, 0) = 0, \end{cases}$$

from which we deduce that H^M satisfies

$$\|H^M(\cdot,t)\|_p \leq \frac{\Gamma\kappa^2}{8\vartheta}\frac{(\pi\Lambda)^{\frac{1}{p}}}{(p-1)^{\frac{1}{p}}}e^{\left(1-\frac{1}{p}\right)T} \quad \text{for all} \quad 2\leq p<\infty. \tag{2.35}$$

Thus, letting $p\to\infty$, we deduce that $\{H^M\}_{M=1}^{\infty}$ is uniformly bounded in $L_t^\infty L_x^\infty$ since each $H^M(\cdot,t)$ is a continuous function. Putting the information obtained from (2.34) and (2.35) together, we find that since

$$f(Q^{M,N,\eta}(x,t)) \leq G^{M,N,\eta}(x,t) + H^{M,N,\eta}(x,t),$$

we may pass to the improved M-independent bound

$$f(Q^M(x,t)) \leq \|f(Q_0)\|_\infty + \frac{\Gamma\kappa^2}{8\vartheta}e^T$$

as $\eta\to 0$ and $N\to\infty$, which holds for all $t\in[0,T]$. Thus, since the sublevel sets of the map f are compact subsets of $\mathsf{D}(f)\subset \mathrm{Sym}_0(2)$, it follows that the compact subset of matrices $K=K(Q_0,T)$ given by

$$K := \left\{ X\in \mathrm{Sym}_0(2) \,:\, f(X)\leq \|f(Q_0)\|_\infty + \frac{\Gamma\kappa^2}{8\vartheta}e^T \right\}$$

contains the range of the approximate maps Q^M for every $M\geq 1$. To conclude, we make the obvious remark that if $Q^M\to Q$ strongly in $L_t^2L_x^2$, then the range of weak solutions also belong to K. □

The result of proposition 2.23 allows us to show that (2.33) holds by an application of the dominated convergence theorem. As such, it is straightforward to show that the limiting equations

$$\begin{cases} \dot{Q}^M + (u^M\cdot\nabla)Q^M - S(Q^M,\nabla u^M) = \Gamma\left(L\Delta Q^M - \vartheta\left\langle\frac{\partial f}{\partial Q}(Q^M)\right\rangle + \kappa\, Q^M\right), \\ \dot{u}^M + \mathbb{P}_M\left[\left(u^M\cdot\nabla\right)u^M\right] = \nu\Delta u^M + \mathbb{P}_M\left[\mathrm{Div}\left(\tau(Q^M)+\sigma(Q^M)\right)\right], \end{cases}$$

hold in the strong sense in $L_t^2L_x^2$ and $L_t^2L_{\mathrm{div}}^2$, respectively.

At this point, we only know strong solutions Q^M to be in $L_t^\infty H_x^1\cap L_t^2H_x^2\cap C([0,T];H^1)$, yet the regularity of the initial datum $Q_0\in H^2$ suggests that these strong solutions should be more regular. The improved regularity of Q^M is brought out in the following manner. By considering the auxiliary equation for the map R,

$$\frac{\partial R}{\partial t} + (u^M\cdot\nabla)R - \Gamma L\Delta R = S(Q,\nabla u^M) - \Gamma\left(\vartheta\left\langle\frac{\partial f}{\partial Q}(Q^M)\right\rangle - \kappa\, Q^M\right),$$

which is supplemented with initial datum $R(\cdot,0)=Q_0\in H^2$, one may construct a unique strong solution $R=R^M$ in the class $L_t^\infty H_x^2\cap L_t^2H_x^3\cap C([0,T];H^2)$, since $\langle(\partial f/\partial Q)(Q^M)\rangle$

is now known to lie in $L^2_t H^2_x$ by the strict physicality of Q^M. By considering the equation satisfied by the difference $Q^M - R^M$, one may show that

$$\frac{d}{dt}\|Q^M(\cdot,t) - R^M(\cdot,t)\|_2^2 \leq 0,$$

and so Q^M and R^M are indeed equal as elements of $L^\infty_t L^2_x$, whence Q^M 'inherits' the regularity of R^M. At this point, we need not worry about the spatial regularity of u^M as it lies in the span of $\{\phi_m\}_{m=1}^M$.

We now seek uniform bounds on (Q^M, u^M) in spaces of more regular maps. Let us now consider the higher-order energy functional $\mathcal{F} : H^2 \times H^1_{\mathrm{div}} \to \mathbb{R}_+$ given by

$$\mathcal{F}(Q^M, u^M) := \int_{I^d} \left(\frac{1}{2}|\nabla u^M|^2 + \frac{L}{2}|\Delta Q^M|^2 \right) dx.$$

By using the convenient identity

$$\int_{I^d} S(Q^M, \nabla u^M) : \Delta Q^M \, dx + \int_{I^d} \left(Q^M \Delta Q^M - \Delta Q^M Q^M \right) : \nabla u^M \, dx = 0,$$

one may show, by means of Ladyzhenskaya's inequality that $\mathcal{F}_M(t) := \mathcal{F}(Q^M(\cdot,t), u^M(\cdot,t))$ satisfies the differential inequality

$$\frac{d\mathcal{F}_M}{dt} \leq C\left(\mathcal{F}_M(t)^2 + 1\right),$$

where $C > 0$ is an M-independent constant. Multiplying throughout the above by the integrating factor

$$\exp\left(-C\int_0^t \mathcal{F}_M(s)\, ds\right),$$

one may infer that

$$\frac{d}{dt}\left(\mathcal{F}_M(t)\exp\left(-C\int_0^t \mathcal{F}_M(s)\, ds\right)\right) \leq C.$$

Thus,

$$\|\nabla u^M(\cdot,t)\|_2^2 + \left\|\Delta Q^M(\cdot,t)\right\|_2^2 \leq C(T)$$

for a constant $C(T) > 0$ independent of M and linear in T, since $\mathcal{F}_M$ is uniformly bounded in $L^1(0,T)$, Q^M and u^M being uniformly bounded in $L^2_t H^2_x$ and $L^2_t H^1_{\mathrm{div}}$, respectively. Returning to the equation for Q^M, one may use these improved bounds to infer that

$$\left\{Q^M\right\}_{M=1}^\infty \quad \text{is uniformly bounded in} \quad L^\infty_t H^2_x \cap L^2_t H^3_x \cap L^\infty_t L^\infty_x, \tag{2.36}$$

and

$$\left\{u^M\right\}_{M=1}^\infty \quad \text{is uniformly bounded in} \quad L^\infty_t H^1_{\mathrm{div}} \cap L^2_t H^2_{\mathrm{div}}. \tag{2.37}$$

It is now straightforward to pass to a limiting system. One may easily show that

$$\dot{Q} + (u\cdot\nabla)Q - S(Q,\nabla u) = \Gamma\left(L\Delta Q - \vartheta\left\langle \frac{\partial f}{\partial Q}(Q)\right\rangle + \kappa\, Q\right)$$

holds in $L^2_t L^2_x$. Using those convergence results which are consequences of (2.36) and (2.37), it follows that

$$\lim_{M\to\infty}\int_0^T\int_{I^d}\left(\dot{u}^M+\mathbb{P}_M\left[(u^M\cdot\nabla)u^M\right]-\nu\Delta u^M-\mathbb{P}_M\left[\mathrm{Div}\left(\tau(Q^M)+\sigma(Q^M)\right)\right]\right)\cdot\omega\,dxdt$$
$$=\int_0^T\int_{I^d}\left(\dot{u}+(u\cdot\nabla)u-\nu\Delta u-\mathrm{Div}\left(\tau(Q)+\sigma(Q)\right)\right)\cdot\omega\,dxdt$$

holds for all $\omega\in L^2_t H^1_{\mathrm{div}}$. A simple density argument yields that

$$\dot{u}+(u\cdot\nabla)u=\nu\Delta u+\mathrm{Div}\left(\tau(Q)+\sigma(Q)\right)$$

holds in $L^2_t L^2_{\mathrm{div}}$, and so the construction is complete.

The General Smoothing Effect of (S) in Two-dimensions

We now make use of the previous results to show that the Beris-Edwards system has the parabolic smoothing effect on initial data in two spatial dimensions. Once again, we merely provide a sketch of the proof, highlighting the main points of difference to avoid laborious repetition.

Theorem 2.24. *Suppose $k\geq 1$. For given initial data $(Q_0,u_0)\in H^{k+1}\times H^k_{\mathrm{div}}$ such that*

$$Q_0 \text{ is strictly physical, i.e. } f(Q_0)\in L^\infty,$$

then there exists a strong solution $Q\in L^\infty_t H^{k+1}_x\cap L^2_t H^{k+2}_x$, $u\in L^\infty_t H^k_x\cap L^2_t H^{k+1}_x$.

Proof. Let us start this time at the M-level of regularity. Since the initial datum Q_0 lies in H^{k+1}, we can show by a bootstrap argument that $Q^M\in L^\infty_t H^{k+1}_x\cap L^2_t H^{k+2}_x$. With the higher regularity of approximate maps established, we now construct uniform bounds on Q^M in $L^2_t H^{k+2}_x$ and u^M in $L^2_t H^{k+1}_{\mathrm{div}}$ by the following iterative procedure.

Following the argument of theorem 2.22, one can show that

$$\{Q^M\}_{M=1}^\infty \text{ is uniformly bounded in } L^\infty_t H^2_x\cap L^2_t H^3_x$$

and

$$\{u^M\}_{M=1}^\infty \text{ is uniformly bounded in } L^\infty_t H^1_{\mathrm{div}}\cap L^2_t H^2_{\mathrm{div}}.$$

Moreover, by the fortuitous cancellation of higher derivatives

$$\int_{I^d} S(Q^M,\nabla\Delta^{k-1}u^M):\Delta Q^M\,dx+\int_{I^d}\left(Q^M\Delta Q^M-\Delta Q^M Q^M\right):\nabla\Delta^{k-1}u^M\,dx=0,$$

for $k\geq 1$, we can infer that the energy functional

$$\mathcal{F}^{(2)}_M(t):=\|u^M(\cdot,t)\|^2_{H^2_{\mathrm{div}}}+\|Q^M(\cdot,t)\|^2_{H^3}$$

is uniformly bounded in M in $L^\infty(0,T)$, since

$$\frac{d\mathcal{F}_M^{(2)}}{dt} \leq C\left(\mathcal{F}_M^{(2)}+1\right)^2$$

for $t \in (0,T)$. Returning to the evolution equations for Q^M and u^M (which hold in the strong sense), one may use this information to infer that

$$\left\{Q^M\right\}_{M=1}^{\infty} \text{ is uniformly bounded in } L_t^\infty H_x^3 \cap L_t^2 H_x^4$$

and

$$\left\{u^M\right\}_{M=1}^{\infty} \text{ is uniformly bounded in } L_t^\infty H_{\mathrm{div}}^2 \cap L_t^2 H_{\mathrm{div}}^3.$$

By repeating this procedure for the higher energy functionals

$$\mathcal{F}_M^{(j)}(t) := \|u^M(\cdot,t)\|_{H_{\mathrm{div}}^j}^2 + \|Q^M(\cdot,t)\|_{H^{j+1}}^2,$$

for $j = 3,...,k$, one may construct uniform bounds up to the maximal level of allowed regularity. This, in turn, allows us to demonstrate that global strong solutions (Q,u) lie in the regularity class $L_t^\infty H_x^{k+1} \cap L_t^2 H_x^{k+2} \times L_t^\infty H_{\mathrm{div}}^k \cap L_t^2 H_{\mathrm{div}}^{k+1}$. We make the obvious remark that strong solutions are indeed global, since the integration factors

$$\exp\left(-C\int_0^t \mathcal{F}_M^{(j)}(s)\,ds\right)$$

allow one to construct uniform bounds on $\mathcal{F}_M^{(j)}$ in $L^\infty(0,T)$ which are linear in $T>0$. □

Remark 2.7. *Let us briefly remark that the issue of uniqueness of solutions of (S) in two dimensions is far from straightforward. The customary approach is to consider the behaviour of differences of distinct solutions (Q,u) and (R,v) which share the same initial datum, namely*

$$e(t) := \|Q(\cdot,t)-R(\cdot,t)\|_{H^1}^2 + \|u(\cdot,t)-v(\cdot,t)\|_{L_{\mathrm{div}}^2}^2$$

by appealing to the structure of the system (S)*. Note that one needs to consider H^1-norms for the tensor fields due to the presence of third-order spatial derivatives in the stress tensors appearing in the Navier-Stokes equations.*

At present, we are unable to control contributions from the anti-symmetric part σ of the stress tensor in a manner that would yield the differential inequality

$$e'(t) \leq h(t)e(t),$$

for some L^1 function h, to which we could then apply Gronwall's lemma. We hope to address the issue of uniqueness in future work.

2.9 Comments on the Existence Theory for $\xi \neq 0$

The presence of a non-zero ξ introduces analytical difficulties not only for the maximum principle argument used to obtain strict physicality of weak solutions, but also for the existence theory itself. In particular, the methods we employ appear to be suitable only for establishing the local-in-time existence of weak solutions of (S). Let us now highlight the point in the construction at which the time of existence is impeded.

We begin our discussion at the (M, N, η)-level of regularity, at the point when we wish to establish the uniform bound on $\{Q^{M,N,\eta}\}_{\eta>0}$ in $L^\infty_t L^2_x$ that sets the construction of weak solutions into motion. Multiplying throughout the equation

$$\frac{\partial Q^{M,N,\eta}}{\partial t} + \left(u^{M,N,\eta} \cdot \nabla\right) Q^{M,N,\eta} - S(Q^{M,N,\eta}, \nabla u^{M,N,\eta}) = -\Gamma \frac{\delta E_N}{\delta Q}(Q^{M,N,\eta})$$

by $\kappa\, Q^{M,N,\eta}$ and integrating over space, we find

$$\begin{aligned}\frac{\kappa}{2}\frac{d}{dt}\|Q^{M,N,\eta}(\cdot,t)\|_2^2 + \Gamma L\kappa\|\nabla Q^{M,N,\eta}(\cdot,t)\|_2^2 = \kappa\int_{I^d} S(Q^{M,N,\eta}, \nabla u^{M,N,\eta}) : Q^{M,N,\eta}\, dz \\ -\Gamma\vartheta\kappa\int_{I^d}\frac{\partial f_N}{\partial Q}(Q^{M,N,\eta}) : Q^{M,N,\eta}\, dz + \Gamma\kappa^2\|Q^{M,N,\eta}(\cdot,t)\|_2^2.\end{aligned} \tag{2.38}$$

Firstly, since

$$-\left(\frac{\partial f_N}{\partial Q}(Q^{M,N,\eta}) - \frac{\partial f_N}{\partial Q}(0)\right) : Q \leq 0,$$

by monotonicity of $\partial f_N/\partial Q$ on $\mathbb{R}^{d\times d}$, we find

$$-\Gamma\vartheta\int_{I^d}\frac{\partial f_N}{\partial Q}(Q^{M,N,\eta}) : Q^{M,N,\eta}\, dz \leq \frac{\Gamma\vartheta}{2}\left|\frac{\partial f_N}{\partial Q}(0)\right|^2 + \frac{\Gamma\vartheta}{2}\|Q^{M,N,\eta}(\cdot,t)\|_2^2,$$

which together with property **(M5)** of f_N yields the bound

$$-\Gamma\vartheta\int_{I^d}\frac{\partial f_N}{\partial Q}(Q^{M,N,\eta}) : Q^{M,N,\eta}\, dz \leq \frac{\Gamma\vartheta}{2}\left|\frac{\partial f}{\partial Q}(0)\right|^2 + \frac{\Gamma\vartheta}{2}\|Q^{M,N,\eta}(\cdot,t)\|_2^2 + 1$$

that holds for all $N \geq N_0$ for some appropriately large N_0. It is the presence of those terms in the $S(Q^{M,N,\eta}, \nabla u^{M,N,\eta})$ contribution which are premultiplied by ξ that introduce difficulties in the following manner. Since we have the bound

$$\begin{aligned}&\int_{I^d} S(Q^{M,N,\eta}(x,t), \nabla u^{M,N,\eta}(x,t)) : Q^{M,N,\eta}(x,t)\, dx \\ &\leq \frac{\nu}{2}\|\nabla u^{M,N,\eta}(\cdot,t)\|_2^2 + C(\xi,\nu)\left(\|Q^{M,N,\eta}(\cdot,t)\|_{H^1}^2 + 1\right)^3,\end{aligned}$$

it follows by adding (2.38) above to the energy identity (2.18) that we find the differential inequality

$$\frac{d\mathcal{G}^{M,N,\eta}}{dt} \leq C\left(\mathcal{G}^{M,N,\eta} + 1\right)^3, \tag{2.39}$$

for some constant C independent of M, N and η, where

$$\mathcal{G}^{M,N,\eta}(t) := \frac{1}{2}\|u^{M,N,\eta}\|_2^2 + \frac{L}{2}\|\nabla Q^{M,N,\eta}\|_2^2 + \vartheta \int_{I^d} \left(f_0 + f_N(Q^{M,N,\eta})\right)\, dx + \frac{\kappa}{2}\|Q^{M,N,\eta}\|_2^2.$$

Thus by Gronwall's inequality one may show that

$$\{Q^{M,N,\eta}\}_{\eta>0} \quad \text{is uniformly bounded in} \quad L^\infty(0,T^*;H^1)$$

and

$$\{u^{M,N,\eta}\}_{\eta>0} \quad \text{is uniformly bounded in} \quad L^\infty(0,T^*;L^2_{\text{div}}),$$

where $T^* = T^*(Q_0, u_0)$ is a (possible) blow-up time obtained from solving (2.39) above.

One possible way of lifting this restriction is that *if* we knew the approximate system

$$\begin{cases} \dot{Q}^M + (u^M \cdot \nabla)Q^M - S(Q^M, \nabla u^M) = \Gamma\left(L\Delta Q^M - \vartheta\left\langle \dfrac{\partial f}{\partial Q}(Q^M)\right\rangle - \kappa\, Q^M\right), \\ \dot{u}^M + \mathbb{P}_M\left[(u^M \cdot \nabla)u^M\right] = \nu\Delta u^M + \mathbb{P}_M\left[\text{Div}\left(\tau(Q^M) + \sigma(Q^M)\right)\right], \end{cases}$$

held in the strong sense in $L^2_t L^2_x$ and that $Q^M(x,t) \in \mathsf{D}(f)$ almost everywhere, one could reduce the cubic bound in (2.39) to a linear one, from which we would be able to infer the global-in-time existence of weak solutions when $\xi \neq 0$. This is an issue to which we hope to return in future work.

2.10 Discussion

There are a number of questions that one can ask in the hope of extending some of the results obtained in this chapter. One obvious question relates to understanding how one should modify the maximum principle argument in order to demonstrate that weak solutions are strictly physical in the case when $\xi \neq 0$. Yet another is to understand the possibility of establishing the analogue of theorem 2.12 in the presence of boundaries, i.e. when we work on a domain Ω with suitably-smooth boundary $\partial\Omega$ equipped with, for instance, uniaxial boundary conditions. Finally, there is no result in the literature at the time of writing which incorporates the effects of the elastic terms L_2, L_3 and L_4 in dynamics. As such, it would be of interest to study system (S) when replacing $L\Delta Q$ by the more general differential operator

$$2L_1\Delta Q_{ij} + 2(L_2+L_3)\frac{\partial^2 Q_{ik}}{\partial x_j \partial x_k} + L_4\left[\frac{\partial}{\partial x_\ell}\left(Q_{\ell k}\frac{\partial Q_{ij}}{\partial x_k}\right) + \frac{\partial}{\partial x_k}\left(Q_{\ell k}\frac{\partial Q_{ij}}{\partial x_\ell}\right) + \frac{\partial Q_{\ell k}}{\partial x_i}\frac{\partial Q_{\ell k}}{\partial x_j}\right],$$

for $1 \leq i, j \leq 3$.

There are also a number of interesting questions one can ask in the static theory. Let us once again consider the full four elastic constant theory,

$$E[Q] := \int_{I^d} \left(w(Q, \nabla Q) + \vartheta\, f(Q) - \frac{\kappa}{2}|Q|^2\right) dx, \tag{2.40}$$

where w is

$$w(Q, \nabla Q) = L_1|\nabla Q|^2 + L_2 Q_{ik,j} Q_{ij,k} + L_3 Q_{ij,j} Q_{ik,k} + L_4 Q_{\ell k} Q_{ij,\ell} Q_{ij,k}.$$

It remains an open problem to generalise the result of propositon 2.7 to the case of non-vanishing constants L_2, L_3 and L_4, namely to show that global minimisers are pointwise physical on Ω if the boundary conditions themselves are.

Quite separate from our results of this chapter, but relevant to the discussion in section 2.1 of this chapter, one can enquire about the connection between the static Landau-de Gennes theory and the well-known Oseen-Frank theory. Recall that if one considers the uniaxial ansatz

$$(Q(n))(x) = s\left(n(x) \otimes n(x) - \frac{1}{3}I\right)$$

for a given constant $s \in \mathbb{R}$ and substitutes it into the four elastic constant energy density w, one discovers that

$$w(Q(n), \nabla Q(n)) = K_1 (\nabla \cdot n)^2 + K_2 (n \cdot \nabla \wedge n)^2$$
$$+K_3 |n \wedge \nabla \wedge n|^2 + (K_2 + K_4)\left[\mathrm{tr}\left((\nabla n)^2\right) - (\nabla \cdot n)^2\right],$$

where

$$K_1 = 2L_1 s^2 + L_2 s^2 + L_3 s^2 - \frac{2}{3} L_4 s^3, \quad K_2 = 2L_1 s^2 - \frac{2}{3} L_4 s^3,$$
$$K_3 = 2L_1 s^2 + L_2 s^2 + L_3 s^2 + \frac{4}{3} L_4 s^3, \quad K_4 = L_3 s^2,$$

which is precisely the Oseen-Frank energy density. As we have learned from our earlier discussions, the work of Majumdar and Zarnescu [61] established such a connection in the case of only one elastic constant. In particular, it was established that global minimisers of the cubic Landau-de Gennes theory were well approximated, in various topologies, by global minimisers of the one-constant Oseen-Frank theory, otherwise known as the Dirichlet energy. If one wishes to explore the analogous question in the case of four elastic constants, one must replace the cubic nonlinearity by f_{BM} in order to guarantee well-posedness of the theory: recall propositions 2.4 and 2.8. Thus, it would be interesting to investigate whether or not global minimisers of (2.40) can be well approximated by global minimisers of

$$E_{\mathrm{OF}}[n] := \int_\Omega \Big(K_1 (\nabla \cdot n)^2 + K_2 (n \cdot \nabla \wedge n)^2 + K_3 |n \wedge \nabla \wedge n|^2$$
$$+(K_2 + K_4)\left[\mathrm{tr}\left((\nabla n)^2\right) - (\nabla \cdot n)^2\right]\Big)\, dx$$

as the elastic constants L_i tend to zero in an approriate fashion. This question is interesting as it would help one to understand the 'geometric' properties global minimisers of Landau-de Gennes, thanks to the *bend, splay* and *twist* interpretation of the K_1-, K_2- and K_3-terms present in E_{OF}: for more on this point, we invite the reader to consult Stewart [80]. This constitutes a challenging problem for the future.

2.11 Appendix: Properties of the Ball-Majumdar Potential f

In this section, we consider the proof of proposition 2.6, which catalogues those properties of $f : \mathrm{Sym}_0(d) \to \mathbb{R} \cup \{\infty\}$ that are important to us in establishing the existence of weak solutions of (S). Before we do this, let us consider the following important lemma taken from Ball and Majumdar [7]. From this point onwards, we work in 3 dimensions for simplicity.

Proposition 2.25. *For any given $Q \in \mathrm{Sym}_0(3)$ with the property that its eigenvalues satisfy the constraints*

$$-\frac{1}{3} < \lambda_i(Q) < \frac{2}{3} \quad \textit{for} \quad i = 1, 2, 3,$$

the minimisation problem

$$\inf_{\rho \in \mathcal{A}(Q)} \int_{\mathbb{S}^2} \rho(\omega) \log \rho(\omega)\, d\omega$$

has a unique minimiser ρ_Q^* in the class

$$\mathcal{A}(Q) := \left\{ \rho : \mathbb{S}^2 \to \mathbb{R}_+ \,:\, \int_{\mathbb{S}^2} \rho = 1 \;\; \textit{and} \;\; \int_{\mathbb{S}^2} \left(\omega \otimes \omega - \frac{1}{3} I \right) \rho(\omega)\, d\omega = Q \right\},$$

given explicitly by

$$\rho_Q^*(\omega) := \frac{\exp\left(\sum_{k=1}^3 \mu_k \omega_k^2 \right)}{Z(\mu_1, \mu_2, \mu_3)} \quad \textit{for} \quad \omega = (\omega_1, \omega_2, \omega_3) \in \mathbb{S}^2.$$

The constants μ_1, μ_2, μ_3 are Lagrange multipliers associated with the constraint that Q be the normalised matrix of second-order moments of ρ^*, while $Z = Z(\mu_1, \mu_2, \mu_3)$ is a so-called partition function given by

$$Z(\mu_1, \mu_2, \mu_3) := \int_{\mathbb{S}^2} \exp\left(\sum_{k=1}^3 \mu_k \omega_k^2 \right) d\omega,$$

which satisfies the following system of ODEs:

$$\frac{1}{Z} \frac{\partial Z}{\partial \mu_i} = \lambda_i + \frac{1}{3} \quad \textit{for} \quad i = 1, 2, 3. \tag{2.41}$$

Proof. The proof of this result is somewhat involved, and so we choose to omit it. One could consult ([7], proposition 1) for an outline of the proof. □

Proof of (P0): Isotropy

It can be shown (see [7], proposition 2) that for any $Q \in \mathsf{D}(f)$, $f(Q)$ has the representation

$$f(Q) = \vartheta(\mu_1 - \mu_3) \left(\lambda_1 + \frac{1}{3} \right) + \vartheta(\mu_2 - \mu_3) \left(\lambda_2 + \frac{1}{3} \right)$$

$$-\vartheta \log \left[\int_{\mathbb{S}^2} \exp\left((\mu_1 - \mu_3)\omega_1^2 + (\mu_2 - \mu_3)\omega_2^2 \right) \, d\omega \right],$$

where, importantly, μ_1, μ_2 and μ_3 satisfy the system (2.41) above. Moreover, the set of eigenvalues of $\mathsf{R}Q\mathsf{R}^T$ equals that of Q, since the coefficients of the associated characteristic polynomial

$$\lambda^3 - \frac{1}{2}\mathrm{tr}\left(Q^2\right)\lambda - \det\left(Q\right) = 0$$

are isotropic functions of the Q-tensor. It therefore follows that $f(\mathsf{R}Q\mathsf{R}^T) = f(Q)$ for all $\mathsf{R} \in \mathrm{O}(3)$.

Proof of (P1): Smoothness

The following argument is due to Zarnescu [87]. We once again recall that $f(Q)$ has the form

$$f(Q) = \vartheta(\mu_1 - \mu_3)\left(\lambda_1 + \frac{1}{3}\right) + \vartheta(\mu_2 - \mu_3)\left(\lambda_2 + \frac{1}{3}\right)$$
$$-\vartheta \log \left[\int_{\mathbb{S}^2} \exp\left((\mu_1 - \mu_3)\omega_1^2 + (\mu_2 - \mu_3)\omega_2^2 \right) \, d\omega \right],$$

whenever $Q \in \mathsf{D}(f)$. As a result, if we can show that the RHS of the above is a smooth function of the eigenvalue arguments (on a suitable linear subspace of $\mathbb{R}^3$, to avoid certain degeneracies), it will follow that f is indeed a smooth function of Q: see, for instance, Ball [6].

We noted above that the Lagrange multipliers μ_1, μ_2, μ_3 are unique up to a constant. For the purposes of establishing smoothness of the map

$$f : Q \mapsto \min_{\rho \in \mathcal{A}(Q)} \int_{\mathbb{S}^2} \rho(\omega) \log \rho(\omega) \, d\omega$$

on the open set

$$\mathsf{D}(f) = \left\{ Q \in \mathrm{Sym}_0(3) \, : \, -\frac{1}{3} < \lambda_i(Q) < \frac{2}{3} \ \text{ for } \ i = 1, 2, 3. \right\}, \tag{2.42}$$

it will prove useful to remove this degeneracy. Thus, let us consider the set

$$X := \left\{ x \in \mathbb{R}^3 \, : \, x \cdot (1,1,1) = 0 \right\},$$

and let us further define the map $F(\lambda, \mu) : X \times X \to X$ by

$$F(\lambda, \mu) := \left(\frac{\partial \log Z}{\partial \mu_1} - \lambda_1 - \frac{1}{3}, \frac{\partial \log Z}{\partial \mu_2} - \lambda_2 - \frac{1}{3}, \frac{\partial \log Z}{\partial \mu_3} - \lambda_3 - \frac{1}{3} \right).$$

One may quickly check that $\mu \mapsto Z(\mu)$ is a C^∞ function, and that $F(\lambda, \mu)$ indeed belongs to X for all $\lambda = (\lambda_1, \lambda_2, \lambda_3) \in X$ and $\mu = (\mu_1, \mu_2, \mu_3) \in X$. Therefore, supposing that $\overline{\lambda} \in X$ and $\overline{\mu} \in X$ satisfy

$$F(\overline{\lambda}, \overline{\mu}) = 0,$$

it is our aim to apply the analytic implicit function theorem to show that μ is a smooth vector function of λ in a suitably-small neighbourhood of $\overline{\lambda}$ in X.

Following a change of variables, one can show that $\mu = \mu(\lambda)$ is a C^∞ function of λ in a neighbourhood of $\overline{\lambda}$ in X if

$$\det(N) \neq 0, \qquad \text{where} \qquad N := \begin{pmatrix} \dfrac{\partial^2 \log Z}{\partial \mu_1^2} & \dfrac{\partial^2 \log Z}{\partial \mu_1 \partial \mu_2} \\ \dfrac{\partial^2 \log Z}{\partial \mu_1 \partial \mu_2} & \dfrac{\partial^2 \log Z}{\partial \mu_2^2} \end{pmatrix}.$$

In particular, this condition will hold if we can demonstrate that N is a positive definite matrix at $\overline{\mu}$, i.e. $(Ny) \cdot y \geq 0$ for all $y \in \mathbb{R}^2$, with equality if and only if $y = 0$. Using the definition of Z, one may show that

$$(Ny) \cdot y = \frac{1}{Z^2} \left[\left(\int_{\mathbb{S}^2} (\omega_1 y_1 + \omega_2 y_2)^2 e^{\overline{\mu}_k \omega_k^2} \, d\omega \right) \left(\int_{\mathbb{S}^2} e^{\overline{\mu}_k \omega_k^2} \, d\omega \right) - \left(\int_{\mathbb{S}^2} (\omega_1 y_1 + \omega_2 y_2) e^{\overline{\mu}_k \omega_k^2} \, d\omega \right)^2 \right] \geq 0$$

by an application of the Cauchy-Schwarz inequality. In particular, equality holds if and only if $y = 0$, whence $\mu(\lambda)$ is C^∞ in a neighbourhood of $\overline{\lambda}$. Finally, using the fact that

$$f(Q) = (\mu_1 - \mu_3) \left(\lambda_1 + \frac{1}{3} \right) + (\mu_2 - \mu_3) \left(\lambda_2 + \frac{1}{3} \right) - \log \left[\int_{\mathbb{S}^2} \exp \left((\mu_1 - \mu_3) \omega_1^2 + (\mu_2 - \mu_3) \omega_2^2 \right) \, d\omega \right],$$

it follows by arbitrariness of $\overline{\lambda}$ that f is a smooth function of Q on $\mathsf{D}(f)$.

Proof of (P2): Boundedness

As the minimising density $\rho_Q^*(\omega) \neq 0$ for all $\omega \in \mathbb{S}^2$, and also

$$-\frac{1}{e} \leq t \log t \quad \text{for all} \quad t > 0,$$

it follows that

$$-\frac{1}{e} \left| \mathbb{S}^2 \right| \leq f(Q) \quad \text{for all} \quad Q \text{ satisfying } (2.42),$$

and so the lower bound is independent of Q.

Proof of (P3): Logarithmic Blow-up

The proof of this property of f is again somewhat involved. We refer the reader to ([7] proposition 2, corollaries 3 and 4) for details.

Proof of (P4): Convexity

We use the fact that $t \mapsto t \log t$ is a strictly convex function on $(0, \infty)$. Also, we make use of the fact that

$$\mathsf{D}(f) := \left\{ Q \in \mathrm{Sym}_0(3) \,:\, -\frac{1}{3} < \lambda_i(Q) < \frac{2}{3} \;\text{ for }\; i = 1, 2, 3. \right\}$$

is a convex subset of $\mathbb{R}^{3\times 3}$. This is due to the fact that the map $Q \mapsto \lambda_{\min}(Q)$ which takes Q to its minimum eigenvalue is a concave function of Q, and similarly that $Q \mapsto \lambda_{\max}(Q)$ is a convex function of Q.

Suppose $Q_0, Q_1 \in \mathsf{D}(f)$. By the above observations, $Q_s := sQ_1 + (1-s)Q_0 \in \mathsf{D}(f)$ for all $0 \leq s \leq 1$. Now consider

$$\rho_0^* := \arg \min_{\rho \in \mathcal{A}(Q_0)} \int_{\mathbb{S}^2} \rho(\omega) \log \rho(\omega)\, d\omega \quad \text{and} \quad \rho_1^* := \arg \min_{\rho \in \mathcal{A}(Q_1)} \int_{\mathbb{S}^2} \rho(\omega) \log \rho(\omega)\, d\omega.$$

One may verify that $s\rho_1^* + (1-s)\rho_0^* \in \mathcal{A}(Q_s)$ for $0 \leq s \leq 1$. Thus,

$$f(Q_s) < s \int_{\mathbb{S}^2} \rho_1^*(\omega) \log \rho_1^*(\omega)\, d\omega + (1-s) \int_{\mathbb{S}^2} \rho_0^*(\omega) \log \rho_0^*(\omega)\, d\omega,$$

for $0 \leq s \leq 1$, whence

$$f(sQ_1 + (1-s)Q_0) < sf(Q_1) + (1-s)f(Q_0),$$

and so f is indeed a strictly convex function on $\mathsf{D}(f)$.

Chapter 3

Dynamic Statistical Scaling

Outline. In this chapter, we study a problem in phase transition theory related to the long time behaviour of nematic systems following the onset of the isotropic-nematic phase transition. In particular, we show that the two-point spatial correlation function

$$c_{\mu_0}(r,t) := \frac{\displaystyle\int_H \int_{\mathbb{R}^3} \operatorname{tr}\left(Q(x+r)Q(x)\right)\, dx d\mu_t(Q)}{\displaystyle\int_H \int_{\mathbb{R}^3} \operatorname{tr}\left(Q(x)^2\right)\, dx d\mu_t(Q)}$$

evolving (in an appropriate sense) under the $L^2(\mathbb{R}^3)$-gradient flow of $E^{(L)}_{\mathrm{LdG}}$ given by

$$\frac{\partial Q}{\partial t} = L\Delta Q - a(\vartheta)Q + b\left(Q^2 - \frac{1}{3}\operatorname{tr}\left(Q^2\right) I\right) - c\operatorname{tr}\left(Q^2\right) Q,$$

exhibits asymptotic self-similar behaviour, namely

$$\left\| c_{\mu_0}(r,t) - e^{-\frac{|r|^2}{8t}} \right\|_{L^\infty(\mathbb{R}^3, dr)} = \mathcal{O}\left(t^{-\frac{1}{2}}\right) \quad \text{as } t \to \infty,$$

whenever μ_0 is supported on a certain class of 'small' initial data. We also pass comment on different scaling behaviour for $c_{\mu_0}(r,t)$ corresponding to certain classes of 'large' initial data. The reader should note that we no longer enforce eigenvalue restrictions on Q in this chapter.

The results in this chapter have been written up as an article in Kirr, Wilkinson and Zarnescu [50], entitled "*Dynamic Statistical Scaling in the Landau-de Gennes Theory of Nematic Liquid Crystals*," which has been submitted for publication.

3.1 Introduction

Thermotropic nematic liquid crystals are a well-studied subclass of nematics whose optical properties change dramatically with variation of system temperature. We recall from our discussion in chapter 1 that it is observed in the laboratory that above a certain temperature threshold depending on the particular material under study, the rod-like molecules exhibit no local orientation preference; as discussed in the introductory chapter, this is commonly known as the *isotropic* phase of the material. However, reducing the temperature of the material below this threshold results in the molecules arranging themselves along locally preferred directions, yielding the *nematic* phase.

Models for the dynamics of this transition from isotropy to a nematic phase in liquid crystals present many challenging mathematical questions, both in continuum theories and also in statistical mechanics. In the laboratory, the transition between the isotropic and nematic phases is observed to be effected by the seeding and subsequent growth of nematic 'islands' in the ambient isotropic phase. Figure 3.1 below presents a sequence of snapshots taken from a video of an isotropic-nematic phase transition captured by the Cambridge group, which can be found at *http://www.doitpoms.ac.uk/tlplib/liquid_crystals/phase_transitions.php*. It is unknown whether or not the video elapses in real time, so we simply work with the time units of the video.

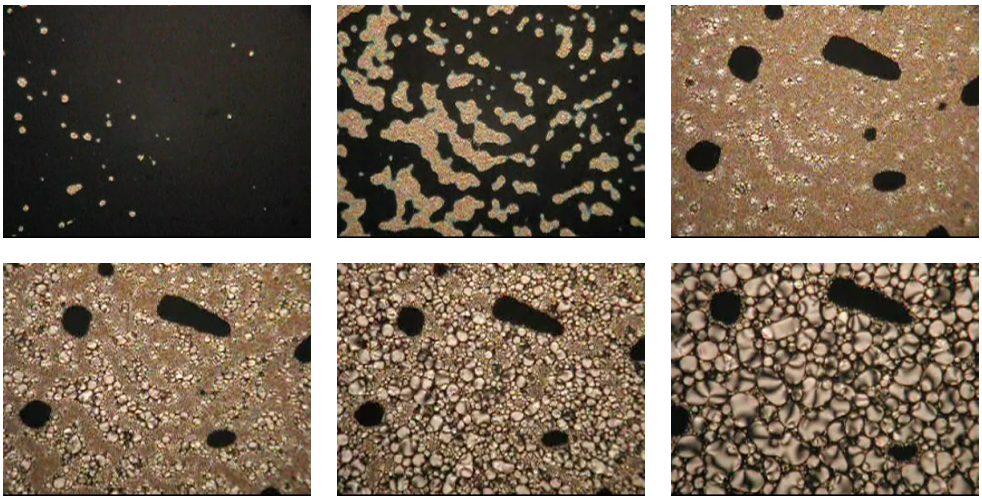


Figure 3.1: Snapshots of the phase transition running from 0, 4, 12, 18, 24 to 34 seconds.

The characteristic length scale $L \equiv L(t)$ of these island-like structures increases with time once the system is coerced into a transition of phase. It is argued in the physics literature (see Bray [16]) that the domain coarsening of the nematic phase is a scaling phenomenon, namely the *structure* of the nematic profile at late times looks *statistically self-similar* to those profiles at an earlier time, up to a simple rescaling in space. Indeed,

we invite the reader to consult the extensive review article of Bray [16] for a helpful introduction to this area of condensed matter physics. With regards to liquid crystal phase transitions, laboratory experiments performed by Pargellis et al. [67], in which a nematic system was contrived to resemble a dynamic XY-model, support this argument.

It is the aim of this chapter to study a model which captures such behaviour of thermotropic nematic systems in a mathematically rigorous manner. In particular, we wish to show that the average large-time behaviour of solutions of a suitable model equation is self similar, in an average sense. We work within the framework of continuum PDE theory, as opposed to the forbidding setting of statistical mechanics.

As the isotropic-nematic phase transition is inherently dynamic, we require an appropriate evolution equation to model this phenomenon. The model we employ in this chapter is the L^2-gradient flow of the well-studied Landau-de Gennes energy introduced in chapter 1. We recall that, in the case when the underlying spatial domain is the whole space $\mathbb{R}^3$, this energy is given by

$$E_{\mathrm{LdG}}[Q] := \int_{\mathbb{R}^3} \left(\frac{1}{2}|\nabla Q|^2 + \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\mathrm{tr}\left(Q^2\right)Q \right) dx \tag{3.1}$$

for appropriately regular maps Q, the gradient flow of which is

$$\frac{\partial Q}{\partial t} = \Delta Q - a(\vartheta)\,Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}\left(Q^2\right)I\right) - c\,\mathrm{tr}\left(Q^2\right)Q. \tag{3.2}$$

This evolution equation evidently has the form of a nonlinear reaction-diffusion system.

In order to achieve our goal, we must first state in precise quantitative terms what we mean by *structure* of nematic profiles and also by *statistical self-similarity*. Indeed, both of these concepts lead us naturally to the mathematical problem of obtaining a phase portrait for a quantity (a correlation function) describing the average behaviour of solutions of the gradient flow of (3.1) above. We argue that one might view this as a convenient simplification of the infinite-dimensional dynamics generated by this PDE on its natural phase space, which captures one essential qualitative property of solutions.

Before we formulate a precise mathematical statement of the problem in question, we should first discuss the notion of correlation function (related to structure), and also statistical solutions of PDEs (related to statistical self-similarity).

'Structure' of Nematic Profiles: Correlation Functions

The measure of structure of nematic profiles $Q : \mathbb{R}^3 \times (0,\infty) \to \mathrm{Sym}_0(3)$ we employ in this chapter is the normalised two-point spatial correlation function $c : \mathbb{R}^3 \times (0,\infty) \to \mathbb{R}$ defined

by

$$c(r,t) := \frac{\displaystyle\int_{\mathbb{R}^3} \operatorname{tr}\left(Q(x+r,t)Q(x,t)\right)\,dx}{\displaystyle\int_{\mathbb{R}^3} \operatorname{tr}\left(Q(x,t)^2\right)\,dx}. \tag{3.3}$$

One may think of c as quantifying how correlated different regions of a nematic profile are with one another and thus as some measure of the spatial structure of the system as it evolves over time. For further information on the use of correlation functions in condensed matter physics, we recommend that the reader consult Sethna ([77], chapter 10).

As mentioned above, it is argued in the physics literature (see for instance Denniston et al. [27] or Zapotocky et al. [86]) that once a system is coerced into an isotropic-nematic phase transition the correlation function assumes a self-similar form asymptotically in time. In summary,

$$\langle c(r,t)\rangle \sim \Gamma\left(\frac{r}{L(t)}\right) \quad \text{in an appropriate topology as} \quad t \longrightarrow \infty,$$

where Γ is some 'universal' scaling function and $L(t)$ is the aforementioned characteristic length scale of nematic domains which invade the isotropic phase. The angular brackets $\langle\cdot\rangle$ signify that one considers a suitable average value of the correlation function computed over many repeated experimental trials, a process which 'smoothes out' anomalous data gathered from experiment. If one then wishes information on the structure of this system for large values of time t, one need only rescale in the spatial variable r to compute the appropriate value of $\langle c(r,t)\rangle$.

In order to model such an averaging procedure in a mathematically rigorous manner, we employ the notion of statistical solution of evolution equations introduced by Foiaş [36] and also by Vishik and Fursikov [39]. This notion of solution to nonlinear PDE, which can simply be seen as a kind of weak notion of solution of a PDE, has been studied many authors in the mathematical theory of the Navier-Stokes equations to explore aspects of turbulence theory. We now outline the significance of statistical solutions in our study of phase transitions.

'Statistical Self-similarity': Statistical Solutions of PDEs

One can show that the semiflow $\{S(t)\}_{t\geq 0}$ of the gradient flow (3.2) of E_{LdG} possesses neither a global attractor nor an inertial manifold in the natural phase space $H := L^2(\mathbb{R}^3)\cap L^6(\mathbb{R}^3)$, which is unfortunate as both objects are well suited to revealing asymptotic structure of dynamics. For more information on such attracting sets in PDE phase space problems, one could consult Constantin, Foiaş, Nicolaenko and Temam [22] or Robinson [72]. This is essentially due to the fact that (3.2) has solutions, starting from initial data in

H, whose $\|\cdot\|_H$-norm increases without bound with time: see Section 3.5 for details on such solutions. Since we are interested in studying the time asymptotics of the correlation function, this presents a significant challenge. Thus, acknowledging the structure of the ensemble of solution trajectories

$$\mathcal{M} := \bigcup_{Q_0 \in H} \Big\{ \{Q(\cdot,t)\}_{t\geq 0} \,:\, Q(\cdot,0) = S(0)Q_0 = Q_0 \Big\},$$

as being rather complicated, we ask what one could say if one turns instead to the ensemble of measure-valued statistical solutions

$$\mathcal{N} := \bigcup_{\mu_0 \in \mathsf{M}_0(H)} \Big\{ \{\mu_t\}_{t\geq 0} \,:\, \mu_t|_{t=0} = \mu_0 \Big\},$$

where $\mathsf{M}_0(H)$ denotes the set of all Borel probability measures on H. The ensemble $\mathcal{N}$ is 'coarser' than $\mathcal{M}$ in terms of information, in the sense that each such statistical solution μ_t of (3.2) at time t is insensitive to changes on sets of μ_t-measure 0. In order to make use of this insensitivity to 'fine structure' of the trajectory ensemble $\mathcal{M}$, and to characterise one qualitative aspect of solutions of (3.2) on H, we redefine the correlation function c previously introduced in (3.3) as

$$c_{\mu_0}(r,t) := \frac{\displaystyle\int_H \int_{\mathbb{R}^3} \mathrm{tr}\left(Q(x+r)Q(x)\right)\, dx d\mu_t(Q)}{\displaystyle\int_H \int_{\mathbb{R}^3} \mathrm{tr}\left(Q(x)^2\right)\, dx d\mu_t(Q)}, \tag{3.4}$$

where μ_0 is a Borel probability measure on H. It is with this definition of the correlation function we work throughout this paper, as opposed to the earlier-given definition which is supported only on single trajectories in $\mathcal{M}$. Moreover, it allows us to give good mathematical sense to the average $\langle\cdot\rangle$ discussed above, namely $\langle c(r,t)\rangle := c_{\mu_0}(r,t)$.

As we mentioned before, the gradient flow (3.2) takes the shape of a nonlinear heat system for the evolution of nematic profiles Q. As this equation generates a strongly-continuous semigroup of solution operators $\{S(t)\}_{t\geq 0}$ on phase space H, it is possible to deal more concretely with the evolution of initial measures as opposed to the so-called Liouville equation formalism, which can be adopted when a semigroup of solution operators is not readily available: see Foiaş et al. [37], chapter V for more information on this more general definition of statistical solution. To be precise, for a given suitable initial Borel measure μ_0 supported on H, we construct in Section 3.4 an associated one-parameter family of measures $\{\mu_t\}_{t\geq 0}$ with the property that

$$\mu_t(E) = \lim_{k\to\infty} \sum_{j=1}^{N(k)} \vartheta_j^{(k)} \delta_{S(t)\overline{Q}_j^{(k)}}(E)$$

for measurable subsets $E \subseteq H$, nematic profiles $\overline{Q}_j^{(k)} \in H$ and $t \geq 0$, where for each fixed k, we have $\sum_{j=1}^{N(k)} \vartheta_j^{(k)} = 1$ and $\vartheta_j^{(k)} \in [0,1]$ for $j = 1, ..., N(k)$. One can then view each statistical solution $\{\mu_t\}_{t\geq 0} \in \mathcal{N}$ as a convenient concatenation of individual solutions $\{Q(\cdot,t)\}_{t\geq 0} \in \mathcal{M}$.

In the study of long time behaviour of dynamical systems generated by evolution equations, one is often interested in constructing a *phase portrait* for all solution trajectories, including the location of any attracting sets of the dynamics. We store some remarks on the construction of a phase portrait for the correlation function c_{μ_0} in the closing section of this chapter.

The Mathematical Model

We reiterate that we consistently employ the Einstein summation convention over repeated lower indices in the sequel. Let us now recall the main features of the models (3.1) and (3.2) which make them suitable for the study of phase transitions.

In accordance with the Landau theory of phase transitions, the free energy density f is assumed to be a smooth map which is frame indifferent, in our case invariant under the action of the group O(3):

$$f\left(T_{\mathsf{R}}D, \mathsf{R}Q\mathsf{R}^T\right) = f\left(D, Q\right) \tag{3.5}$$

where $Q \in \mathrm{Sym}_0(3)$ and $(T_{\mathsf{R}}D)_{ijk} := R_{i\ell}R_{jm}R_{kn}D_{\ell mn}$ for all $\mathsf{R} \in \mathrm{O}(3)$ whenever D is a rank 3 tensor. We assume that the corresponding free energy has the form

$$\int_{\mathbb{R}^3} f(\nabla Q(x), Q(x))\, dx = \int_{\mathbb{R}^3} \left(w(\nabla Q(x), Q(x)) + f_{\mathrm{B}}(Q(x))\right) dx$$

in which the elastic and bulk terms are decoupled. We recall from chapter 1 that one may show by invariant theory that any such smooth isotropic map f_{B} is a smooth function of the principle invariants of O(3)

$$\mathrm{tr}\left(Q^2\right) \qquad \text{and} \qquad \mathrm{tr}\left(Q^3\right),$$

recalling that $\mathrm{tr}(Q) = 0$. As stated above, we consider the energy functional $E_{\mathrm{LdG}} \equiv E^{(1)}_{\mathrm{LdG}}$, namely

$$E_{\mathrm{LdG}}[Q] := \int_{\mathbb{R}^3} \left(\frac{1}{2}|\nabla Q(x)|^2 + \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\left(\mathrm{tr}\left(Q^2\right)\right)^2\right) dx,$$

to which the elastic energy contribution is simply the Dirichlet energy, although one could work with more a general elastic energy of the form

$$L_1|\nabla Q|^2 + L_2 Q_{ij,j}Q_{ik,k} + L_3 Q_{ik,j}Q_{ij,k} + L_4 Q_{k\ell}Q_{ij,k}Q_{ij,\ell},$$

which is compatible with the hemitropy symmetry (3.5) above. Moreover, we have chosen to employ the simplest bulk energy density f_{B} that is able to predict a first order isotropic-nematic phase transition, namely

$$f_{\mathrm{B}}(Q) := \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\left(\mathrm{tr}\left(Q^2\right)\right)^2, \tag{3.6}$$

where $a = \alpha(\vartheta - \vartheta_*)$, $\vartheta_* > 0$ is the so-called *supercooling* temperature and $\vartheta \in \mathbb{R}$ is a temperature parameter controlling the depths of the nematic energy wells. In the low-temperature regime in which the nematic phase is energetically favourable, the material-dependent constants (a, b, c) belong to the region of *uniaxial bistability*

$$\mathcal{D} := \left\{(a, b, c) \in (0, \infty)^3 \,:\, b^2 > 24ac\right\}$$

of parameter space $(0, \infty)^3$. The model for the dynamics of nematic liquid crystals we study is the L^2-gradient flow of the functional E_{LdG},

$$\frac{\partial Q}{\partial t} = \Delta Q - a(\vartheta)\, Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}\left(Q^2\right) I\right) - c\,\mathrm{tr}\left(Q^2\right) Q. \tag{3.7}$$

Furthermore, we model the temperature quench which renders the isotropic phase less energically-favourable than the nematic as *instantaneous*, i.e. the parameters (a, b, c) are fixed and lie in the region $\mathcal{D}$ and do not depend on an evolving temperature field ϑ. Before the quench is effected at time $t = 0$, one thinks of the parameters (a, b, c) as lying in the complementary region $(0, \infty)^3 \setminus \mathcal{D}$: in this case, the isotropic phase $Q \equiv 0$ is a global minimiser of the bulk energy density (3.6) above. Of course, one could consider the more physically-relevant problem where ϑ evolves under an appropriate evolution equation, however we believe this to be an unnecessary complication for investigating the asymptotic self-similarity of solutions Q.

We work over the whole space $\mathbb{R}^3$ as opposed to a bounded domain $\Omega \subset \mathbb{R}^3$ so we need not worry about restricting the spatial argument r of the correlation function (3.4). One may interpret this in physical terms as modelling behaviour of a liquid crystal in the bulk of the material, far from any boundaries where complicated boundary effects could come into play.

The main result of this chapter is captured by the following statement.

Theorem 3.1. *For any given $\delta > 0$ there exist $\eta > 0$, depending only on δ and the parameters $(a, b, c) \in \mathcal{D}$, and an open dense subset of*

$$\left\{R \in L^\infty(\mathbb{R}^3, \mathrm{Sym}_0(3)) \,:\, \operatorname*{ess\,sup}_{x \in \mathbb{R}^3} (1 + |x|)^{8+\delta}\, |R(x)| < \eta\right\},$$

such that for any Borel probability measure supported in this open dense set, the associated correlation function c_{μ_0} (3.4) exhibits asymptotic self-similar behaviour, viz

$$\left\| c_{\mu_0}(r, t) - e^{-\frac{|r|^2}{8t}} \right\|_{L^\infty(\mathbb{R}^3,\, dr)} = \mathcal{O}\left(t^{-\frac{1}{2}}\right) \quad \text{as} \quad t \to \infty.$$

In the final section of this chapter, we explore an alternative scaling regime for the correlation function $c_{\mu_0}(\cdot, t)$ as $t \to \infty$, when μ_0 is supported on 'large' initial data in H.

Remark 3.1. *The structure of the open dense subset*

$$\left\{ R \in L^\infty(\mathbb{R}^3, \mathrm{Sym}_0(3)) \,:\, \operatorname*{ess\,sup}_{x\in\mathbb{R}^3} (1+|x|)^{8+\delta} \, |R(x)| < \eta \right\},$$

to which we refer in the statement of theorem 3.1 is described in detail in section 3.4.

Structure of the Chapter

In section 3.2, we record some preliminary results which allow us to establish a representation formula for 'small initial data' solutions of the Q-tensor equation in section 3.3. The main result of the chapter lies in section 3.4, in which we establish asymptotic self-similarity of the correlation function c_{μ_0} by means of the previously established representation formula. In the final section of the chapter, we briefly discuss scaling behaviour of the correlation function corresponding to a class of solutions starting from 'large' initial data, which gives rise to a different scaling regime for the correlation function, namely $L(t) = t$.

Notation

For the convenience of the reader, let us lay out the notation adopted throughout this chapter. For any matrix $A \in \mathrm{Sym}_0(3)$ we denote its Frobenius norm by $|A| := \sqrt{A : A}$, where $A : B \equiv A_{ij}B_{ji}$ for $A, B \in \mathrm{Sym}_0(3)$. In what follows, unless otherwise stated, all Lebesgue spaces have range in $\mathrm{Sym}_0(3)$ and we write $L^p(\mathbb{R}^3, \mathrm{Sym}_0(3))$ simply as $L^p(\mathbb{R}^3)$ for $1 \le p \le \infty$. We also work with the phase space $H := L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$ endowed with the norm $\|Q\| := \max\{\|Q\|_2, \|Q\|_6\}$, where the norms $\|\cdot\|_p$ are given by

$$\|Q\|_p := \begin{cases} \left(\displaystyle\int_{\mathbb{R}^3} \left(\mathrm{tr}\left[Q(x)^2\right] \right)^{\frac{p}{2}} \, dx \right)^{\frac{1}{p}} & \text{when} \quad 1 \le p < \infty, \\ \displaystyle\operatorname*{ess\,sup}_{x\in\mathbb{R}^3} |Q(x)| & \text{when} \quad p = \infty. \end{cases}$$

We denote the fundamental solution of the heat equation on $\mathbb{R}^3$ by Φ, namely

$$\Phi(x,t) := \frac{e^{-|x|^2/4t}}{(4\pi t)^{\frac{3}{2}}},$$

and denote the time-shifted profile $\Phi(x, t+1)$ simply by $\Phi_1(x,t)$. Finally, for any given $\delta > 0$ we denote by $\mathcal{A}$ the space of essentially bounded functions given by

$$\mathcal{A} := \left\{ Q \in L^\infty(\mathbb{R}^3) \,:\, \operatorname*{ess\,sup}_{x\in\mathbb{R}^3} (1+|x|)^{8+\delta} \, |Q(x)| < \infty \right\}, \tag{3.8}$$

and equip it with the natural norm $\|Q\|_{\mathcal{A}} := \operatorname{ess\,sup}_{x\in\mathbb{R}^3}(1+|x|)^{8+\delta}|Q(x)|$. The constant $\delta > 0$ is chosen arbitrarily but remains *fixed*, and we subsequently suppress the dependence of the space $\mathcal{A}$ on δ.

3.2 Some Preliminary Results

We now establish some results which enable us to comment on the long-time behaviour of the correlation function concentrated on individual solutions of the Q-tensor equation, namely the asymptotic behaviour as $t \to \infty$ of the quantity

$$c(r,t) = \frac{\displaystyle\int_{\mathbb{R}^3} \operatorname{tr}\left(Q(x,t)Q(x+r,t)\right)\, dx}{\displaystyle\int_{\mathbb{R}^3} \operatorname{tr}\left(Q(x,t)^2\right)\, dx},$$

where the initial datum $Q_0 \in H$ is chosen appropriately. We begin by proving a simple result on the well-posedness of the Q-tensor equation in the phase space H.

Proposition 3.2. *For each $Q_0 \in H$ there exists a unique global classically-smooth solution Q of the Q-tensor equation (3.7) on $\mathbb{R}^3 \times (0,\infty)$ satisfying $\|Q(\cdot,t)\| < \infty$ for all $t > 0$. Furthermore, the nonlinear semigroup of solution operators $S(t) : H \to H$ defined by*

$$S(t)Q_0 := \begin{cases} Q_0, & \text{if} \quad t = 0 \\ \\ Q(\cdot,t;Q_0) & \text{if} \quad t > 0 \end{cases}$$

for any $Q_0 \in H$ is strongly continuous.

Proof. For any given $Q_0 \in H$, choose the constant $T_0 > 0$ so as to enforce the condition

$$3\left(1 + 4\|Q_0\| + 16\|Q_0\|^2\right)\left(T_0^{\frac{1}{4}} + T_0^{\frac{1}{2}} + T_0\right) \leq \frac{1}{2}. \tag{3.9}$$

We denote by Y the Banach space $C([0,T_0];\, H)$ equipped with the supremum norm $\|U\|_Y := \max_{t\in[0,T_0]} \|U(t)\|$. For the same given $Q_0 \in H$, we define an associated nonlinear operator $G : Y \to Y$ by

$$(GU)(t) := e^{t\Delta}Q_0 - \int_0^t e^{(t-s)\Delta} f(U(\cdot,s))\, ds,$$

for $0 \leq t \leq T_0$, where $\{e^{t\Delta}\}_{t\geq 0}$ denotes the well-known heat semigroup on $L^2(\mathbb{R}^3)$ and the nonlinearity $f : \mathrm{Sym}_0(3) \to \mathrm{Sym}_0(3)$ is defined to be

$$f(U) := -a\,U + b\left(U^2 - \frac{1}{3}\operatorname{tr}\left(U^2\right) I\right) - c\operatorname{tr}\left(U^2\right) U.$$

For any U, V in $C([0,T];\, H)$, we have by the inequalities of Young and Hölder

$$\|(GU)(t)-(GV)(t)\|_r \leq \sum_{k=1}^{3} \int_0^t \|\Phi(\cdot, t-s)\|_{p_k} \left(\|U(s)\|_{kq_k} + \|V(s)\|_{kq_k}\right)^{k-1} \|U(s)-V(s)\|_{kq_k}\, ds,$$

where $1/p_i + 1/q_i = 1 + 1/r$ for appropriately-chosen $p_i, q_i, r \geq 1$ and $i = 1, 2, 3$. Since $U, V \in L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$, we may deduce from this observation the following inequality,

$$\|GU - GV\|_Y \leq 3C_0(U,V) \left(T_0^{\frac{1}{4}} + T_0^{\frac{1}{2}} + T_0\right) \|U - V\|_Y,$$

where

$$C_0(U,V) := \sum_{k=0}^{2} \left(\|U\|_Y + \|V\|_Y\right)^k.$$

Noting that

$$\max_{t\in[0,T_0]} \|e^{t\Delta} Q_0\| \leq \|Q_0\|,$$

which implies that

$$\|GU\|_Y \leq \|Q_0\| + 3\left(1 + \|U\|_Y + \|U\|_Y^2\right) \left(T_0^{\frac{1}{4}} + T_0^{\frac{1}{2}} + T_0\right) \|U\|_Y,$$

by restricting the operator G to the closed (and hence complete) subspace $B := B(0, 2\|Q_0\|) \subset Y$, we find by condition (3.9) that G becomes a contractive operator on the closed metric subspace B with range therein. By applying the Banach fixed point theorem, we deduce the existence of a *unique* element $Q \in C([0,T_0];\, H)$ satisfying the integral equation

$$Q(\cdot, t) = e^{t\Delta} Q_0 - \int_0^t e^{(t-s)\Delta} f(Q(\cdot, s), s)\, ds, \tag{3.10}$$

for $0 < t \leq T_0$. We claim that we may extend this *uniquely* to an element of $C([0,\infty);\, H)$. Noting that $Q \in C([0,T_0];\, H)$ satisfying (3.10) is in fact a smooth solution of the Q-tensor equation on $\mathbb{R}^3 \times (0,\infty)$ by the regularising properties of the heat semigroup $\{e^{t\Delta}\}_{t\geq 0}$, we multiply (3.7) throughout by $(\mathrm{tr}[Q^2])^{p/2-1}Q$, take traces and integrate over the whole space $\mathbb{R}^3$ to produce the identity

$$\begin{aligned} &\frac{1}{p}\frac{d}{dt}\int_{\mathbb{R}^3} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}} - \int_{\mathbb{R}^3} \Delta Q_{ij}\, Q_{ij} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}-1} \\ = \quad &-\int_{\mathbb{R}^3} \left(a\,\mathrm{tr}\left(Q^2\right) - b\,\mathrm{tr}\left(Q^3\right) + c\left(\mathrm{tr}\left(Q^2\right)\right)^2\right) \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}-1}, \end{aligned}$$

for $2 \leq p \leq 6$. Since the solution Q evolves in a space of traceless and symmetric matrices and is smooth everywhere on $\mathbb{R}^3 \times (0,\infty)$, one may construct a map $\mathsf{T} : \mathbb{R}^3 \times (0, T_0) \to \mathrm{O}(3)$ via pointwise diagonalisation with the property that

$$\mathrm{tr}\left(Q^2\right) = \mathrm{tr}\left(\mathsf{T}Q\mathsf{T}^{\mathrm{T}}\mathsf{T}Q\mathsf{T}^{\mathrm{T}}\right) = \mathrm{tr}\left(\mathrm{diag}\left(\lambda, \mu, -(\lambda+\mu)\right)^2\right) = 2\left(\lambda^2 + \lambda\mu + \mu^2\right),$$

for the eigenvalue maps $\lambda, \mu : \mathbb{R}^3 \times (0, T_0) \to \mathbb{R}$, as the Frobenius norm of a matrix is invariant under the action of the group O(3). Similarly, for the same map T we have

$$\mathrm{tr}\left(Q^3\right) = \mathrm{tr}\left(\mathsf{T}Q\mathsf{T}^{\mathrm{T}}\mathsf{T}Q\mathsf{T}^{\mathrm{T}}\mathsf{T}Q\mathsf{T}^{\mathrm{T}}\right) = -3\lambda\mu(\lambda+\mu).$$

For any $\epsilon > 0$, by an application of Young's inequality we have the estimate

$$\mathrm{tr}\left(Q^3\right) = -3\lambda\mu(\lambda+\mu) \leq \frac{3}{2\epsilon}\mathrm{tr}\left(Q^2\right) + \frac{3\epsilon}{8}\left(\mathrm{tr}\left(Q^2\right)\right)^2,$$

and we also have the equality

$$\begin{aligned}-\int_{\mathbb{R}^3} \Delta Q_{ij}\, Q_{ji} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}-1} &= \int_{\mathbb{R}^3} (\nabla Q_{ij} \cdot \nabla Q_{ji}) \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}-1} \\ &\quad + (p-2)\int_{\mathbb{R}^3} (\partial_k Q_{ij}) Q_{ji} (\partial_k Q_{mn}) Q_{nm} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}-2},\end{aligned}$$

from which one may easily deduce

$$-\int_{\mathbb{R}^3} \Delta Q_{ij}\, Q_{ji} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}-1} \geq 0.$$

By the above considerations, we deduce that

$$\frac{1}{p}\frac{d}{dt}\int_{\mathbb{R}^3} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}} \leq \left(\frac{3b}{2\epsilon} - a\right)\int_{\mathbb{R}^3} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}} + \left(\frac{\epsilon b}{3} - c\right)\int_{\mathbb{R}^3} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}+1},$$

and so choosing $\epsilon = 3c/b > 0$, we have

$$\frac{1}{p}\frac{d}{dt}\int_{\mathbb{R}^3} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}} \leq \left(\frac{b^2}{2c} - a\right)\int_{\mathbb{R}^3} \left(\mathrm{tr}\left(Q^2\right)\right)^{\frac{p}{2}}, \tag{3.11}$$

whence

$$\|Q(t)\| \leq \|Q_0\| e^{Ct},$$

for all $t \geq 0$. We may therefore extend our classical solution to *at least* one element of $C([0,\infty);\ H)$. To demonstrate uniqueness of extension, suppose that there exist two extensions Q and $\widetilde{Q}$ which are not identically equal in H on the interval $[T_0, T_1]$ for some $T_1 > 0$. As both such extensions are smooth in space and time, there exists a constant $C_1 > 0$ depending on T_1 such that

$$\max_{t\in[T_0,T_1]} \left(\|Q(t)\| + \|\widetilde{Q}(t)\|\right) \leq C_1.$$

Considering the difference of these extensions, one may derive the inequality

$$\frac{1}{p}\frac{d}{dt}\int_{\mathbb{R}^3} \left(\mathrm{tr}\left((Q-\widetilde{Q})^2\right)\right)^{\frac{p}{2}} \leq C_1 \int_{\mathbb{R}^3} \left(\mathrm{tr}\left((Q-\widetilde{Q})^2\right)\right)^{\frac{p}{2}},$$

and an application of Gronwall's inequality yields the equality of Q and $\widetilde{Q}$ in the space $C([T_0, T_1];\ H)$. From this point onwards, it is straightforward to check that the one-parameter family of solution operators $\{S(t)\}_{t\geq 0}$ defined above is indeed strongly continuous. □

It is our aim to investigate finer properties of 'small initial data' solutions of (3.7), namely we wish to demonstrate a decomposition result for solutions starting from initial data which are small in the $\|\cdot\|_{\mathcal{A}}$-norm. In order to achieve this, we first must examine the long-time behaviour of solutions of the heat equation in $L^p(\mathbb{R}^3)$.

A Remark on the Heat Equation in $\mathbb{R}^d$

Consider the heat equation

$$\frac{\partial u}{\partial t}(x,t) = \Delta u(x,t) \qquad (x,t) \in \mathbb{R}^d \times (0,\infty),$$

where $d \geq 1$ is an integer. For given $L^q(\mathbb{R}^d)$ initial data with $1 \leq q \leq \infty$, it possesses a classically smooth solution on $\mathbb{R}^d \times (0,\infty)$ and this solution $u(x,t)$ may be expressed as a convolution involving the d-dimensional heat kernel $\Phi_d(x,t)$,

$$u(x,t) = (\Phi_d(\cdot,t) * u_0)(x) = \int_{\mathbb{R}^d} \frac{e^{-|x-y|^2/4t}}{(4\pi t)^{d/2}} u_0(y)\, dy,$$

for $t > 0$. In order to obtain an estimate on the time decay of solutions in $L^p(\mathbb{R}^d)$, one can employ Young's inequality in the above to produce

$$\|u(\cdot,t)\|_p \leq \frac{C(r)}{t^{\frac{d}{2}(1-\frac{1}{r})}} \|u_0\|_q,$$

for all $t > 0$ and $1 + 1/p = 1/q + 1/r$. Thus, all solutions of the heat equation with $L^q(\mathbb{R}^d)$ initial data decay to zero *at least* with rate $t^{-d/2+d/2r}$ as $t \to \infty$. We show in what is to come that if we insist the initial data of the heat equation are of *zero mean* i.e. $\int_{\mathbb{R}^d} u_0 = 0$ and possess some mild decay condition at infinity, then we may improve our estimate on the rate of decay of the corresponding solution to 0 in $L^p(\mathbb{R}^d)$ as $t \to \infty$.

We begin with an auxiliary pointwise estimate on solutions of the heat equation that will be of help to us in the following section, and may indeed be of independent interest. We consider only the case of the heat equation in $\mathbb{R}^3$ appropriate to our considerations. The methods used here may be extended without great effort to capture a similar result in $\mathbb{R}^d$ for arbitrary dimension $d \geq 1$.

Proposition 3.3. *Suppose $\beta > 0$, and consider an integrable map $u_0 : \mathbb{R}^3 \to \mathbb{R}$ satisfying*

$$\int_{\mathbb{R}^3} (1+|x|)^{\beta+1} |u_0(x)|\, dx < \infty.$$

The difference

$$\overline{m}(x,t) := (e^{t\Delta} u_0)(x) - \Phi(x,t) \int_{\mathbb{R}^3} u_0(y)\, dy$$

satisfies the estimate

$$|\overline{m}(x,t)| \leq C t^{-2} \left(1 + \frac{|x|}{\sqrt{8t}}\right)^{-\beta} \int_{\mathbb{R}^3} |y| \left(1 + \frac{|y|}{\sqrt{8t}}\right)^{\beta} |u_0(y)|\, dy \tag{3.12}$$

for $x \in \mathbb{R}^3$, $t > 0$. The explicitly-computable constant $C > 0$ depends only on β.

Proof. Define the map $\sigma : [0, 2\pi) \times [0, \pi) \to \mathbb{S}^2$, a standard surface patch parameterisation on the unit sphere, to be

$$\sigma(\vartheta, \varphi) := (\cos\vartheta \sin\varphi, \sin\vartheta \sin\varphi, \cos\varphi)\,,$$

and define $U : [0, \infty) \times [0, 2\pi) \times [0, \pi) \to \mathbb{R}$ by

$$U(r, \vartheta, \varphi) := \int_r^\infty u_0(\rho\cos\vartheta\sin\varphi, \rho\sin\vartheta\sin\varphi, \rho\cos\varphi)\rho^2 \sin\varphi\, d\rho.$$

Now, by a change of co-ordinates and an application of integration by parts, we deduce that

$$\begin{aligned}
&(e^{t\Delta}u_0)(x)\\
=\;& \int_0^\pi \int_0^{2\pi} \int_0^\infty \frac{e^{-|x-r\sigma(\vartheta,\varphi)|^2/4t}}{(4\pi t)^{3/2}} u_0(r\sigma(\vartheta,\varphi))r^2 \sin\varphi\, dr d\vartheta d\varphi\\
=\;& \int_{\mathbb{R}^3} \Phi(x - r\sigma, t) \frac{\partial}{\partial r}\left(-U(r,\vartheta,\varphi)\right)\, dr d\vartheta d\varphi\\
=\;& \Phi \int_0^\pi \int_0^{2\pi} U(0,\vartheta,\varphi)\, d\vartheta d\varphi + \int_{\mathbb{R}^3} \frac{\sigma\cdot(x-r\sigma)}{2t} \Phi(x-r\sigma,t)U(r,\vartheta,\varphi)\, dr d\vartheta d\varphi\\
=\;& \Phi \int_{\mathbb{R}^3} u_0(y)\, dy + \int_{\mathbb{R}^3} \frac{\sigma\cdot(x-r\sigma)}{2t} \Phi(x-r\sigma,t)U(r,\vartheta,\varphi)\, dr d\vartheta d\varphi.
\end{aligned}$$

Applying the elementary inequality $\sqrt{z}\exp(-z) \le \exp(-z/2)$ for $z \ge 0$, we deduce from the above

$$\begin{aligned}
&(e^{t\Delta}u_0)(x) - \Phi(x,t)\int_{\mathbb{R}^3} u_0(y)\, dy\\
\le\;& \frac{1}{(4\pi)^{3/2}}\frac{1}{t^2}\int_{\mathbb{R}^3} e^{-|x-r\sigma|^2/8t}\left(\int_r^\infty |u_0(\rho\sigma)|\rho^2 d\rho\right)\sin\varphi\, dr d\vartheta d\varphi\\
\le\;& Ct^{-2}\int_{\mathbb{R}^3} \sup_{(\vartheta,\varphi)}\left(e^{-|x-r\sigma|^2/8t}\right)\left(\int_r^\infty |u_0(\rho\sigma)|\rho^2 d\rho\right)\sin\varphi\, dr d\vartheta d\varphi\\
=\;& Ct^{-2}\int_{\mathbb{R}^3} e^{-(|x|-r)^2/8t}\left(\int_r^\infty |u_0(\rho\sigma)|\rho^2 d\rho\right)\sin\varphi\, dr d\vartheta d\varphi,
\end{aligned}$$

where $C > 0$ is independent of $t > 0$. A couple of applications of Fubini's theorem then yield

$$\begin{aligned}
\overline{m}(x,t) &\le Ct^{-2}\int_0^\infty e^{-(|x|-r)^2/8t}\int_{|y|\ge r}|u_0(y)|\, dy\, dr\\
&= Ct^{-2}\int_{\mathbb{R}^3}\left(\int_0^\infty (1-\chi_{B(0,r)}(y))e^{-(|x|-r)^2/8t}\, dr\right)|u_0(y)|\, dy,
\end{aligned}$$

where $\chi_{B(0,r)}$ denotes the characteristic function of the open ball $B(0,r) \subset \mathbb{R}^3$. From this we find

$$\overline{m}(x,t) \le Ct^{-2}\int_{\mathbb{R}^3}\left(\int_0^{|y|} e^{-(|x|-r)^2/8t}\, dr\right)|u_0(y)|\, dy. \tag{3.13}$$

We pause at this point to obtain a helpful estimate on the y-integrand in the above.

Lemma 3.4. *For any $\beta > 0$, there exists a constant $C = C(\beta) > 0$ such that*

$$\int_{X-Y}^{X} e^{-\xi^2} d\xi \leq CY \left(\frac{1+Y}{1+X}\right)^{\beta} \quad \text{for } X, Y \geq 0. \tag{3.14}$$

Proof of Lemma. In what follows we fix $Y \geq 0$, considering it as a parameter. We separate the demonstration of the inequality into two cases.

(i) The case where $0 \leq X \leq Y$: One may easily deduce from the chain $0 \leq X \leq Y$ the simple inequality

$$Y \leq Y \left(\frac{1+Y}{1+X}\right)^{\beta},$$

for any $\beta > 0$. Using this, we have

$$\int_{X-Y}^{X} e^{-\xi^2}\, d\xi \leq \int_{X-Y}^{X} \max_{\xi_0} \left(e^{-\xi_0^2}\right)\, d\xi = Y \leq Y \left(\frac{1+Y}{1+X}\right)^{\beta}.$$

Thus, the claimed inequality holds for $0 \leq X \leq Y$.

(ii) The case where $Y \leq X$: This time, we have the estimate

$$\int_{X-Y}^{X} e^{-\xi^2}\, d\xi \leq \int_{X-Y}^{X} \sup_{\xi_0} \left(e^{-\xi_0^2}\right)\, d\xi = Y e^{-(X-Y)^2}.$$

Now, since there exists a constant $C > 1$ dependent only on $\beta > 0$ such that

$$e^{-Z^2} \leq C \left(\frac{1}{1+Z}\right)^{\beta},$$

for all $Z \geq 0$, and noting that

$$\left(\frac{1}{1+Z}\right)^{\beta} \leq \left(\frac{1+Y}{1+Y+Z}\right)^{\beta},$$

for all $Y \geq 0$, it follows from the substitution $Z \mapsto X - Y$ that

$$e^{-(X-Y)^2} \leq C \left(\frac{1+Y}{1+X}\right)^{\beta}.$$

for all $X \geq Y$. This estimate together with the first case estimate yields the result (3.14) above. □

We now return to the estimate (3.13) and close the proof of the proposition. Transforming the y-integrand through a simple change of variables provides

$$\begin{aligned} \overline{m}(x,t) &\leq Ct^{-2} \int_{\mathbb{R}^3} \left(\int_0^{|y|} e^{-(|x|-r)^2/8t}\, dr \right) |u_0(y)|\, dy \\ &= Ct^{-2} \int_{\mathbb{R}^3} \left(\sqrt{8t} \int_{\frac{|x|}{\sqrt{8t}} - \frac{|y|}{\sqrt{8t}}}^{\frac{|x|}{\sqrt{8t}}} e^{-\xi^2}\, d\xi \right) |u_0(y)|\, dy. \end{aligned} \tag{3.15}$$

Finally, setting $X := |x|/(8t)^{1/2}$ and $Y := |y|/(8t)^{1/2}$, we apply the above lemma to (3.15), from which estimate (3.12) follows. □

Remark 3.2. *Raising both sides of* (3.12) *to the power* $p > 1$ *and integrating over the domain* $\mathbb{R}^3$*, one has that*

$$\left\| e^{t\Delta}u_0 - \Phi(\cdot,t)\int_{\mathbb{R}^3} u_0(y)\,dy \right\|_p \leq \frac{C(p,\beta)}{t^{2-\frac{3}{2p}}}\int_{\mathbb{R}^3} |u_0(y)|(1+|y|)^{\beta+1}\,dy,$$

for $t > 0$*. Therefore, if the initial data of the heat equation are of mean zero and lie in* $L^1(\mathbb{R}^3; d\omega_\beta)$*, where* $d\omega_\beta := (1+|x|)^{\beta+1}dx$*, we have improved upon the standard estimate obtained by Young's inequality for the time decay of solutions in* $L^p(\mathbb{R}^3)$*. Estimates of type* (3.12) *are key to obtaining a representation formula in the following section for solutions of* (3.7)*. Let us also remark that the above result leads to a generalisation to higher spatial dimension of the work of* Taskinen [81].

3.3 A Representation Formula

We establish here a helpful structural formula for solutions of the gradient flow starting from 'small' initial data. In particular, we show that the leading order asymptotics (up to order $t^{-3/2}$ in time after rescaling) of such solutions in all L^p-norms are governed by a matrix multiple of the heat kernel. It proves important in our subsequent analysis to consider a transformed version of the gradient flow (3.7). If we set $R(x,t) := e^{at}Q(x,t)$ and substitute R into (3.7) in a formal manner, we obtain the equation

$$\partial_t R = \Delta R + b\,e^{-at}\left(R^2 - \frac{1}{3}\mathrm{tr}\left(R^2\right)\right) - c\,e^{-2at}\mathrm{tr}\left(R^2\right)R, \tag{3.16}$$

which is the principle equation of analysis in the section to come.

Let $\delta > 0$ be arbitrarily chosen but *fixed*. We recall from (3.8) that the space $\mathcal{A}$ is defined to be

$$\left\{ Q \in L^\infty(\mathbb{R}^3) \,:\, \operatorname*{ess\,sup}_{x\in\mathbb{R}^3} (1+|x|)^{8+\delta}\,|Q(x)| < \infty \right\}.$$

Let X_0 denote the set of maps

$$X_0 := \left\{ W \in C(\mathbb{R}^3\times[0,\infty);\,\mathrm{Sym}_0(3)) \;\middle|\; \sup_{(x,t)} \omega(x,t)|W(x,t)| < \infty \right\},$$

where the space-time weight ω is defined to be

$$\omega(x,t) := \left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{4+\frac{\delta}{2}}(t+1)^2.$$

When endowed with the natural norm

$$\|W\|_{X_0} := \sup_{(x,t)} \omega(x,t)|W(x,t)|,$$

one may verify that X_0 admits the structure of a Banach space. We also employ the product space $X := \mathrm{Sym}_0(3)\times X_0$ furnished with the norm $\|\cdot\|_X := |\cdot| + \|\cdot\|_{X_0}$.

Remark 3.3. *The space of maps X_0 with which we work from now on might seem at first glance rather ungainly. However, this space is only auxiliary in the sense that it does not feature in the hypotheses of theorem 3.5 below. In our setting, it is essentially the 'right' space in which to capture the first correction to the leading heat kernel asymptotics of small initial datum solutions of the transformed equation (3.16).*

The main result of this section is contained in the following theorem.

Theorem 3.5. *There exists $\eta > 0$ depending only on $(a, b, c) \in \mathcal{D}$ such that for initial data $Q_0 \in \mathcal{A} \subset H$ satisfying the smallness condition*

$$\|Q_0\|_{\mathcal{A}} \leq \eta, \tag{3.17}$$

the Q-tensor equation (3.7) has a unique smooth solution on $\mathbb{R}^3 \times (0, \infty)$ of the form

$$Q(x,t) = Ae^{-at}\Phi_1(x,t) + e^{-at}V(x,t), \tag{3.18}$$

where $A \in \mathrm{Sym}_0(3)$ and $V \in X_0$.

An Auxiliary System of Integral Equations

With the above-defined Banach spaces in mind, for any given initial data $Q_0 \in \mathcal{A}$ consider the following nonlinear operator $F : X \to X$ associated with Q_0 defined componentwise as $F_1 : X \to \mathrm{Sym}_0(3)$, where

$$F_1(A,V) := \int_{\mathbb{R}^3} Q_0(y)\,dy + \int_0^\infty \int_{\mathbb{R}^3} h(A\Phi_1(y,s) + V(y,s), s)\,dyds, \tag{3.19}$$

and $F_2 : X \to X_0$, where

$$\begin{aligned} F_2(A,V;\cdot,t) \quad := \quad & e^{t\Delta}\left(Q_0 - \frac{e^{-|\cdot|^2/4}}{(4\pi)^{3/2}}\int_{\mathbb{R}^3} Q_0(y)\,dy\right) + \int_0^t e^{(t-s)\Delta} h(A\Phi_1(*,s) + V(*,s), s)\,ds \\ & - \Phi_1(\cdot,t)\int_0^\infty \int_{\mathbb{R}^3} h(A\Phi_1(y,s) + V(y,s), s)\,dyds. \end{aligned} \tag{3.20}$$

The function h is the nonlinearity in the transformed Q-tensor equation (3.16), and is given by

$$h(R,t) := b\,e^{-at}\left(R^2 - \frac{1}{3}\mathrm{tr}\left(R^2\right) I\right) - c\,e^{-2at}\mathrm{tr}\left(R^2\right) R,$$

for $R \in \mathrm{Sym}_0(3)$ and $t \geq 0$.

Suppose that there exists a fixed point (A^*, V^*) of the operator F in X, i.e. that the integral equations

$$A^* = F_1(A^*, V^*) \quad \text{and} \quad V^* = F_2(A^*, V^*)$$

hold in $\mathrm{Sym}_0(3)$ and X_0, respectively. Multiplying throughout the first equality above by $\Phi_1(x,t)$ and then adding the contribution of the second equality, one finds that the integral equation

$$A^*\Phi_1(\cdot,t) + V^*(\cdot,t) = e^{t\Delta}Q_0 + \int_0^t e^{(t-s)\Delta}h(A^*\Phi_1 + V^*, s)\,ds$$

holds for the assumed fixed point (A^*, V^*). Writing $R^* := A^*\Phi_1 + V^*$, we note that the above integral equation implies that R^* is classically smooth and satisfies (3.16) on $\mathbb{R}^3 \times (0,\infty)$. Following the time-dependent transformation effected by $Q^*(x,t) = e^{-at}R^*(x,t)$, one immediately finds that Q^* satisfies (3.7) on the same space-time domain. In turn, we may deduce from proposition 3.2 (uniqueness of solutions) that for the chosen initial datum $Q_0 \in \mathcal{A} \subset H$, the corresponding solution Q^* of the Q-tensor equation admits the decomposition

$$Q^*(x,t) = A^*e^{-at}\Phi_1(x,t) + e^{-at}V^*(x,t),$$

for $t > 0$ as claimed. Therefore, in order to achieve this representation formula it suffices to show that the operator $F : X \to X$ possesses a fixed point in X for given $Q_0 \in \mathcal{A}$. We achieve this for a special class of Q_0 (namely those which satisfy $\|Q_0\|_{\mathcal{A}} < \eta$ for $\eta > 0$ sufficiently small) through an application of Banach's fixed point theorem. Establishing the fact that F is locally Lipschitz on X is a little delicate, and we consider details of this calculation below.

The Operator $F : X \to X$ is Locally Lipschitz

In order to make our presentation more concise, we adopt the following notation. For given $A, B \in \mathrm{Sym}_0(3)$ and $V, W \in X_0$, we define the *contraction modulus* $k_0 \equiv k_0(A, B; V, W)$ to be

$$k_0 := (|A| + |B| + \|V\|_{X_0} + \|W\|_{X_0}) + (|A| + |B| + \|V\|_{X_0} + \|W\|_{X_0})^2,$$

and write $\phi \lesssim \psi$ whenever $\phi \leq Ck_0\psi$ and $C > 0$ is some absolute constant. Moreover, to avoid any confusion which may arise from line to line, we interpret the string $\phi \lesssim \psi \lesssim \omega$ as $\phi \leq C_1k_0\psi \leq C_2k_0\omega$ for some absolute constants $C_1, C_2 > 0$. We demonstrate that the operator F satisfies the difference property

$$\|F(A,V) - F(B,W)\|_X \lesssim \|(A,V) - (B,W)\|_X,$$

for any $A, B \in \mathrm{Sym}_0(3)$ and $V, W \in X_0$, following which we deduce that F is indeed well-defined as an operator on and with range in X and thus is locally Lipschitz on X. Indeed, we gather these goals together in the following proposition.

Proposition 3.6. *The operator F associated with $Q_0 \in \mathcal{A}$ defined on X component-wise in (3.19) and (3.20) is well defined, i.e. has range in X, and also satisfies the local Lipschitz*

condition

$$\|F(A,V)-F(B,W)\|_X \lesssim \|(A,V)-(B,W)\|_X, \tag{3.21}$$

whenever (A,V) *and* (B,W) *belong to some bounded subset of* X*.*

Proof. We begin by stating a useful estimate upon which we call frequently during the course of our proof.

Lemma 3.7. *For* $A,B\in \mathrm{Sym}_0(3)$*,* $V,W\in X_0$*,* $x\in\mathbb{R}^3$ *and* $t\geq 0$*, we have*

$$\begin{aligned} &|h(A\Phi_1(x,t)+V(x,t),t)-h(B\Phi_1(x,t)+W(x,t),t)| \\ \lesssim\ & \left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-8-\delta} e^{-at}(t+1)^{-3}\|(A,V)-(B,W)\|_X. \end{aligned} \tag{3.22}$$

Proof. The proof is skipped and is left to the reader. □

We now look to obtain estimates on the components of F and its differences in the appropriate spaces.

The component $F_1 : X \to \mathrm{Sym}_0(3)$

The treatment of F_1 is straightforward: following an application of the estimate (3.22), we deduce that the inequality

$$|F_1(A,V)-F_1(B,W)|\leq C_1 k_0(A,B;V,W)\|(A,V)-(B,W)\|_X \tag{3.23}$$

holds for any $A,B\in\mathrm{Sym}_0(3)$ and $V,W\in X_0$ and constant $C_1>0$. Furthermore, one can quickly verify that $\mathrm{tr}(F_1(A,V))=0$ and indeed $F_1(A,V)<\infty$ for any $(A,V)\in X$.

We now turn our attention to the component F_2, whose analysis requires considerably more care than that of F_1. In order to deal with the singularity of the heat kernel at $t=0$, we cleave our estimates into one part which is in a neighbourhood of the origin in time, and one other part which is bounded away from zero in time. We now consider the more involved case when time t is bounded away from the origin.

The component $F_2 : X \to X_0$ when $t \geq 1$

A judicious splitting of integrals faciliates a swift analysis. For $(A,V),(B,W)\in X$, we begin by writing the difference as

$$F_2(A,V;x,t)-F_2(B,V;x,t)=I(x,t)+J(x,t),$$

where

$$I(\cdot,t):=\int_{t/2}^{t} e^{(t-s)\Delta}\big(h(A\Phi_1+V,s)-h(B\Phi_1+W,s)\big)\,ds,$$

and

$$J(\cdot,t) := \int_0^{t/2} e^{(t-s)\Delta}\big(h(A\Phi_1+V,s)-h(B\Phi_1+W,s)\big)\,ds \\ -\Phi_1(\cdot,t)\int_0^{\infty}\int_{\mathbb{R}^3}\big(h(A\Phi_1(y,\tau)+V(y,\tau),\tau)-h(B\Phi_1(y,\tau)+W(y,\tau),\tau)\big)\,dyd\tau.$$

We deal initially with the estimate on the term I and consider at first its temporal integrand, given by

$$\int_{\mathbb{R}^3}\frac{e^{-|x-y|^2/4(t-s)}}{(4\pi(t-s))^{3/2}}\left(h(A\Phi_1(y,s)+V(y,s),s)-h(B\Phi_1(y,s)+W(y,s),s)\right)\,dy. \tag{3.24}$$

for $x\in\mathbb{R}^3$, $t\geq 1$ and $t/2\leq s\leq t$. For any given fixed $x\in\mathbb{R}^3$ the inequality

$$\left(1+\frac{|y|}{\sqrt{s+1}}\right)^{-8-\delta}\leq C\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-8-\delta} \tag{3.25}$$

holds for all $\delta>0$, $t/2\leq s\leq t$ and y in the region $\mathcal{R}_1(x)$, where

$$\mathcal{R}_1(x):=\left\{y\in\mathbb{R}^3\,:\,|x-y|\leq\frac{|x|}{2}\right\},$$

and the constant $C>0$ depends only on $\delta>0$. For a fixed $x\in\mathbb{R}^3$, we consider the integral (3.24) but over the region $\mathcal{R}_1(x)$ as opposed to the whole space:

$$\begin{aligned}
&\int_{\mathcal{R}_1(x)}\Phi(x-y,t-s)\left(h(A\Phi_1+V,s)-h(B\Phi_1+W,s)\right)\,ds\\
&\overset{(3.22)}{\lesssim}\frac{\|(A,V)-(B,W))\|_X}{e^{as}(s+1)^3}\int_{\mathcal{R}_1(x)}\Phi(x-y,t-s)\left(1+\frac{|y|}{\sqrt{s+1}}\right)^{-8-\delta}dy\\
&\overset{(3.25)}{\lesssim}\frac{\|(A,V)-(B,W))\|_X}{e^{as}(s+1)^3}\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-8-\delta}\int_{\mathcal{R}_1(x)}\Phi(x-y,t-s)\,dy\\
&\lesssim\frac{\|(A,V)-(B,W))\|_X}{e^{as}(s+1)^3}\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-8-\delta},
\end{aligned}\tag{3.26}$$

using the fact that the heat kernel has unit mass over $\mathbb{R}^3$. For the same fixed $x\in\mathbb{R}^3$, the inequality

$$\exp\left(-\frac{1}{8}\frac{|x-y|^2}{(t-s)}\right)\leq C\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} \tag{3.27}$$

holds for y in the region $\mathcal{R}_2(x):=\mathbb{R}^3\setminus\mathcal{R}_1(x)$, whenever $t/2\leq s\leq t$. Now proceeding in a similar manner as for the region $\mathcal{R}_1(x)$, we find that

$$\begin{aligned}
&\int_{\mathcal{R}_2(x)}\Phi(x-y,t-s)\left(h(A\Phi_1(y,s)+V(y,s),s)-h(B\Phi_1(y,s)+W(y,s),s)\right)\,dy\\
&=\int_{\mathcal{R}_2(x)}\frac{e^{-|x-y|^2/8(t-s)}}{(4\pi(t-s))^{3/2}}e^{-|x-y|^2/8(t-s)}\left(h(A\Phi_1+V,s)-h(B\Phi_1+W,s)\right)\,dy
\end{aligned}$$

$$\overset{(3.27)}{\leq} C\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}}\int_{\mathcal{R}_2(x)}\frac{e^{-|x-y|^2/8(t-s)}}{(4\pi(t-s))^{3/2}}\,|h(A\Phi_1+V,s)-h(B\Phi_1+W,s)|\,dy$$

$$\overset{(3.22)}{\lesssim}\frac{\|(A,V)-(B,W))\|_X}{e^{as}(s+1)^3}\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}}\int_{\mathcal{R}_2(x)}\frac{e^{-|x-y|^2/8(t-s)}}{(4\pi(t-s))^{3/2}}\,dy. \tag{3.28}$$

Combining results (3.26) and (3.28) we obtain

$$\int_{\mathbb{R}^3}\Phi(x-y,t-s)\left(h(A\Phi_1(y,s)+V(y,s),s)-h(B\Phi_1(y,s)+W(y,s),s)\right)\,dy$$
$$\lesssim \frac{1}{e^{as}(s+1)^3}\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}}\|(A,V)-(B,W))\|_X. \tag{3.29}$$

Finally, integrating (3.29) with respect to s over the interval $t/2\leq s\leq t$, we find

$$I(x,t)\lesssim\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}}(t+1)^{-2}\|(A,V)-(B,W)\|_X, \tag{3.30}$$

as desired. Let us progress to the required estimate for J.

It is at this point we utilise the heat equation 'decay improvement' proposition 3.3. For convenience, for our chosen $(A,V),(B,W)\in X$ we denote by $h_0:\mathbb{R}^3\times(0,\infty)\to\mathrm{Sym}_0(3)$ the map

$$h_0(x,t):=h(A\Phi_1(x,t)+V(x,t),t)-h(B\Phi_1(x,t)+W(x,t),t).$$

If we denote by $\overline{M}(x,t,s)$ the quantity

$$\overline{M}(\cdot,t,s):=\int_{\mathbb{R}^3}\frac{e^{-|\cdot-y|^2/4(t-s)}}{(4\pi(t-s))^{3/2}}h_0(y,s)\,dy-\Phi(\cdot,t-s)\left(\int_{\mathbb{R}^3}h_0(y,s)\,dy\right)$$

and also stipulate that $H_0:(0,\infty)\to\mathrm{Sym}_0(3)$ be

$$H_0(t):=\int_t^\infty\int_{\mathbb{R}^3}h_0(y,\tau)\,dyd\tau,$$

one may verify that the identity

$$J(x,t)=\overbrace{\int_0^{t/2}\overline{M}(x,t,s)\,ds}^{J_1(x,t):=}+\overbrace{H_0(0)\big(\Phi(x,t)-\Phi_1(x,t)\big)}^{J_2(x,t):=}-\overbrace{\Phi\left(x,\frac{t}{2}\right)H_0\left(\frac{t}{2}\right)}^{J_3(x,t):=}$$
$$+\underbrace{\int_0^{t/2}\left(\frac{6\pi}{t-s}-\frac{|x|^2}{4(t-s)^2}\right)\Phi(x,t-s)H_0(s)\,ds}_{J_4(x,t):=}$$

holds for all $x\in\mathbb{R}^3$ and $t\geq1$. It is straightforward to show that

$$J_i(x,t)\lesssim\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}}(t+1)^{-2}\|(A,V)-(B,W)\|_X, \tag{3.31}$$

for $i=3,4$ simply by using familiar properties of the heat kernel, inequality (3.22) and the fact that $(t-s)^{-1}\leq4(t+1)^{-1}$ for $t\geq1$ and s in the interval $0\leq s\leq t/2$. The treatment

of the cases $i = 1, 2$ require a little more care. An application of the result of proposition 3.3 to the term J_1 yields

$$\begin{aligned}
&\int_0^{t/2} \overline{M}(x,t,s)\,ds \\
&\overset{(3.12)}{\leq} C\int_0^{t/2}\int_{\mathbb{R}^3} \frac{|y|}{(t-s)^2}\left(\frac{1+|y|/\sqrt{8(t-s)}}{1+|x|/\sqrt{8(t-s)}}\right)^{4+\frac{\delta}{2}} |h(A\Phi_1+V,s)-h(B\Phi_1+W,s)|\,dyds, \\
&\overset{(3.22)}{\lesssim} \int_0^{t/2}\frac{e^{-as}}{(s+1)^3}\int_{\mathbb{R}^3}\frac{|y|}{(t-s)^2}\left(1+\frac{|y|}{\sqrt{8(t-s)}}\right)^{4+\frac{\delta}{2}}\left(1+\frac{|y|}{\sqrt{s+1}}\right)^{-8-\delta} dyds \\
&\qquad \times \left(1+\frac{|x|}{\sqrt{8(t-s)}}\right)^{-4-\frac{\delta}{2}} \|(A,V)-(B,W))\|_X.
\end{aligned}$$

Now, noticing that for $0 \leq s \leq t/2$ and $t \geq 1$ we have the string of inequalities $(t-s)^{-1/2} \leq \sqrt{2}t^{-1/2} \leq C(t+1)^{-1/2} \leq C(s+1)^{-1/2}$, we deduce from the above that

$$\begin{aligned}
&\int_0^{t/2} \overline{M}(x,t,s)\,ds \\
&\lesssim \int_0^{t/2}\left(1+\frac{|x|}{\sqrt{8(t-s)}}\right)^{-4-\frac{\delta}{2}} \frac{e^{-as}}{(s+1)}\frac{1}{(t-s)^2}\left(\int_{\mathbb{R}^3}(1+|y|)^{-3-\frac{\delta}{2}}\,dy\right) ds \\
&\qquad \times \|(A,V)-(B,W))\|_X \\
&\lesssim \left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} (t+1)^{-2}\|(A,V)-(B,W))\|_X, \qquad (3.32)
\end{aligned}$$

since $\delta > 0$ gives us the required integrability of $(1+|\cdot|)^{-3-\delta/2}$ in dimension three. It remains to verify such an estimate holds for the term J_2, and for this we require the following simple lemma.

Lemma 3.8. *For $x \in \mathbb{R}^3$ and $t \geq 1$, the heat kernel difference $\Phi_1(x,t) - \Phi(x,t)$ satisfies the inequality*

$$|\Phi_1(x,t) - \Phi(x,t)| \leq \frac{2e^{-|x|^2/8(t+1)}}{(t+1)^{5/2}}. \qquad (3.33)$$

Proof. Consider the smooth map ψ defined by

$$\psi(z,t) := e^{-\frac{z^2}{4}\left(\frac{1}{2(t+1)}\right)} - e^{-\frac{z^2}{4}\left(\frac{2+t}{2t(t+1)}\right)}.$$

For any fixed $t \geq 1$, by considering the equation $\psi_z(z,t) = 0$ one may show that $z \mapsto \psi(z,t)$ is controlled by its unique global maximum over the set $[1,\infty)$, namely

$$\psi(z,t) \leq 2\left(\frac{1}{\frac{2}{t}+1}\right)^{t/2}\frac{1}{t+1}.$$

Upon setting $z = |x|$, we readily deduce from the above

$$e^{-|x|^2/4(t+1)} - e^{-|x|^2/4t} \leq \frac{2e^{-|x|^2/8(t+1)}}{(t+1)},$$

from which estimate (3.33) quickly follows. □ □

Piecing this together with the estimates (3.31) and (3.32), we obtain

$$J(x,t) \lesssim \|(A,V)-(B,W)\|_X \left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} (t+1)^{-2},$$

which along with (3.30) provides

$$|F_2(A,V;x,t) - F_2(B,W;x,t)| \lesssim \|(A,V)-(B,W)\|_X \left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} (t+1)^{-2}, \quad (3.34)$$

for $x \in \mathbb{R}^3$ and $t \geq 1$.

The component $F_2 : X \to X_0$ when $0 \leq t \leq 1$

This case follows almost immediately from (3.22) and the fact that our time interval of interest in this instance is compact. Thus, combining this with (3.34), rearranging and taking norms in X_0, we find that

$$\|F_2(A,V) - F_2(B,W)\|_{X_0} \leq C_2 k_0(A,B;V,W)\|(A,V)-(B,W)\|_X \quad (3.35)$$

for some constant $C_2 > 0$. We have therefore verified the difference property (3.21).

The operator $F_2 : X \to X_0$ is well defined

All that remains to be checked is that the map

$$(x,t) \mapsto \int_{\mathbb{R}^3} \frac{e^{-|x-y|^2/4t}}{(4\pi t)^{3/2}} \left(Q_0(y) - \frac{e^{-|y|^2/4}}{(4\pi)^{3/2}} \int_{\mathbb{R}^3} Q_0(z)\,dz\right) dy$$

is an element of X_0. The case when $t \geq 1$ may be tackled using inequality (3.12) and lemma 3.8. On the other hand, for the case when $0 \leq t \leq 1$, we need only concern ourselves with the behaviour of the heat term $e^{t\Delta}Q_0$ near the origin in time. We obtain the required estimates by writing

$$(e^{t\Delta}Q_0)(x) = \int_{\mathcal{R}_1(x)} \Phi(x-y,t)Q_0(y)\,dy + \int_{\mathcal{R}_2(x)} \Phi(x-y,t)Q_0(y)\,dy$$

and applying inequalities (3.25) and (3.27) in the manner previously outlined over the regions $\mathcal{R}_1(x)$ and $\mathcal{R}_2(x)$, respectively.

Finally, setting $(B,W) = 0$ in (3.35) completes the proof that $F : X \to X$ is both well-defined and locally Lipschitz on X. □

Let $\mathfrak{B} := \overline{B(0,\varepsilon_0)} \subset X$ denote the closed ball of radius $\varepsilon_0 > 0$ in X, where ε_0 is yet to be fixed. To close the proof of theorem 3.5 by means of an application of Banach's fixed point theorem, it remains to show that $F : \mathfrak{B} \to \mathfrak{B}$ is a strictly contractive operator for ε_0 chosen sufficiently small. To this end, fix ε_0 to be the positive root of the quadratic equation associated with the contraction constraint

$$\max\{C_1, C_2\}\left(2\varepsilon + 4\varepsilon^2\right) = \frac{1}{4},$$

where C_1 and C_2 are those constants appearing in (3.23) and (3.35), respectively. Taking into account the definition of the contraction modulus k_0, we deduce from (3.23) and (3.35) that

$$\|F(A,V) - F(B,W)\|_X \leq \frac{1}{2}\|(A,V) - (B,W)\|_X,$$

for all $(A,V),(B,W) \in \mathfrak{B}$. Given that we also have the estimate

$$\begin{aligned}\|F(A,V)\|_X \leq \quad & \sup_{(x,t)}\left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{4+\frac{\delta}{2}}(t+1)^2\left|e^{t\Delta}\left(Q_0 - \frac{e^{-|\cdot|^2/4}}{(4\pi)^{3/2}}\int_{\mathbb{R}^3} Q_0(z)\,dz\right)(x)\right| \\ & + \left|\int_{\mathbb{R}^3} Q_0(y)\,dy\right| + \frac{1}{2}\|(A,V)\|_X,\end{aligned}$$

for any $(A,V) \in \mathfrak{B}$, it is clear we may find $\eta > 0$ to ensure that the quantity

$$\sup_{(x,t)}\left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{4+\frac{\delta}{2}}(t+1)^2\left|e^{t\Delta}\left(Q_0 - \frac{e^{-|\cdot|^2/4}}{(4\pi)^{3/2}}\int_{\mathbb{R}^3} Q_0(z)\,dz\right)(x)\right| + \left|\int_{\mathbb{R}^3} Q_0(y)\,dy\right|$$

is less than or equal to $\varepsilon_0/2$ for all $Q_0 \in \mathcal{A}$ satisfying $\|Q_0\|_{\mathcal{A}} \leq \eta$. Thus, for all such Q_0 satisfying this 'smallness' condition, the associated nonlinear operators F are strictly contractive with range in $\mathfrak{B}$. By the Banach fixed point theorem, there exists a unique (relabeled) fixed point $(A,V) \in \mathfrak{B}$ and so from the discussion in section 3.3 follows the proof of theorem 3.5, namely

$$Q(x,t) = Ae^{-at}\Phi_1(x,t) + e^{-at}V(x,t),$$

for some $A \in \mathrm{Sym}_0(3)$ and $V \in X_0$ satisfying $\|(A,V)\|_X \leq \varepsilon_0$.

Remark 3.4. *We henceforth denote by $\mathcal{A}^\circ \subset \mathcal{A}$ the open subset of all initial data $Q_0 \in \mathcal{A}$ for which the above decomposition result holds, namely*

$$\mathcal{A}^\circ := \left\{R \in L^\infty(\mathbb{R}^3) \,:\, \operatorname*{ess\,sup}_{x\in\mathbb{R}^3}(1+|x|)^{8+\delta}\,|R(x)| < \eta\right\}.$$

3.4 The Scaling Regime $L(t) = t^{1/2}$

Before we discuss the behaviour of the correlation function $c_{\mu_0}(r,t)$ as $t \to \infty$, we comment on the behaviour of the correlation function concentrated on *individual* solutions. Utilising the decomposition formula $Q(x,t) = Ae^{-at}\Phi_1(x,t) + e^{-at}V(x,t)$ obtained in theorem 3.5, we investigate how the quantity

$$c(r,t) = \frac{\displaystyle\int_{\mathbb{R}^3} \operatorname{tr}\left[Q(x+r,t)Q(x,t)\right]\,dx}{\displaystyle\int_{\mathbb{R}^3} \operatorname{tr}\left[Q(x,t)^2\right]\,dx}$$

behaves for large time. Firstly, noting that we have the equality

$$\int_{\mathbb{R}^3} \Phi_1(x+r,t)\Phi_1(x,t)\,dx = \frac{1}{\sqrt{8}}\frac{e^{-|r|^2/8(t+1)}}{(4\pi(t+1))^{3/2}},$$

and also that any $V \in X_0$ has the norm decay property

$$\|V(\cdot,t)\|_2 \leq C\|V\|_{X_0}(t+1)^{-5/4},$$

one may then verify that

$$\frac{\sqrt{8}e^{2at}(4\pi(t+1))^{3/2}}{\operatorname{tr}(A^2)}\left|\int_{\mathbb{R}^3} \operatorname{tr}\left[Q(x+r,t)Q(x,t)\right]\,dx\right| \leq e^{-|r|^2/8(t+1)} + \omega(t), \tag{3.36}$$

for $r \in \mathbb{R}^3$ *provided* $A \neq 0$, where the function ω is bounded and continuous on $[1,\infty)$ and decays at least as quickly at $t^{-1/2}$ as $t \to \infty$. Setting $r = 0$ in (3.36) above and taking the appropriate quotient, one quickly finds after subtracting off the contribution $\exp(-|r|^2/8t)$ that

$$c(r,t) - e^{-|r|^2/8t} \leq \frac{1}{1+\omega(t)}\left(e^{-|r|^2/8(t+1)} - e^{-|r|^2/8t}\right) - \frac{\omega(t)}{1+\omega(t)}e^{-|r|^2/8t} + \frac{\omega(t)}{1+\omega(t)},$$

from which we deduce

$$\left\| c(r,t) - e^{-\frac{|r|^2}{8t}} \right\|_{L^\infty(\mathbb{R}^3;\,dr)} = \mathcal{O}\left(t^{-1/2}\right) \quad \text{as} \quad t \longrightarrow \infty. \tag{3.37}$$

Let us emphasise once more that the above calculation is only valid whenever the constant matrix A is non-zero. If $A = 0$, one discovers that the correlation function has the form

$$c(r,t) = \frac{\displaystyle\int_{\mathbb{R}^3} \operatorname{tr}\left(V(x+r,t)V(x,t)\right)\,dx}{\displaystyle\int_{\mathbb{R}^3} \operatorname{tr}\left(V(x,t)^2\right)\,dx},$$

from which no scaling information on $c(r,t)$ can be gleaned. This is, of course, not the case when $A \neq 0$ as the map $(r,t) \mapsto e^{-|r|^2/8t}$ is manifestly self-similar on $\mathbb{R}^3 \times (0,\infty)$. We now demonstrate that the set of all initial data in $\mathcal{A}^\circ$ which possibly give rise to solutions for which $A = 0$ in the decomposition (3.18) is rare, in the sense that it is a closed subset of $\mathcal{A}^\circ$ containing no open $\|\cdot\|_{\mathcal{A}}$-ball, i.e. it has empty interior. In particular, the complement of this set in $\mathcal{A}^\circ$ is dense in $\mathcal{A}^\circ$.

The matrix A cannot be zero on 'large' sets of initial data in $\mathcal{A}^\circ$

It is our aim to show that the scaling behaviour of solutions is generic amongst all those evolving from initial data satisfying the smallness condition (3.17). Let us reiterate that our notion of 'generic' here is that the set of all such initial data in $\mathcal{A}^\circ$ giving rise to solutions with constant matrix $A = 0$ constitute a closed set containing no open ball.

Firstly, we note that as each $Q_0 \in \mathcal{A}^\circ$ gives rise to a unique solution of the shape

$$Q(x,t) = Ae^{-at}\Phi_1(x,t) + e^{-at}V(x,t), \tag{3.38}$$

where each matrix A satisfies the explicit identity (c.f. formula (3.19))

$$A = \int_{\mathbb{R}^3} Q_0(y)\,dy + \int_0^\infty \int_{\mathbb{R}^3} h(Q(y,\tau),\tau)\,dyd\tau,$$

we may ask about the nature of the resulting map between $\mathcal{A}^\circ$ and $\mathrm{Sym}_0(3)$ which yields A from Q_0. It is well known that real-analytic maps between open connected sets of Banach spaces cannot be constant on open subsets unless they are identically constant on the whole set: see, for instance, Buffoni and Toland [18], theorem 4.3.9. Thus, if we demonstrate the map $Q_0 \mapsto A$ is real-analytic on $\mathcal{A}^\circ$ and is indeed not identically the zero map, it follows that the set of all initial data which produce the result $A = 0$ in the decomposition (3.38) is closed in $\mathcal{A}^\circ$ and contains no $\|\cdot\|_{\mathcal{A}}$-open ball.

In this direction, consider the map $\mathcal{F}_0 : \mathcal{X} \times \mathcal{A} \to \mathcal{X}$ defined by

$$\mathcal{F}_0(Z(\cdot,t),z) := e^{t\Delta}z + \int_0^t e^{(t-s)\Delta}h(Z(\cdot,s),s)\,ds - Z(\cdot,t),$$

for $Z \in \mathcal{X}$, $z \in \mathcal{A}$ and $t \geq 0$, where $\mathcal{X}$ is the Banach space of maps

$$\mathcal{X} := \left\{ U \in C(\mathbb{R}^3 \times [0,\infty); \mathrm{Sym}_0(3)) \,:\, \sup_{(x,t)} \left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{4+\frac{\delta}{2}} (t+1)^{3/2}|U(x,t)| < \infty \right\}$$

endowed with the natural weighted supremum norm $\|\cdot\|_{\mathcal{X}}$. We also recall that the space $\mathcal{A}$ is endowed with the norm $\|R\|_{\mathcal{A}} = \operatorname{ess\,sup}_{x\in\mathbb{R}^3}(1+|x|)^{8+\delta}|R(x)|$. In what follows, we wield results from the theory of analytic Banach space-valued maps. We refer the reader to Zeidler [89] for the basic definitions and results. As a helpful first step, we establish the following proposition.

Proposition 3.9. *The map $\mathcal{F}_0 : \mathcal{X} \times \mathcal{A} \to \mathcal{X}$ is real-analytic.*

Proof. By considering the difference

$$\mathcal{F}_0[(R,\rho) + (\Xi_1,\xi_1)] - \mathcal{F}_0[(R,\rho)],$$

one may check that the first Fréchet derivative $d\mathcal{F}_0$ of $\mathcal{F}_0$ at $(R,\rho) \in \mathcal{X} \times \mathcal{A}$ satisfies

$$(d\mathcal{F}_0[(R,\rho)])(\Xi_1,\xi_1) = e^{t\Delta}\xi_1 + b\int_0^t e^{(t-s)\Delta}e^{-as}\left(R\Xi_1 + \Xi_1 R - \frac{2}{3}\mathrm{tr}\,(R\Xi_1)\,I\right)ds$$

$$- c \int_0^t e^{(t-s)\Delta} e^{-2as} \left(2 \operatorname{tr} (R\Xi_1)\, R + \operatorname{tr} \left(R^2 \right) \Xi_1 \right)\, ds - \Xi_1(\cdot, t),$$

for all $(\Xi_1, \xi_1) \in \mathcal{X} \times \mathcal{A}$. Moreover, one has that

$$(d^2 \mathcal{F}_0[(R,\rho)])((\Xi_1,\xi_1),(\Xi_2,\xi_2)) = b \int_0^t e^{(t-s)\Delta} e^{-as} \left(\Xi_1\Xi_2 + \Xi_2\Xi_1 - \frac{2}{3} \operatorname{tr} (\Xi_1\Xi_2)\, I \right) ds$$
$$-2c \int_0^t e^{(t-s)\Delta} e^{-2as} \left(\operatorname{tr}(\Xi_1\Xi_2) R + \operatorname{tr}(R\Xi_1)\Xi_2 + \operatorname{tr}(R\Xi_2)\Xi_1 \right)\, ds,$$

and

$$(d^3 \mathcal{F}_0[R,\rho])((\Xi_1,\xi_1),(\Xi_2,\xi_2),(\Xi_3,\xi_3))$$
$$= -2c \int_0^t e^{(t-s)\Delta} e^{-2as} \left(\operatorname{tr}(\Xi_1\Xi_2)\Xi_3 + \operatorname{tr}(\Xi_3\Xi_1)\Xi_2 + \operatorname{tr}(\Xi_2\Xi_3)\Xi_1 \right)\, ds$$

for for $(R,\rho), (\Xi_1,\xi_1)..., (\Xi_3,\xi_3) \in \mathcal{X} \times \mathcal{A}$. Owing to the fact that the nonlinearity h in the operator $\mathcal{F}_0$ is of cubic order, the higher Fréchet derivatives satisfy

$$\left(d^k \mathcal{F}[(R,\rho)]\right) \left((\Xi_1,\xi_1),...,(\Xi_k,\xi_k)\right) = 0 \quad \text{in} \quad \mathcal{X},$$

for $(R,\rho), (\Xi_1,\xi_1)..., (\Xi_k,\xi_k) \in \mathcal{X} \times \mathcal{A}$ and $k \geq 4$. Furthermore, for constants C, K and r depending on the point (R,ρ), the estimates

$$\| d^k \mathcal{F}_0[(Z,z)] \| \leq \frac{Ck!}{K^k}, \quad \text{whenever} \quad \|(Z,z) - (R,\rho)\|_{\mathcal{X}\times\mathcal{A}} < r$$

hold for $0 \leq k < 4$, where norms are taken in the appropriate space of multilinear operators. By triviality of the higher Fréchet derivatives, the map $\mathcal{F}_0$ is real-analytic on $\mathcal{X} \times \mathcal{A}$. □

Having established that the map $\mathcal{F}_0 : \mathcal{X} \times \mathcal{A} \to \mathcal{X}$ is analytic, this result aids us in establishing the useful fact that the solution map $\mathcal{F} : Q_0 \mapsto Q$ from $\mathcal{A}^\circ$ to $\mathcal{X}$ is itself a real-analytic map.

Theorem 3.10. *The solution map $\mathcal{F} : \mathcal{A}^\circ \to \mathcal{X}$ is real-analytic.*

Proof. In what follows, we call $(R,\rho) \in \mathcal{X} \times \mathcal{A}$ a *solution pair* if and only if $R \in \mathcal{X}$ is the unique solution of (3.16) corresponding to the initial datum $\rho \in \mathcal{A}$. We denote the corresponding *solution map* which yields R from ρ by $\mathcal{F}$. We make the important observation that for any point $(R,\rho) \in \mathcal{X} \times \mathcal{A}$,

$$\mathcal{F}_0[(R,\rho)] = 0 \qquad \text{if and only if} \qquad (R,\rho) \text{ is a solution pair.} \tag{3.39}$$

Suppose (R,ρ) chosen from the open subset $\mathcal{X} \times \mathcal{A}^\circ \subset \mathcal{X} \times \mathcal{A}$ is a solution pair. We claim that the partial derivative $d_Z \mathcal{F}_0[(R,\rho)] \in \mathcal{L}(\mathcal{X})$ is a homeomorphism.

We prove the claim as follows. As the partial Fréchet derivative $d_Z\mathcal{F}_0$ satisfies

$$(d_Z\mathcal{F}_0[(R,\rho)])(\Xi) = b\int_0^t e^{(t-s)\Delta}e^{-as}\left(R\Xi + \Xi R - \frac{2}{3}\mathrm{tr}\,(R\Xi)\,I\right)\,ds$$
$$- c\int_0^t e^{(t-s)\Delta}e^{-2as}\left(2\,\mathrm{tr}\,(R\Xi)\,R + \mathrm{tr}\left(R^2\right)\Xi\right)\,ds - \Xi(\cdot,t)$$

for all $\Xi \in \mathcal{X}$, one may then verify that the inequality

$$\|d_Z\mathcal{F}_0[(R,\rho)] - J\|_{L(\mathcal{X})} < 1$$

holds by 'smallness' in the $\|\cdot\|_{\mathcal{X}}$-norm of those solutions of (3.16) starting from $\mathcal{A}^\circ$ initial data. Furthermore, the map $J : \mathcal{X} \to \mathcal{X}$ given by $J\Xi := -\Xi$ clearly has unit norm in $\mathcal{L}(\mathcal{X})$. It then follows from the theory of Neumann series that $d_Z\mathcal{F}_0[(R,\rho)] \in L(\mathcal{X})$ is a homeomorphism. Thus, by the analytic implicit function theorem, one may infer the existence of an open neighbourhood $\mathcal{V} \subset \mathcal{A}^\circ$ of ρ, an open neighbourhood $\mathcal{U} \subset \mathcal{X} \times \mathcal{A}^\circ$ of the point (R,ρ) and a real-analytic map $\phi : \mathcal{V} \to \mathcal{X}$ with the property that

$$\{(\phi(\rho),\rho) \,:\, \rho \in \mathcal{V}\} = \mathcal{F}_0^{-1}(0) \cap \mathcal{U}.$$

By observation (3.39), it is clear that the set $\mathcal{F}_0^{-1}(0)$ is simply that of all solution pairs $(\mathcal{F}\rho,\rho)$ such that $\rho \in \mathcal{A}$. Therefore, the map $\phi : \mathcal{V} \to \mathcal{X}$ is identically equal to the restriction $\mathcal{F}|_{\mathcal{V}}$ of the solution operator to the set $\mathcal{V} \subset \mathcal{A}^\circ$.

As the point (R,ρ) was arbitrarily chosen, it then follows that the solution operator $\mathcal{F} : \mathcal{A}^\circ \to \mathcal{X}$ is real-analytic. □

Now that we have established the basic result that the solution operator $\mathcal{F} : \mathcal{A}^\circ \to \mathcal{X}$ is real-analytic, we define some other relevant operators. We define $\mathcal{G} : \mathcal{A}^\circ \to \mathcal{A}^\circ \times \mathcal{X}$ by

$$\mathcal{G}Q_0 := (Q_0, \mathcal{F}Q_0) \qquad \text{for all} \qquad Q_0 \in \mathcal{A}^\circ.$$

By virtue of the last theorem, it is clear that $\mathcal{G}$ is real-analytic on $\mathcal{A}^\circ$. Moreover, by a routine calculation, one may also verify that the map $\mathcal{H} : \mathcal{A}^\circ \times \mathcal{X} \to \mathrm{Sym}_0(3)$ defined by

$$\mathcal{H}(z,Z) := \int_{\mathbb{R}^3} z(y)\,dy + \int_0^\infty \int_{\mathbb{R}^3} h(Z(y,\tau),\tau)\,dyd\tau$$

is also real analytic. With these facts in mind, one may view the right-hand side of the equality

$$A = \int_{\mathbb{R}^3} Q_0(y)\,dy + \int_0^\infty \int_{\mathbb{R}^3} h(Q(y,\tau),\tau)\,dyd\tau$$

as a composition of analytic maps taking $\mathcal{A}^\circ$ to $\mathrm{Sym}_0(3)$, namely

$$A = (\mathcal{H} \circ \mathcal{G})Q_0.$$

As compositions of real analytic maps are themselves real analytic (see BUFFONI AND TOLAND [18], theorem 4.5.7), we deduce that the map $\mathcal{H} \circ \mathcal{G} : Q_0 \mapsto A$ is real analytic on $\mathcal{A}^\circ$.

We need only now show that the map $\mathcal{H} \circ \mathcal{G}$ is non-zero on $\mathcal{A}^\circ$. To this end, we provide a non-empty set of initial data contained in $\mathcal{A}^\circ$ for which the matrix A in the decomposition (3.18) is non-zero. Together with the fact that the coefficient matrix A depends in a continuous manner on initial data, we have the existence of an open set of initial data for which $A \neq 0$.

Proposition 3.11. *For $\alpha \geq 0$, let $\lambda_\alpha : \mathbb{R}^3 \to \mathbb{R}$ denote the map*

$$\lambda_\alpha(x) := -\frac{\alpha}{(1+|x|)^{8+\delta}}, \tag{3.40}$$

and set $Q_{0,\alpha} := \operatorname{diag}(\lambda_\alpha, \lambda_\alpha, -2\lambda_\alpha)$. There exists $\alpha_0 > 0$ such that $A \neq 0$ in the decomposition (3.18) for all $0 < \alpha < \alpha_0$.

Proof. By uniqueness of solutions of the gradient flow (3.7), it follows that solutions starting from uniaxial data

$$Q_0(x) = \begin{pmatrix} \lambda_0(x) & 0 & 0 \\ 0 & \lambda_0(x) & 0 \\ 0 & 0 & -2\lambda_0(x) \end{pmatrix}$$

remain of uniaxial form

$$Q(x,t) = \begin{pmatrix} \lambda(x,t) & 0 & 0 \\ 0 & \lambda(x,t) & 0 \\ 0 & 0 & -2\lambda(x,t) \end{pmatrix}$$

for $t > 0$, where $\lambda(x,t)$ satisfies the scalar nonlinear heat equation

$$\frac{\partial \lambda}{\partial t} = \Delta\lambda - a\,\lambda - b\,\lambda^2 - 6c\,\lambda^3 \tag{3.41}$$

on $\mathbb{R}^3 \times (0,\infty)$. Suppose that we consider solutions of (3.41) starting from initial data of the form (3.40). By THEOREM 3.5, there exists $\overline{\alpha} > 0$ such that if $|\lambda_0(x)| < \alpha < \overline{\alpha}$, then

$$|\lambda(x,t)| \leq C\alpha \quad \text{on} \quad \mathbb{R}^3 \times (0,\infty),$$

for some constant $C > 0$ depending only on $(a,b,c) \in \mathcal{D}$.

Let us make the transformation $\nu(x,t) := e^{at}\lambda(x,t)$. Now, one can find $\alpha_0 > 0$ small enough satisfying $\overline{\alpha} \geq \alpha_0 > 0$ such that

$$-b\,e^{-at}\,(\nu(x,t))^2 - c\,e^{-2at}\,(\nu(x,t))^3 \leq 0 \quad \text{on} \quad \mathbb{R}^3 \times (0,\infty).$$

Furthermore, since ν can easily be shown to satisfy the equation

$$\nu(\cdot,t) = e^{t\Delta}\lambda_0 - \int_0^t e^{(t-s)\Delta}\left(b\,e^{-as}\left(\nu(\cdot,s)\right)^2 + 6c\,e^{-2as}\left(\nu(\cdot,s)\right)^3\right)\,ds,$$

by integrating across over space, we deduce that

$$\int_{\mathbb{R}^3}\nu(x,t)\,dx \leq \int_{\mathbb{R}^3}\lambda_0(x,t)\,dx < 0,$$

for all $t > 0$. Thus, the $L^1(\mathbb{R}^3)$-norm of the original solutions λ cannot decay to 0 as $t \to \infty$, and so for the set of initial data

$$\left\{\mathrm{diag}(\lambda_0,\lambda_0,-2\lambda_0)\,:\,\lambda_0(x) = -\frac{\alpha}{(1+|x|)^{8+\delta}} \quad \text{for} \quad 0<\alpha<\alpha_0\right\} \subset \mathcal{A}^\circ,$$

the corresponding matrix A in the solution decomposition (3.18) cannot be zero. □

To complete our demonstration that $\mathcal{H}\circ\mathcal{G}$ is not identically the zero map on $\mathcal{A}^\circ$, we argue as follows. For α chosen from the interval $(0,\alpha_0)$ determined from the above proposition, we denote the coefficient matrix in the decomposition formula (3.18) corresponding to the solution with uniaxial initial datum $Q_{0,\alpha} = \mathrm{diag}(\lambda_\alpha,\lambda_\alpha,-2\lambda_\alpha)$ by $A(\alpha)$. Since $A(\alpha) \neq 0$, there exists an open ball of matrices $\mathbb{B}(\alpha) \subset \mathrm{Sym}_0(3)$ with centre $A(\alpha)$ that does not contain the zero matrix. Since $\mathcal{H}\circ\mathcal{G}$ is analytic, it follows that $(\mathcal{H}\circ\mathcal{G})^{-1}(\mathbb{B}(\alpha))$ is an open set of initial data in $\mathcal{A}^\circ$. From this we conclude that $\mathcal{H}\circ\mathcal{G}$ cannot be the zero map on $\mathcal{A}^\circ$, from which it follows that the set of all those Q_0 in $\mathcal{A}^\circ$ which yield $A = 0$ in (3.38) is closed and contains no open ball.

Remark 3.5. *We subsequently denote the set of all maps in $\mathcal{A}^\circ$ for which the coefficient matrix A is 0 by $\mathcal{B}$.*

Asymptotic Behaviour of $c_{\mu_0}(r,t)$ as $t \to \infty$

As discussed in the introduction, we express the notion of averaging over initial conditions in a rigorous manner by evaluating the correlation function with respect to a suitable time-dependent family of Borel probability measures. We construct statistical solutions of (3.7) in the following proposition, whose proof is a modification of a construction contained in Foias, Manley, Rosa and Temam ([37], Appendix A1). We quickly recall the definition a Dirac delta measure on the space $L^2(\mathbb{R}^3)$.

Definition 3.1. *Let $\mathcal{P}(L^2(\mathbb{R}^3))$ denote the power set of $L^2(\mathbb{R}^3)$. For any given $Q \in L^2(\mathbb{R}^3)$, the associated map $\delta_Q : \mathcal{P}(L^2(\mathbb{R}^3)) \to \{0,1\}$ defined by*

$$\delta_Q(A) := \begin{cases} 1 & \text{if} \quad Q \in A, \\ \\ 0 & \text{otherwise}, \end{cases}$$

is the Dirac delta measure *concentrated at $Q \in L^2(\mathbb{R}^3)$.*

Proposition 3.12. *Suppose $0 < \gamma < \infty$. For any given Borel probability measure $\overline{\mu}$ supported on the set*

$$\left\{Q \in L^2(\mathbb{R}^3) \,:\, \|Q\|_2 \leq \gamma\right\} \cap H,$$

there exists a corresponding one-parameter family of Borel probability measures $\{\mu_t\}_{t\geq 0}$ and an approximating sequence of families

$$\left\{\{\mu_t^{(k)}\}_{t\geq 0} \,:\, k = 1, 2, 3, ...\right\} \quad \textit{with} \quad \mu_t^{(k)} := \sum_{j=1}^{N(k)} \vartheta_j^{(k)} \delta_{S(t)\overline{Q}_j^{(k)}}$$

for some $N(k) \in \mathbb{N}$ and $\vartheta_j^{(k)} \in (0, 1]$, such that

$$\mu_t(E) = \lim_{k\to\infty} \mu_t^{(k)}(E) \tag{3.42}$$

for all $t \geq 0$ and all μ_t-measurable subsets $E \subseteq \{Q \in L^2(\mathbb{R}^3) \,:\, \|Q\|_2 \leq \gamma\} \cap H$. For each $k \geq 1$, the coefficients $\vartheta_j^{(k)} \geq 0$ respect the sum $\sum_j \vartheta_j^{(k)} = 1$, and $S(t)\overline{Q}_j^{(k)}$ denotes the action of the semigroup of proposition 3.2 on initial data $\overline{Q}_{k,j}$.

Proof. We establish the spaces which we use to construct the family of measures $\{\mu_t\}_{t\geq 0}$. We endow the set

$$K := \left\{Q \in L^2(\mathbb{R}^3) \,:\, \|Q\|_2 \leq \gamma\right\}$$

with the weak topology inherited from $L^2(\mathbb{R}^3)$, with respect to which it is a compact topological space. Furthermore, this space is metrisable with metric d_w, given by

$$d_w(Q, R) := \sum_{k=1}^{\infty} \frac{1}{2^k} \left| \int_{\mathbb{R}^3} Q : \chi_k - \int_{\mathbb{R}^3} R : \chi_k \right|,$$

where $\{\chi_k\}_{k=1}^{\infty}$ is a countable dense subset of the set $K \subset L^2(\mathbb{R}^3)$. We write $\mathsf{M}_0(K)$ to denote the set of all Borel probability measures carried by subsets of K, and furnish $\mathsf{M}_0(K)$ with the subspace weak-$*$ topology inherited from $C(K)'$, whence $\mathsf{M}_0(K)$ is a convex, compact Hausdorff topological space by the Banach-Alaoglu theorem.

Let $T > 0$ be given. The estimate

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^3} \mathrm{tr}\left(Q^2\right) \leq \left(\frac{b^2}{2c} - a\right) \int_{\mathbb{R}^3} \mathrm{tr}\left(Q^2\right),$$

which may be derived from (3.11), implies that there exists $\gamma' = \gamma'(T, \gamma) > 0$ such that the solution $Q(\cdot, t)$ satisfies

$$Q(\cdot, t) \in K' := \left\{R \in L^2(\mathbb{R}^3) \,:\, \|R\|_2 \leq \gamma'\right\},$$

for all $0 \leq t \leq T$ whenever $Q(\cdot, 0) = Q_0 \in K \cap H$. With this in mind, we write σ_T to denote the set of solution trajectories

$$\sigma_T := \left\{Q \in C([0, T], K') \,:\, Q(x, t) \text{ solves (3.7) and } Q(\cdot, 0) \in K \cap H\right\}.$$

Using standard energy estimates associated with (3.7), by the Arzelà-Ascoli theorem, one may show that σ_T is a compact topological space with respect to the topology induced from $(C([0,T];K'),d_\infty)$, where

$$d_\infty(Q_1,Q_2) := \max_{0\le t\le T} d_w(Q_1(t),Q_2(t)).$$

Similarly, the space $\mathsf{M}_0(\sigma_T)$ of all Borel probability measures on σ_T is also a convex, compact Hausdorff topological space.

Let us now begin our construction. For a given $\overline{\mu}\in\mathsf{M}_0(K)$ supported on $K\cap H$, by the Krein-Milman theorem we know there exists a sequence of families of Dirac delta measures $\{\delta_{\overline{Q}_j^{(k)}}\}_{j=1}^{N(k)}$ for $k=1,2,3,...$ satisfying

$$\int_K \varphi\, d\overline{\mu} = \lim_{k\to\infty}\sum_{j=1}^{N(k)} \vartheta_j^{(k)} \int_K \varphi\, d\delta_{\overline{Q}_j^{(k)}} \quad \text{for all} \quad \varphi\in C(K).$$

Using this approximating sequence of measures, we define a new sequence of probability measures $\{\mu^{(k)}\}_{k=1}^\infty\subset\mathsf{M}_0(\sigma_T)$ by

$$\mu^{(k)} := \sum_{j=1}^{N(k)} \vartheta_j^{(k)} \delta_{Q\left(\cdot\,;\overline{Q}_j^{(k)}\right)},$$

where $Q(\cdot\,;\overline{Q}_j^{(k)})$ denotes the solution trajectory starting from the initial datum $\overline{Q}_j^{(k)}$. This defines a sequence of elements in $\mathsf{M}_0(\sigma_T)$, so by compactness there exists a measure $\mu\in\mathsf{M}_0(\sigma_T)$ to which a (relabeled) subsequence of $\{\mu^{(k)}\}_{k=1}^\infty$ converges in the weak-$*$ topology. We now focus on this limiting measure μ.

For each fixed $s\in[0,T]$, the map

$$\varphi\mapsto\int_{\sigma_T}\varphi(Q(s))\,d\mu$$

is well defined, positive and linear on $C(K)$, so by the Riesz-Kakutani theorem there exists a Borel probability measure μ_s (depending on the choice of $s\in[0,T]$) satisfying

$$\int_{\sigma_T}\varphi(Q(s))\,d\mu(Q) = \int_K \varphi(R)\,d\mu_s(R)$$

for all $\varphi\in C(K)$. By direct computation, one may show for the sequence of approximants $\{\mu^{(k)}\}_{k=1}^\infty$ that the equality

$$\int_{\sigma_T}\varphi(Q(s))\,d\mu^{(k)}(Q) = \int_K \varphi(R)\,d\mu_s^{(k)}(R)$$

holds for all $\varphi\in C(K)$, where

$$\mu_s^{(k)} := \sum_{j=1}^{N(k)} \vartheta_j^{(k)} \delta_{S(s)\overline{Q}_j^{(k)}}.$$

Using the fact that $\mu^k \rightharpoonup \mu$ weakly-star in $\mathsf{M}_0(\sigma_T)$, we find

$$\int_K \varphi(R)\, d\mu_t = \int_{\sigma_T} \varphi(Q(t))\, d\mu(Q) = \lim_{k\to\infty} \int_{\sigma_T} \varphi(Q(t))\, d\mu^{(k)} = \lim_{k\to\infty} \int_K \varphi(R)\, d\mu_t^{(k)}(R).$$

From this we deduce the result

$$\mu_t(E) = \lim_{k\to\infty} \mu_t^{(k)}(E),$$

for all μ_t-measurable subsets $E \subseteq K$. The proof of the theorem is concluded by noting that $\lim_{t\to 0} \mu_t(E) = \overline{\mu}(E)$ for all E by the left continuity of the semigroup $\{S(t)\}_{t\geq 0}$, and also that the transport of the measure $\overline{\mu}$ may be extended globally in time as the semigroup $\{S(t)\}_{t\geq 0}$ is defined globally in time. □

Assembling all that has come before, we now approach the proof of our main result, which follows rather swiftly from previous results.

Theorem 3.13. *For any given $\delta > 0$, there exists $\eta > 0$ depending only on δ and the parameters $(a, b, c) \in \mathcal{D}$ such that for any Borel probability measure μ_0 supported in the dense open set*

$$\mathcal{A}^\circ \setminus \mathcal{B} = \left\{ R \in L^\infty(\mathbb{R}^3) \,:\, \operatorname*{ess\,sup}_{x\in\mathbb{R}^3} (1+|x|)^{8+\delta} \, |R(x)| < \eta \right\} \setminus \mathcal{B},$$

where $\mathcal{B}$ was defined in remark 3.5, the associated correlation function (3.4) exhibits asymptotic self-similar behaviour:

$$\left\| c_{\mu_0}(r,t) - e^{-\frac{|r|^2}{8t}} \right\|_{L^\infty(\mathbb{R}^3,\, dr)} = \mathcal{O}(t^{-1/2}) \quad \text{as} \quad t \to \infty.$$

Proof. By the previous result (3.42), we know that

$$\sum_{j=1}^{N_k} \vartheta_j^k \delta_{S(t)\overline{Q}_{k,j}}(E) \to \mu_t(E)$$

as $k \to \infty$ for any measurable subset $E \subset \mathcal{A}^\circ \setminus \mathcal{B}$. Since we have that

$$c_{\mu_0}(r,t) = \lim_{k\to\infty} \frac{\displaystyle\sum_{j=1}^{N(k)} \vartheta_j^{(k)} \int_H \int_{\mathbb{R}^3} \operatorname{tr}\left(Q(x+r)Q(x)\right)\, dx d\delta_{S(t)\overline{Q}_j^{(k)}}(Q)}{\displaystyle\sum_{j=1}^{N(k)} \vartheta_j^{(k)} \int_H \int_{\mathbb{R}^3} \operatorname{tr}\left(Q(x)^2\right)\, dx d\delta_{S(t)\overline{Q}_j^{(k)}}(Q)}.$$

the result then follows by employing a similar calculation as the one used to achieve (3.37). □

3.5 The Scaling Regime $L(t) = t$: An Observation

We now present evidence to support the existence of another scaling regime for the correlation function c_{μ_0}, namely $L(t) = t$, when μ_0 is concentrated on initial profiles whose $L^2(\mathbb{R}^3)$-norm is *not* restricted in magnitude in the manner of theorem 3.5.

Suppose that we offer initial data $Q_0 \in H$ of the form $Q_0 = \operatorname{diag}(\lambda_0, \lambda_0, -2\lambda_0)$ for equation (3.7). By uniqueness (proposition 3.2) we know the solution Q remains of diagonal form $Q = \operatorname{diag}(\lambda, \lambda, -2\lambda)$, where λ satisfies the *scalar* nonlinear heat equation

$$\begin{cases} \dfrac{\partial \lambda}{\partial t} = \Delta\lambda - a\,\lambda - b\,\lambda^2 - 6c\,\lambda^3, \\ \lambda(\cdot, 0) = \lambda_0. \end{cases}$$

For any $R > 0$ we denote by $\lambda_{0,R} : \mathbb{R}^3 \to \mathbb{R}$ the map

$$\lambda_{0,R}(x) := \begin{cases} \lambda^* & \text{if} \quad |x| < R, \\ 0 & \text{otherwise,} \end{cases}$$

where λ^* is the global minimiser of the bulk potential associated with (3.5), namely

$$\lambda^* = \arg\min_{\lambda \in \mathbb{R}} \left(\frac{a}{2}\lambda^2 + \frac{b}{3}\lambda^3 + \frac{3c}{2}\lambda^4 \right).$$

In order to comment on the asymptotic behaviour of the correlation function concentrated on such solutions, we require the following result (which we state without proof) that is based on the observations of Aronson and Weinberger [3] and Poláčik [69] that equation (3.5) supports *pulse-like* solutions.

Proposition 3.14. *There exist $R_0 > 0$ and $\overline{c} > 0$ such that solutions of (3.5) subject to initial data $\lambda_{0,R}$ for $R \geq R_0$ satisfy*

$$\lim_{t \to \infty} \|\lambda(\cdot, t) - \lambda^*\|_{L^\infty(B(0, \overline{c}t))} = 0, \tag{3.43}$$

where $B(0, \overline{c}t) \subset \mathbb{R}^3$ denotes the ball of radius $\overline{c}t$ and centre 0. Furthermore, for any $t_0 > 0$ there exists $\vartheta = \vartheta(t_0)$ such that the solution λ satisfies the bounds

$$0 \leq \lambda(x, t) \leq Ce^{-\sigma(|x| - \overline{c}t + \vartheta)} \quad \text{on} \quad \mathbb{R}^3 \times [t_0, \infty), \tag{3.44}$$

for some positive constants C and σ.

Utilising the results (3.43) and (3.44) above, one may verify that the correlation function

$$c_{\delta_{Q_0}}(r, t) = \frac{\displaystyle\int_{\mathbb{R}^3} \lambda(x + r, t)\lambda(x, t)\, dx}{\displaystyle\int_{\mathbb{R}^3} \lambda(x, t)\lambda(x, t)\, dx}$$

concentrated on solutions with initial data $Q_0 = \mathrm{diag}(\lambda_{0,R}, \lambda_{0,R}, -2\lambda_{0,R})$ for $R \geq R_0$ satisfies

$$\lim_{t\to\infty} \left\| c_{\delta_{Q_0}}(r,t) - P\left(\frac{|r|}{t}\right) \right\|_{L^\infty(\mathbb{R}^3,\, dr)} = 0,$$

where P is a cubic polynomial of the shape

$$P(z) = \frac{1}{13\overline{c}^3}\,(4\overline{c}+z)\,(2\overline{c}-z)^2\,.$$

Thus, for this one-parameter family of initial data, whose H-norm may be made arbitrarily large, we obtain *both* a different universal scaling function (a polynomial, as opposed to the exponential map) and a different form for the coarsening length scale $L(t)$. Some effort would be required to establish the stability of such profiles, leading to a result for the correlation function c_{μ_0}, where μ_0 is a non-atomic measure supported on an appropriate set of 'large' initial data. Finally, it would be of some interest to establish asymptotic self-similarity of c_{μ_0} when μ_0 is supported on the class of 'large' initial data which look like the union of nematic 'islands' previously alluded to in the introduction of this chapter. We hope to investigate this problem in future work.

3.6 Closing Remarks

In this chapter, we have been able to obtain asymptotic information for $c_{\mu_0}(\cdot,t)$ in $L^\infty(\mathbb{R}^3)$ for μ_0 probing a rather restricted region of phase space H. Ideally, one would like to be able to decompose phase space $H = \cup_{j\in J} H_j$ in such a manner that given the knowledge $\operatorname{supp}\mu_0 \subseteq H_i \subset H$, one could find non-trivial $\Gamma_i : \mathbb{R}^3 \to \mathbb{R}$ and $L_i : (0,\infty) \to (0,\infty)$ such that

$$\lim_{t\to\infty} \left\| c_{\mu_0}(r,t) - \Gamma_i\left(\frac{|r|}{L_i(t)}\right) \right\|_{L^\infty(\mathbb{R}^3, dr)} = 0.$$

It is in this sense we hope to construct a *phase portrait* for c_{μ_0} on H in future work.

Chapter 4

Concluding Remarks

In this thesis, we have addressed two problems in the mathematical Q-tensor theory of nematic liquid crystals. There remains, however, much interesting work to be done. We have highlighted some of these problems at the end of chapters 2 and 3, which we hope to tackle in the future.

One problem that we find of particular interest, already mentioned at the beginning of chapter 1, relates to understanding how an evolution equation for the Q-tensor Q arises in a mathematically-rigorous manner from an underlying kinetic theory for a probability distribution function ϱ. Following the work on hydrodynamic limits of the Boltzmann equation due to Bardos, Golse and Levermore [10, 11], we hope to discern the possibility of obtaining an *analytic closure* for the hierarchy of orientational moments of ϱ, in contrast to the more commonly employed *algebraic closures*, such as the quadratic closure of Doi: see, for instance, Doi and Edwards [28].

Bibliography

[1] H. Abels, G. Dolzmann, and Y. Liu, *Private communication.*

[2] R. Adams and J. F. Fournier, *Sobolev spaces*, vol. 140, Elsevier/Academic Press, Amsterdam, 2003.

[3] D. G. Aronson and H. F. Weinberger, *Multidimensional nonlinear diffusion arising in population genetics*, Adv. in Math. **30** (1978), no. 1, 33–76. MR 511740 (80a:35013)

[4] J. M. Ball, *Défauts dans les cristaux et dans les cristaux liquides (Paris lecture slides)*, http://people.maths.ox.ac.uk/ball/Teaching/parisox.pdf.

[5] ———, *The mathematics of liquid crystals (Cambridge lecture slides)*, http://people.maths.ox.ac.uk/ball/Teaching/cambridge.pdf.

[6] ———, *Differentiability properties of symmetric and isotropic functions*, Duke Math. J. **51** (1984), 699–728.

[7] J. M. Ball and A. Majumdar, *Nematic liquid crystals: From Maier-Saupe to a continuum theory*, Mol. Cryst. Liq. Cryst. **525** (2010), 1–11.

[8] ———, *Passage from the mean-field Maier-Saupe to the continuum Landau-de Gennes theory for nematic liquid crystals*, Preprint (2012).

[9] V. Barbu, *Nonlinear differential equations of monotone types in Banach spaces*, Springer Monographs in Mathematics, Springer, New York, 2010. MR 2582280 (2011d:34001)

[10] C. Bardos, F. Golse, and D. Levermore, *Fluid dynamic limits of kinetic equations. I. Formal derivations*, J. Statist. Phys. **63** (1991), no. 1-2, 323–344.

[11] ———, *Fluid dynamic limits of kinetic equations. II. Convergence proofs for the Boltzmann equation*, Comm. Pure Appl. Math. **46** (1993), 667–753.

[12] A. Belleni-Morante and A. C. McBride, *Applied nonlinear semigroups*, Wiley Series in Mathematical Methods in Practice, vol. 3, John Wiley & Sons Ltd., 1998.

[13] A. N. Beris and B. J. Edwards, *Thermodynamics of flowing systems with internal microstructure*, vol. 36, Oxford University Press, 1994.

[14] F. Bethuel, H. Brezis, and F. Hélein, *Ginzburg-Landau vortices*, Progress in Nonlinear Differential Equations and their Applications, 13, Birkhäuser Boston Inc., Boston, MA, 1994. MR 1269538 (95c:58044)

[15] B. Bollobás, *Linear analysis*, 2nd ed. ed., Cambridge University Press, Cambridge, 1999. MR 1711398 (2000g:46001)

[16] A. J. Bray, *Theory of phase ordering kinetics*, Advances in Physics **51** (2002), 481–587.

[17] H. Brezis, *Opérateurs maximaux monotones et semi-groupes de contractions dans les espaces de Hilbert*, North-Holland Publishing Co., Amsterdam, 1973, North-Holland Mathematics Studies, No. 5. Notas de Matemática (50). MR 0348562 (50 #1060)

[18] B. Buffoni and J. Toland, *Analytic theory of global bifurcation*, Princeton Series in Applied Mathematics, Princeton University Press, Princeton, NJ, 2003, An introduction. MR 1956130 (2004b:47117)

[19] C. Cercignani, R. Illner, and M. Pulvirenti, *The mathematical theory of dilute gases*, Applied Mathematical Sciences, vol. 106, Springer-Verlag, 1994.

[20] S. Chandrasekhar, *Liquid crystals*, Cambridge University Press, 1993.

[21] H. J. Coles, *Laser and electric field induced birefringence studies on the cyanobiphenyl homologues*, Mol. Cryst. Liq. Cryst. **49** (1978), 67–74.

[22] P. Constantin, C. Foiaş, B. Nicolaenko, and R. Temam, *Integral manifolds and inertial manifolds for dissipative partial differential equations*, Applied Mathematical Sciences, vol. 70, Springer-Verlag, New York, 1989. MR 966192 (90a:35026)

[23] P. Constantin, A. Kiselev, L. Ryzhik, and A. Zlatoš, *Diffusion and mixing in fluid flow*, Ann. of Math. (2) **168** (2008), no. 2, 643–674. MR 2434887 (2009e:58045)

[24] P. G. De Gennes and J. Prost, *The physics of liquid crystals*, International Series of Monographs on Physics, vol. 83, Oxford University Press, 1993.

[25] C. Denniston, E. Orlandini, and J. M. Yeomans, *Lattice Boltzmann simulations of liquid crystal hydrodynamics*, Phys. Rev. E **63** (2000), 056702.

[26] ———, *Phase ordering in nematic liquid crystals*, Phys. Rev. E **64** (2001), 021701.

[27] C. Denniston, E. Orlandini, and J. M. Yeomans, *Phase ordering in nematic liquid crystals*, Phys. Rev. E **64** (2001), 021701.

[28] M. Doi and S. F. Edwards, *The theory of polymer dynamics*, vol. 73, Oxford University Press, 1988.

[29] R. M. Dudley, *Real analysis and probability*, Cambridge Studies in Advanced Mathematics, vol. 74, Cambridge University Press, Cambridge, 2002, Revised reprint of the 1989 original. MR 1932358 (2003h:60001)

[30] J. L. Ericksen, *Conservation laws for liquid crystals*, Trans. Soc. Rheology **5** (1961), 23–34.

[31] ———, *Continuum theory of liquid crystals of nematic type*, Mol. Cryst. **7** (1969), no. 1, 153–164.

[32] L. C. Evans, *Partial differential equations*, second ed., Graduate Studies in Mathematics, vol. 19, American Mathematical Society, Providence, RI, 2010. MR 2597943 (2011c:35002)

[33] I. Fatkullin and V. Slastikov, *On spatial variations of nematic ordering*, Phys. D **237** (2008), 2577–2586.

[34] ———, *Vortices in two-dimensional nematics*, Commun. Math. Sci. **7** (2009), no. 4, 917–938. MR 2604622 (2011f:82017)

[35] E. Feireisl, E. Rocca, G. Schimperna, and A. Zarnescu, *Evolution of non-isothermal Landau-de Gennes nematic liquid crystals flows with singular potential*, arXiv:1207.1643 (2012).

[36] C. Foiaş, *Solutions statistiques des équations d'évolutions non linéaires*, Problems in Non-Linear Analysis (C.I.M.E., IV Ciclo, Varenna, 1970), Edizioni Cremonese, Rome, 1971, pp. 129–188. MR 0287390 (44 #4596)

[37] C. Foias, O. Manley, R. Rosa, and R. Temam, *Navier-Stokes equations and turbulence*, Encyclopedia of Mathematics and its Applications, vol. 83, Cambridge University Press, Cambridge, 2001. MR 1855030 (2003a:76001)

[38] M. Frémond, *Non-smooth thermomechanics*, Springer-Verlag, Berlin and Heidelberg, 2002.

[39] A. W. Fursikov and M. I. Vishik, *Mathematical problems of statistical hydrodynamics*, Kluwer Academic Publisher, 1988.

[40] F. Golse, *The Boltzmann equation and its hydrodynamic limits*, Evolutionary equations. Vol. II, Handb. Differ. Equ., Elsevier/North-Holland, Amsterdam, 2005, pp. 159–301. MR 2182829 (2007e:35025)

[41] E. F. Gramsbergen, L. Longa, and W. H. de Jeu, *Landau theory of the nematic-isotropic phase transition*, Physics Reports **135** (1986), no. 4, 195–257.

[42] R. Hardt, D. Kinderlehrer, and F.-H. Lin, *Existence and partial regularity of static liquid crystal configurations*, Comm. Math. Phys. **105** (1986), no. 4, 547–570. MR 852090 (88a:35207)

[43] P. Hartman, *Ordinary differential equations*, Classics in Applied Mathematics, vol. 38, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2002, Corrected reprint of the second (1982) edition [Birkhäuser, Boston, MA; MR0658490 (83e:34002)], With a foreword by Peter Bates. MR 1929104 (2003h:34001)

[44] D. Henry, *Geometric theory of semilinear parabolic equations*, Lecture Notes in Mathematics, vol. 840, Springer-Verlag, 1981.

[45] D. Hilbert, *Theory of algebraic invariants*, Cambridge University Press, 1993.

[46] R. Ignat, L. Nguyen, V. Slastikov, and A. Zarnescu, *Stability of the vortex defect in the Landaude Gennes theory for nematic liquid crystals*, Comptes Rendus Mathematique (2013).

[47] G. Iyer, *A stochastic Lagrangian proof of global existence of the Navier-Stokes equations for flows with small Reynolds number*, Ann. Inst. H. Poincaré Anal. Non Linéaire **26** (2009), no. 1, 181–189. MR 2483818 (2010f:76022)

[48] G. Iyer, X. Xu, and A. Zarnescu, *Private communication.*

[49] J. Katriel, G. F. Kventsel, G. R. Luckhurst, and T. J. Sluckin, *Free energies in the Landau and molecular field approaches*, Liq. Cryst. **1** (1986), 337–355.

[50] E. Kirr, M. Wilkinson, and A. Zarnescu, *Dynamic statistical scaling in the Landau-de Gennes theory of nematic liquid crystals (submitted)*, arXiv:1211.4427.

[51] L. Landau and E. Lifschitz, *Statistical physics, volume 9*, Cambridge University Press, 1993.

[52] F. M. Leslie, *Some constitutive equations for liquid crystals*, Arch. Rational Mech. Anal. **28** (1968), 265–283.

[53] E. H. Lieb and M. Loss, *Analysis*, second ed., Graduate Studies in Mathematics, vol. 14, American Mathematical Society, Providence, RI, 2001. MR 1817225 (2001i:00001)

[54] F.-H. Lin and C. Liu, *Existence of solutions for the Ericksen-Leslie system*, Arch. Ration. Mech. Anal. **154** (2000), no. 2, 135–156. MR 1784963 (2003a:76014)

[55] F.-H. Lin, C. Liu, and P. Zhang, *On hydrodynamics of viscoelastic fluids*, Comm. Pure Appl. Math. **58** (2005), no. 11, 1437–1471. MR 2165379 (2006d:76005)

[56] F.-H. Lin and C. Wang, *The analysis of harmonic maps and their heat flows*, World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2008. MR 2431658 (2011a:58030)

[57] J.-L. Lions, *Quelques méthodes de résolution des problèmes aux limites non linéaires*, Dunod, 1969, pp. xx+554. MR 0259693 (41 #4326)

[58] L. Longa, D. Monselesan, and H.-R. Trebin, *An extension of the Landau-Ginzburg-de Gennes theory for liquid crystals*, Liq. Cryst. **2** (1987), no. 6, 769–796.

[59] A. Majumdar, *Equilibrium order parameters of nematic liquid crystals in the Landau-de Gennes theory*, European J. Appl. Math. **21** (2010), no. 2, 181–203. MR 2596543 (2011c:82077)

[60] ———, *The Landau-de Gennes theory of nematic liquid crystals: uniaxiality versus biaxiality*, Commun. Pure Appl. Anal. **11** (2012), 1303–1337.

[61] A. Majumdar and A. Zarnescu, *Landau-De Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond*, Arch. Ration. Mech. Anal. **196** (2010), no. 1, 227–280. MR 2601074 (2011g:82122)

[62] N. J. Mottram and C. Newton, *Introduction to Q-tensor theory*, University of Strathclyde, Department of Mathematics Research Report **10** (2004).

[63] L. Nguyen and A. Zarnescu, *Refined approximation for minimizers of a Landau-de Gennes energy functional*, Calc. Var. Partial Differential Equations **47** (2013), no. 1-2, 383–432. MR 3044143

[64] L. Onsager, *The effects of shape on the interaction of colloidal particles*, Annals of the New York Academy of Sciences **51** (1949), no. 4, 627–659.

[65] M. Paicu and A. Zarnescu, *Global existence and regularity for the full coupled Navier-Stokes and Q-tensor system*, SIAM J. Math. Anal. **43** (2011), no. 5, 2009–2049. MR 2837493 (2012m:35262)

[66] ———, *Energy dissipation and regularity for a coupled Navier-Stokes and Q-tensor system*, Arch. Ration. Mech. Anal. **203** (2012), no. 1, 45–67. MR 2864407 (2012m:76012)

[67] A. N. Pargellis, S. Green, and B. Yurke, *Planar XY-model dynamics in a nematic liquid crystal system*, Phys. Rev. E **49** (1994), 4250–4257.

[68] A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, Applied Mathematical Sciences, vol. 44, Springer-Verlag, New York, 1983. MR 710486 (85g:47061)

[69] P. Poláčik, *Threshold solutions and sharp transitions for nonautonomous parabolic equations on* $\mathbb{R}^N$, Arch. Ration. Mech. Anal. **199** (2011), no. 1, 69–97. MR 2754337 (2011m:35197)

[70] P. Pucci and J. Serrin, *The maximum principle*, Progress in Nonlinear Differential Equations and their Applications, 73, Birkhäuser Verlag, Basel, 2007. MR 2356201 (2008m:35001)

[71] T. Qian and P. Sheng, *Generalized hydrodynamic equations for nematic liquid crystals*, Phys. Rev. E **58** (1998), 7475–7485.

[72] J. C. Robinson, *Infinite-dimensional dynamical systems*, Cambridge Texts in Applied Mathematics, Cambridge University Press, Cambridge, 2001, An introduction to dissipative parabolic PDEs and the theory of global attractors. MR 1881888 (2003f:37001a)

[73] R. T. Rockafellar, *Convex analysis*, Princeton Landmarks in Mathematics, Princeton University Press, Princeton, NJ, 1997, Reprint of the 1970 original, Princeton Paperbacks. MR 1451876 (97m:49001)

[74] L. Saint-Raymond, *Hydrodynamic limits of the Boltzmann equation*, Lecture Notes in Mathematics, vol. 1971, Springer-Verlag, Berlin, 2009. MR 2683475 (2012f:82079)

[75] E. Sandier and S. Serfaty, *Vortices in the magnetic Ginzburg-Landau model*, Progress in Nonlinear Differential Equations and their Applications, 70, Birkhäuser Boston Inc., Boston, MA, 2007. MR 2279839 (2008g:82149)

[76] R. Schoen and K. Uhlenbeck, *A regularity theory for harmonic maps*, J. Differential Geom. **17** (1982), no. 2, 307–335. MR 664498 (84b:58037a)

[77] J. P. Sethna, *Statistical mechanics: Entropy, order parameters, and complexity*, Oxford Master Series in Statistical, Computational, and Theoretical Physics.

[78] R. E. Showalter, *Monotone operators in Banach space and nonlinear partial differential equations*, Mathematical Surveys and Monographs, vol. 49, American Mathematical Society, Providence, RI, 1997. MR 1422252 (98c:47076)

[79] A. M. Sonnet and E. G. Virga, *Dissipative ordered fluids*, Springer, 2012.

[80] I. W. Stewart, *The static and dynamic continuum theory of liquid crystals*, CRC Press, 2004.

[81] J. Taskinen, *Asymptotical behaviour of a class of semilinear diffusion equations*, J. Evol. Equ. **7** (2007), no. 3, 429–447. MR 2328933 (2008g:35104)

[82] R. Temam, *Navier-Stokes equations and nonlinear functional analysis*, second ed., CBMS-NSF Regional Conference Series in Applied Mathematics, vol. 66, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1995. MR 1318914 (96e:35136)

[83] G. Tóth, C. Denniston, and J. M. Yeomans, *Hydrodynamics of domain growth in nematic liquid crystals*, Phys. Rev. E **67** (2003), 051705.

[84] E. G. Virga, *Variational theories for liquid crystals*, Applied Mathematics and Mathematical Computation, vol. 8, Chapman & Hall, 1994.

[85] M. Wilkinson, *Strict physicality of global weak solutions of a Navier-Stokes Q-tensor system with singular potential*, arXiv:1211.6083 (2012).

[86] M. Zapotocky, P.M. Goldbart, and N. Goldenfeld, *Kinetics of phase ordering in uniaxial and biaxial nematic films*, Phys. Rev. E **51** (1995), 1216.

[87] A. Zarnescu, *Private communication.*

[88] ———, *Topics in the Q-tensor theory of liquid crystals*, Topics in mathematical modeling and analysis, Jindřich Nečas Cent. Math. Model. Lect. Notes, vol. 7, 2012, pp. 187–252.

[89] E. Zeidler, *Nonlinear functional analysis and its applications. I*, Springer-Verlag, New York, 1986, Fixed-point theorems, Translated from the German by Peter R. Wadsack. MR 816732 (87f:47083)