A Bifurcation Analysis of Models of Liquid Crystals

Michaela A. C. Vollmer
The Queen's College

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To my husband Sebastian, my daughter Jana-Elin and my son Jakob.

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Abstract

In this thesis we provide a deeper insight into the fundamental phase transition between isotropic and nematic states of liquid crystals. In particular, we focus on the problem of classifying all minimising states of the Onsager free-energy functional in three dimensions, a problem which has drawn a lot of attention since 1949. We study the bifurcation diagram of the Onsager free-energy functional for liquid crystals with orientation parameter on the sphere. In particular, we concentrate on the bifurcations from the isotropic solution for a general class of two-body interaction potentials including the Onsager kernel. Reformulating the problem as a non-linear eigenvalue problem for the kernel operator, we prove that spherical harmonics are the corresponding eigenfunctions and we present a direct relationship between the coefficients of the Taylor expansion of this class of interaction potentials and their eigenvalues. We find explicit expressions for all bifurcation points corresponding to bifurcations from the isotropic state of the Onsager free-energy functional equipped with the Onsager interaction potential. A substantial amount of our analysis is based on the use of spherical harmonics and a special algorithm for computing expansions of products of spherical harmonics in terms of spherical harmonics is presented. Using a Lyapunov-Schmidt reduction, we derive a bifurcation equation depending on five state variables. The dimension of this state space is further reduced to two dimensions by using the rotational symmetry of the problem and the invariant theory of groups. On the basis of these results, we show that the first bifurcation from the isotropic state of the Onsager interaction potential is a transcritical bifurcation and that the corresponding solution is uniaxial. In addition, we prove some global properties of the bifurcation diagram such as the fact that the trivial solution is the unique local minimiser if the bifurcation parameter is high, that it is not a local minimiser if the bifurcation parameter is small, the boundedness of all equilibria of the functional and that the bifurcation branches are either unbounded or that they meet another bifurcation branch.

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Chapter 1

Introduction

There are three classical states of matter: the solid, the liquid and the gas phase. A phase transition from one phase to another occurs, for example, by an increase of temperature leading to a gain of kinetic energy of the constituent particles in a material. The particles in a crystalline solid are in thermal motion while still strongly interacting with each other due to intermolecular forces. If the energy of the system has reached a particular threshold, these thermal motions give rise to breaks in the crystal structure and the particles start moving around in space while their intermolecular forces are still significant over the average distance between them. The resulting phase is called the liquid phase. Once the kinetic energy of the particles is so high that they cannot maintain strong intermolecular forces between them over an average distance, they expand into the whole volume that is available to them. This third state of matter is called the gas phase.

However, some materials, called liquid crystals, exhibit an intermediate state of matter between the solid and the liquid phase, hence the name liquid crystals. Such an intermediate state of matter is called a mesophase and occurs in a particular range of temperature and concentration. There are two types of liquid crystalline phases, thermotropic liquid crystals, which exhibit a phase transition when the temperature of the material is changed, and lyotropic liquid crystals whose transformation into another liquid crystalline phase depends on both a change in temperature and concentration. Liquid crystals flow like incompressible viscous liquids while retaining optical properties that are a characteristic of crystals [**?**].

An onset of the liquid crystal phase has been characterised in experiments by a cloudy appearance of the substance occurring at a first melting point before the material transforms into a liquid state of matter at a second higher melting point, called the clearing point. This observation has first been made in 1888 by F. Reinitzer and O. Lehmann who studied cholesteryl benzonate. Since then, thousands of liquid crystals have been discovered and their different characteristics have been studied.

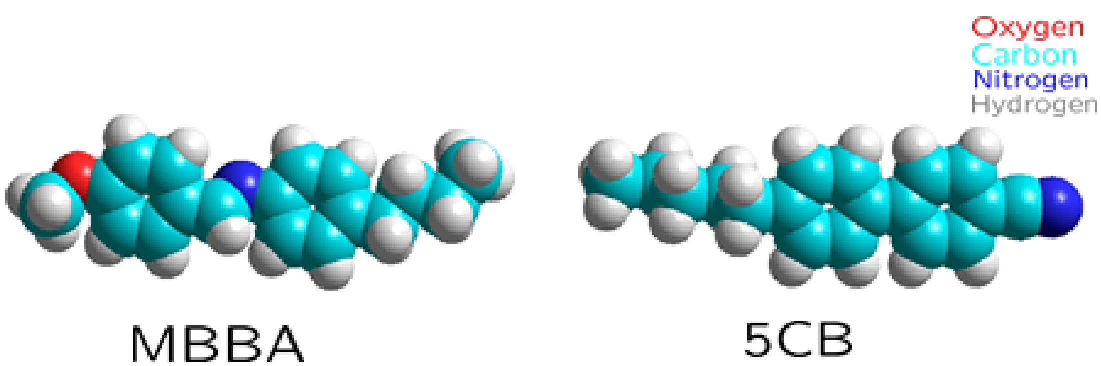


Figure 1.1: Schematic representation of two well-known liquid crystal molecules, the N-(4-Methoxybenzylidene)-4-butylaniline $C_{18}H_{21}NO$ (MBBA) and the 4-Cyano-4'-pentylbiphenyl $C_{18}H_{19}N$ (5CB) (by courtesy of Professor Claudio Zannoni).

The prototype of a molecule that can form a liquid crystalline phase exhibits a highly anisotropic structure which is often assumed to be ellipsoidal or rod-like. Two well-known liquid crystal components are the N-(4-Methoxybenzylidene)-4-butylaniline (MBBA) and the 4-Cyano-4'-pentylbiphenyl (5CB) molecules, see Figure 1.1. The MBBA is a nematic liquid crystal at room temperature and it undergoes a phase transition to an isotropic state at 43°C. The liquid crystal 5CB transforms from a crystalline state to a nematic state at 18°C and further to an isotropic state at 35°C [?].

On the basis of the different qualitative features of the molecules which form a liquid crystalline phase, we distinguish between three different categories of liquid crystals which are called nematic, cholesteric and smectic. A schematic representation of the three most important liquid crystalline phases for rod-like molecules with a statistical head-to-tail symmetry can be found in Figure 1.2. Mathematically, any physical state of matter of a material can be described by the behaviour of its constituent particles and therefore by their corresponding translational and orientational motion. The solid phase is a highly ordered phase in which the atoms form a crystal lattice. Hence their lattice vectors have similar orientations and their locations are following a very regular pattern across the material. In contrast, if the particles exhibit the liquid phase, both their centres of mass and their molecular orientation vectors are much more randomly distributed. Within the nematic phase of a liquid crystal, the molecules do not exhibit a long-range positional order while they induce a partial orientational order at a microscopic level. The particles are distributed in the space available to them meaning that

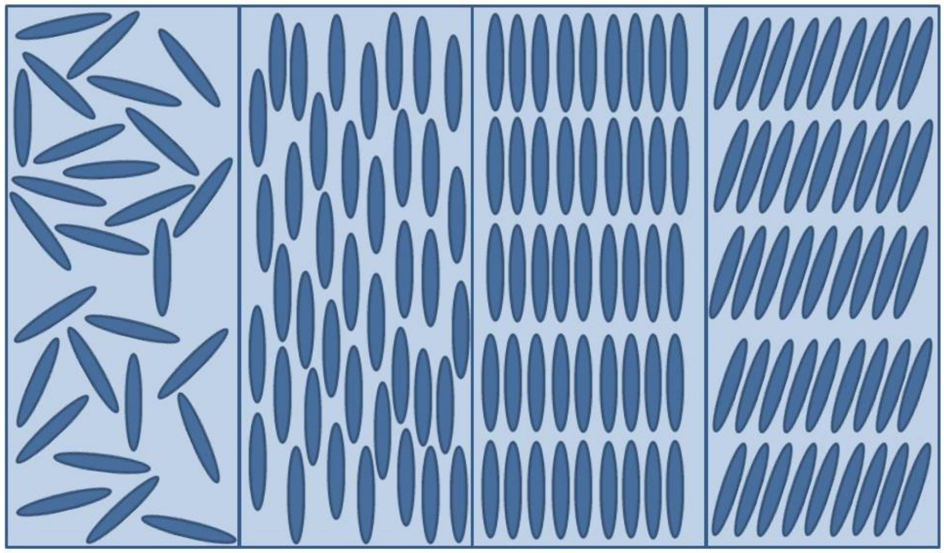


Figure 1.2: Schematic representation of molecular order in the liquid, nematic and smectic phases

their centres of mass are much more randomly distributed while their molecular axes are still approximately parallel. However, locally they exhibit some positional order due to the local packing of molecules, a correlation that is visualised by the radial distribution function [?]. Another liquid crystal phase, called the smectic phase, is characterised by an interplay of positional and orientational order. All molecules have roughly the same orientation and are locally approximately parallel to each other in different layers lying on top of each other.

A third phase of liquid crystals is the cholesteric phase. ln this phase all molecules are built up in helices which have either a left or right orientation. They

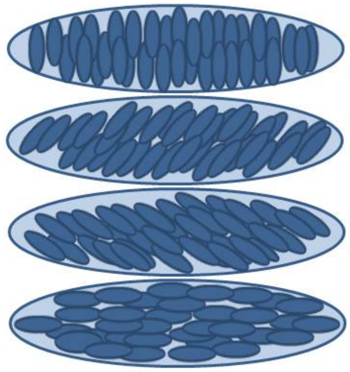


Figure 1.3: Schematic representation of a cholesteric phase

are twisted perpendicular to their intermolecular vector giving rise to a vertical periodicity with the period being equal to the length of a full rotation. The helical structure of a right oriented cholesteric liquid crystal is shown in Figure 1.3.

An important application of liquid crystals are liquid crystal displays which consist of two polarizing filters perpendicular to each other. Due to the orthogonality of the two filters, the light passing through the first polarizer is blocked by the second and no output occurs. However, if we fill the space between the filters with liquid crystal molecules, their orientation will align with the direction of the surface of the polarizer and thus they will form a helical structure which allows light to pass through the device. By an application of an external electric field, the orientation of the molecules can be influenced and a particular output on the screen can be achieved [**?**].

One of the major aims in the mathematical modelling of liquid crystals is to predict when a material undergoes a phase transition if either the temperature or the concentration in the solvent is changed. Because physical systems usually tend to the state of minimal free-energy, the problem turns mathematically into a minimization problem of the calculus of variations. The main mathematical ingredient is a probability density which describes the behaviour of the molecules. The particles considered throughout this thesis have cylindrical symmetry. It depends on the positional and orientational vector of each of its constituent particles, that is

$$x = (\underbrace{r_1, r_2, r_3}_{\text{position}}, \underbrace{p_1, p_2, p_3}_{\text{orientation}}) \quad \text{where } r \in \mathbb{R}^3 \text{ and } p \in \mathbb{S}^2.$$

The probability density $\rho : \mathbb{R}^3 \times \mathbb{S}^2 \to \mathbb{R}$ assigns to any point in the phase space (r, p) a probability stating how likely it is that there exists a particle whose configuration can be described by the pair (r, p). In the following discussion, we are interested in the prediction of the nematic phase, in which the particles admit an orientational but no significant positional order and therefore ρ will only depend on the orientation p of the molecules. Hence $\rho : \mathbb{S}^2 \to \mathbb{R}$.

1.1 The Onsager model for phase transitions

The isotropic-to-nematic phase transition of rod-like molecules is one of the most studied phenomena in the theory of liquid crystals. It is characterised by an onset of orientational order when either the concentration of molecules is increased or the temperature of the system is decreased. The first model describing such a phase transition was introduced by Onsager in 1949 [?]. Let $\rho : \mathbb{S}^2 \to \mathbb{R}$ be a probability density function characterising the orientation of the molecules, that is

$$\rho(p) \geq 0 \quad \text{for all } p \in \mathbb{S}^2 \qquad \text{and} \qquad \int_{\mathbb{S}^2} \rho(p)\, dp = 1. \tag{1.1}$$

Using a second virial approximation, Onsager derived an expression for the Helmholtz free-energy per molecule which is given as a sum of an entropy term and a second term modelling the two-body interactions

$$\mathcal{F}(\rho) := \epsilon_0 \int_{\mathbb{S}^2} \left(\lambda \rho(p) \ln(\rho(p)) + \frac{1}{2} U(\rho)(p)\rho(p) \right) \, dp. \tag{1.2}$$

The parameter λ, which appears in the entropy term, incorporates the thermal or athermal effects between the molecules. In this thesis, we assume that $\lambda \sim k_B \frac{T}{c}$ where T denotes the temperature and c the concentration. The parameter ϵ_0 has been introduced in order to keep the Onsager free-energy functional dimensionless. The operator $U : L^1(\mathbb{S}^2) \to L^\infty(\mathbb{S}^2)$

$$U(\rho)(p) := \int_{\mathbb{S}^2} K(p, q)\rho(q)\, dq \tag{1.3}$$

is called the interaction operator. It depends on the interaction kernel $K(\cdot, \cdot) : \mathbb{S}^2 \times \mathbb{S}^2 \to \mathbb{R}$ which models the two-body interactions between any two hard core molecules. Based on the assumptions we impose on the characteristics of the interactions, different types of interaction kernels arise. One of the first interaction kernels that has been derived is the so called Onsager kernel

$$K_O(p,q) = |p \times q| = \sqrt{1-(p\cdot q)^2}. \tag{1.4}$$

It describes the excluded volume effect given by the repulsive interactions between any two slender polymer rods in the system. The excluded volume is the volume which is inaccessible to a particle due to the presence of another particle in the system [?]. Even though the Onsager kernel admits a relatively simple form, the equilibria of the energy functional in (1.2) cannot be computed explicitly due to the singularity of this particular interaction potential. Subsequently, other theories and interaction kernels have been formulated and considered. One of the most popular interaction kernels is the Maier-Saupe potential [?]

$$K_{\mathrm{MS}}(p,q) = \frac{1}{3} - (p\cdot q)^2. \tag{1.5}$$

It is based on a mean-field approach to dispersion forces, attractive interactions between non-polar molecules. A third well-known intermolecular potential is the dipolar potential for polar molecules

$$K_d(p,q) = -p\cdot q. \tag{1.6}$$

Most of the mathematical analysis has so far been focussed on the Maier-Saupe and the dipolar potential, the main reason being that the Onsager potential is not differentiable because of its 'cusp' singularity at zero.

1.2 Bifurcation theory

In this thesis we show that for large values of λ the unique minimiser of the Onsager free-energy functional is given by the uniform probability density $\rho_0 = \frac{1}{4\pi}$. However, as λ decreases, new minimisers may form. In mathematical terms such a phenomenon is called bifurcation. Bifurcations can usually be described as

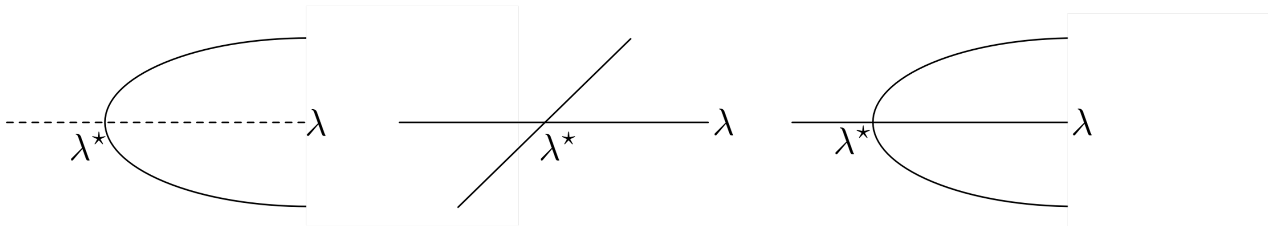


Figure 1.4: Schematic representation of the number of distinct solutions varying with respect to a change of the parameter λ. The graphics show a saddle node (left), a transcritical (middle) and a pitchfork (right) bifurcation.

either occurring as local or global bifurcations. The former can be analysed by an investigation of the local stability properties of all critical points when the bifurcation parameter crosses a critical threshold. In contrast, global bifurcations are not associated with the stability properties of the critical points. Therefore they include bifurcations that appear out of nowhere and are not arising from already existing solutions [?]. The three basic types of local bifurcations are called saddle-node, transcritical and pitchfork bifurcation and are illustrated in Figure 1.4. A saddle-node bifurcation is a bifurcation in which two equilibria exist which collide in one point. Hence if $\lambda \leq \lambda^\star$, then there exists only one equilibrium, if $\lambda > \lambda^\star$, then there exist two equilibria, one of which is stable, the other one is unstable. In case of a transcritical bifurcation there exist two fixed points for all values of λ except for $\lambda = \lambda^\star$ when there is only one. The two branches interchange stability at $\lambda^\star$. A pitchfork bifurcation is a local bifurcation in which three equilibria emerge at $\lambda^\star$. The purpose of local bifurcation theory is to study the qualitative changes of the characteristics of a parameter dependent family of equations when the parameter value is changed. In particular, we are interested in the number of equilibria of the Onsager free-energy functional when the parameter λ, which models both the athermal and thermal effects, is changed. Classically, its equilibria can be computed by solving the corresponding Euler-Lagrange equation

$$E(\rho, \lambda)(p) = 0.$$

We know that this equation has locally a unique solution branch if the implicit function theorem applies. Vice versa multiple solutions may exist if the implicit function theorem fails to apply at a particular point (ρ, λ). Hence the implicit function theorem will be at the centre of our analysis in order to find the local bifurcation structure of the Onsager free-energy functional.

1.3 Literature review

The equilibrium states of the free-energy functional above equipped with the Maier-Saupe kernel in (1.5) have been studied extensively in the past. Among the first researchers who became interested in this problem was Freiser [**?**], who extended the Maier-Saupe interaction potential to the case of asymmetric molecules. He proved both the existence of a first-order phase transition to a nematic state and a second-order phase transition to a biaxial state. Constantin, Kevrekidis and Titi [?] established the equivalence of the equilibrium states of the Onsager functional with the Maier-Saupe potential in three dimensions to the solutions of a transcendental matrix equation, and thus derived the high concentration asymptotics in terms of the eigenvalues of this particular matrix. A complete classification of the equilibrium states in three dimensions has been provided independendly by Fatkullin and Slastikov [?] and by Liu, Zhang and Zhang [?]. Using the properties of spherical harmonics, both groups derived explicit formulae for all critical points and proved their axial symmetry. Similarly, Fatkullin and Slastikov also obtained results for the dipolar interaction potential in (1.6).

One of the first approaches to the original problem involving the Onsager kernel in (1.4) has been undertaken by Kayser and Raveché [?]. By reformulating the problem as an eigenvalue problem, they derive an iterative scheme that allows them to compute all axially symmetric equilibria of the functional. Using the Fourier coefficients of the Onsager potential in two dimensions, Wang and Zhou [?, ?] showed that there exist in fact infinitely many bifurcation branches with different symmetries. Revisiting the same question, Chen, Li and Wang [?] also proved that all solutions are axially symmetric in 2D. For a class of interaction potentials involving only a finite number of Fourier modes, Lucia and Vukadinovic [?] verified the existence of continuous branches in two dimensions and they characterised the structure of the bifurcation diagram in terms of the size of the spectral gaps of the interaction operator. A very recent approach to the same problem has also been undertaken by Niksirat and Yu [?] who obtained the local bifurcation structure of all equilibrium states in two dimensions and the uniqueness of the trivial solution if the bifurcation parameter is large.

1.4 Outline of this thesis

Chapter 2 - The Onsager free-energy functional. The purpose of this chapter is to set up the foundational framework to which we will refer to in the remaining parts of this thesis. We will step back for a moment and review the Onsager free-energy functional based on ideas in statistical mechanics. Having obtained an explicit expression for the Helmholtz free-energy functional, we are then in a position to concentrate on the two most famous two-body interaction potentials, the Maier-Saupe interaction potential and the Onsager interaction potential. While the former is based on a mean-field approach to the problem where all interactions of the molecules are viewed as a single effect acting on every single particle, the latter is based on the purely repulsive interactions between the particles. In order to complete the picture, we conclude this chapter by a very brief introduction to the dipolar interaction potential which models materials with a dipole moment.

Chapter 3 - Existence and boundedness of minimisers of the three-dimensional Onsager model. Before beginning with our bifurcation analysis of the Onsager free-energy functional, we prove the existence of minimisers using the direct method of the calculus of variations. Moreover, we show that every minimiser is in fact bounded from below and above, while the lower bound is in fact positive. These facts let us reduce the state space of the problem to the Hilbert space $L^2(\mathbb{S}^2)$ which will be essential for our forthcoming analysis.

Chapter 4 - A complete description of all bifurcation points of the Onsager free-energy functional. The problem of classifying all critical points of the Onsager free-energy functional with the Onsager interaction kernel in three dimensions has not yet been addressed. The Euler-Lagrange equation corresponding to the Onsager free-energy functional is given by

$$E(\phi, \lambda) = \lambda\phi(p) - \frac{1}{Z(\phi)}\int_{\mathbb{S}^2} k(p \cdot q)\exp(-\phi(q))dq$$

where $\phi \in H^2(\mathbb{S}^2)$ denotes the thermodynamical potential associated to the probability distribution ρ. In this chapter, we rewrite the problem as an eigenvalue problem for the interaction operator U and we solve it for all eigenvalues. In particular, we are interested in all non-zero solutions (η, λ) of

$$\int_{\mathbb{S}^2} k(p \cdot q)\eta(q)dq = -4\pi\lambda\eta(p)$$

and therefore in the nullspace of the operator $\mathcal{L}_\lambda := \int_{\mathbb{S}^2} k(p \cdot q)\eta(q)dq$. Writing an interaction kernel $k(\cdot)$ as a series of spherical harmonics, we find a method to compute its eigenvalues. On the basis of this result, we obtain a complete set of all bifurcation points corresponding to bifurcations of the Onsager free-energy functional from the isotropic state. In particular, we prove the following statement.

Theorem 1.1 (Bifurcation points of the Onsager free-energy functional). *Let the Onsager free-energy functional $\mathcal{F}$ in (1.2) be equipped with the Onsager kernel $K_O(p,q) = \sqrt{1-(p\cdot q)^2}$. Then all local bifurcations from the trivial solution occur at the bifurcation points*

$$\lambda_l = \frac{\Gamma(l/2+\frac{1}{2})\Gamma(l/2-1/2)}{8\Gamma(l/2+1)\Gamma(l/2+2)}$$

where $l \in 2\mathbb{N}$. Moreover, the corresponding eigenfunctions of the Onsager interaction operator

$$U(\rho) = \int_{\mathbb{S}^2} k(p\cdot q)\rho(q)dq$$

are given by the spherical harmonics Y_l^m of even degree.

Chapter 5 - Bifurcations of the three-dimensional Onsager model. Having found explicit expressions for all bifurcation points, we derive the bifurcation equation of the bifurcation point corresponding to the first phase transition occurring at the biggest value of λ. In Section 6.3.2, we prove the existence of a transcritical bifurcation. Our results about the local bifurcation structure of the Onsager free-energy functional are summarised in the following theorem.

Theorem 1.2 (Local bifurcations of the Onsager free-energy functional). *Let the Onsager free-energy functional $\mathcal{F}$ in (1.2) be equipped with the Onsager kernel $K_O(p,q) = \sqrt{1-(p\cdot q)^2}$. Then a transcritical bifurcation from the trivial solution*

$\rho = \frac{1}{4\pi}$ *occurs locally at the bifurcation point*

$$\lambda_\star = \frac{\pi}{32}$$

(up to rotational symmetry).

The proof of this theorem consists of two crucial steps. The derivation of the bifurcation equation up to sufficiently high order and the exploitation of the symmetry properties inherent to the problem - we will concentrate on this second step of the proof in Chapter 6.

We restrict our attention to bifurcations of the Euler-Lagrange equation of the Onsager free-energy functional from the isotropic state $\rho = \frac{1}{4\pi}$ equipped with the Onsager kernel. However, our approach is generally applicable to any physical two-body interaction potential that satisfies the following assumptions.

Assumption 1.3. *The interaction potential* $K(\cdot,\cdot) : \mathbb{S}^2 \times \mathbb{S}^2 \to \mathbb{R}$ *satisfies*

(a) $K(\cdot,\cdot)$ *is continuous in both variables;*

(b) $K(\cdot,\cdot)$ *is rotationally symmetric, that is* $K(p,q) = K(Rq,Rp)$ *for all* $R \in SO(3)$ *and* $p, q \in \mathbb{S}^2$.

An important consequence of rotational symmetry is the following proposition which is based on the basic representation theorem of simultaneous invariants of vectors due to Cauchy.

Proposition 1.4. [?, page 29] *The interaction potential is rotationally symmetric* *if and only if it can be written as a function of a scalar* $K(p, q) = k(p \cdot q)$ *where* $k : \mathbb{R} \to \mathbb{R}$.

Remark 1.5. *Within this thesis, we use the notations* $K(p, q)$ *and* $k(p \cdot q)$ *interchangeably to denote the interaction kernel of interest.*

Remark 1.6. *Notice that by Proposition 1.4, rotational symmetry implies the symmetry of the interaction kernel.*

The particular combination of methods that we are using in this chapter and in Chapter 6 allows us a derivation of an expansion of the bifurcation equation which can be repeated equivalently for any other kernel, see Remark 5.6 for more details. Hence a characterisation of the local bifurcation can be achieved for many other cases by following an adaptation of the steps presented in this thesis.

Other well-known kernels such as the dipolar and the Maier-Saupe kernel have been considered by [**?**]. However, they also fit into this framework as outlined in Remark 4.9.

Similar results about the local bifurcation structure of the Onsager free-energy functional with interaction potential satisfying Assumption 1.3 can also be found in the unpublished thesis of Jakob Wachsmuth [**?**], which was only drawn to the attention of the author after completion of our work on the bifurcation structure of the Onsager free-energy functional. The major differences between his and our work have been outlined in Appendix C.

Chapter 6 - Solutions of the bifurcation equation of the Onsager free-energy functional. Having derived the bifurcation equation for the Onsager free-energy functional equipped with the Onsager kernel in Chapter 5, we reduced the initial problem from an infinite state space to a system of five equations with six variables. However, this system is still too complicated to solve so we will reduce the dimension of its state space further by using the symmetry properties inherent to the problem. In particular, due to the rotational symmetry of the kernel and thus of the Onsager free-energy functional, we identify any two solutions if they are related by an application of a rotation. This problem is equivalent to finding the representatives of the orbit space of the group action $SO(3)$ acting on $\mathbb{R}^5$ which is the space of solutions to the bifurcation equation. In particular, we find a representation of this group action and we derive two invariant polynomials associated to it which separate its orbit, that means that two solutions a and b can be mapped onto each other by an application of a rotation in $SO(3)$ if and only if

$$(I_1(a), I_2(a)) = (I_1(b), I_2(b))$$

where I_1 and I_2 denote the two invariant polynomials. We will show that there exists a two-dimensional set $\mathcal{S}$ for which the images of I_1 and I_2 are surjective and that it is therefore sufficient to consider only the two-dimensional set $\mathcal{S}$ as state space for possible solutions to the bifurcation equation.

This approach involving invariant theory for groups is generally applicable to bifurcation problems for functions defined on the sphere and is of interest on its own, for details see Sections 6.2.

The final part of this chapter is to solve the reduced two-dimensional bifurcation equation by identifying the equivalent recognition problem which can then be solved. In particular, we find non-degeneracy conditions which will ensure the one-to-one correspondence between solutions of the two-dimensional bifurcation equation and an algebraic equation of simple form of lower order. Based on these results we will finalise our bifurcation analysis by concluding that there exists a transcritical bifurcation up to rotations from the isotropic solution.

Chapter 7 - Other properties of the bifurcation diagram. Chapter 7 is devoted to a brief analysis of some additional local and global properties of the bifurcation diagram. First of all, we prove the local uniaxiality of all solutions corresponding to the first bifurcation branch which has been shown to admit a transcritical bifurcation in the Chapters 5 and 6. This result has already been of interest to many experts in the field. Moreover, we show the uniqueness of the trivial solution as local minimiser if the bifurcation parameter is high and the continuity of all bifurcation branches. These results are summarised in the following theorem.

Theorem 1.7 (Bifurcations of the Onsager free-energy functional)**.** *Let $K(\cdot,\cdot) : \mathbb{S}^2 \times \mathbb{S}^2 \to \mathbb{R}$ be an interaction kernel satisfying Assumption 1.3. Then*

- *all solutions corresponding to the transcritical bifurcation branch found in Section 6.3.2 are locally uniaxial;*
- *the uniform distribution $\rho_0(p) = \frac{1}{4\pi}$ is a critical point for all values of λ. In*

particular, if λ is such that

$$8\pi M \exp\left(\frac{16M}{\lambda}\right) \leq \lambda$$

where $M = \max_{p,q\in\mathbb{S}^2} K(p,q)$, then the uniform distribution is in fact the unique solution of the Onsager free-energy functional in three dimensions;

- *the trivial solution $\rho = \frac{1}{4\pi}$ is a local minimiser for all $\lambda > \frac{\pi}{32}$ and it is not a local minimiser for $\lambda < \frac{\pi}{32}$;*
- *all bifurcation branches either meet infinity or they meet another bifurcation branch.*

Chapter 8 - Conclusion. In the final chapter of this thesis, we summarise our results about the bifurcation diagram of the Onsager free-energy functional with physical interaction operator. These results are also summarised in Figure 1.5 and they have been published by the Archive for Rational Mechanics and Analysis [**?**].

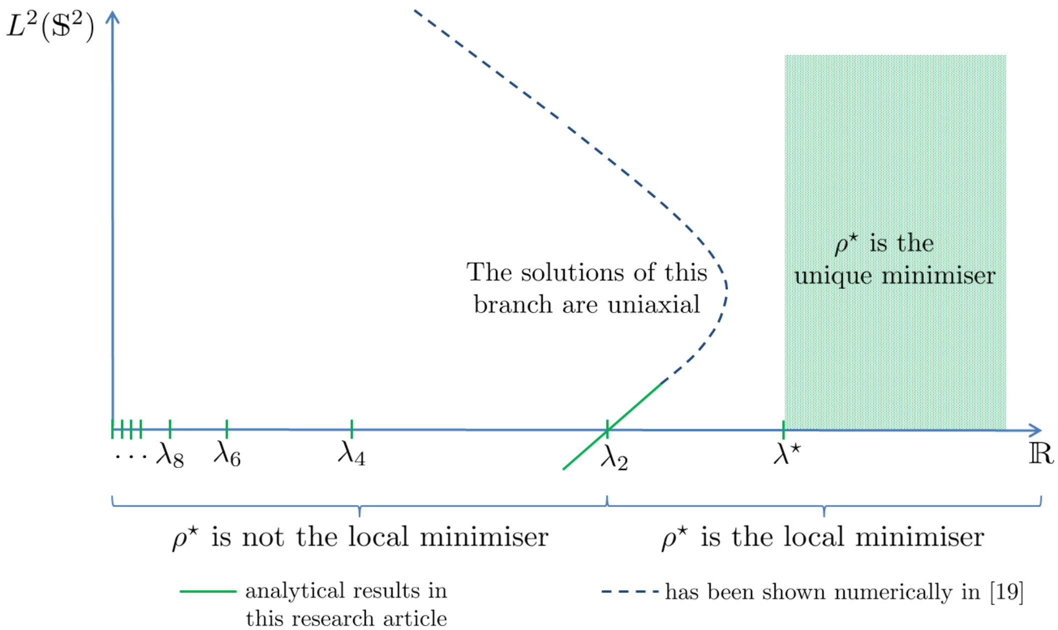


Figure 1.5: Summary of our results

CHAPTER 2

The Onsager free-energy functional

The following review of the Onsager free-energy functional with Maier-Saupe and Onsager interaction potential goes back to [?] and [?]. We consider a dynamical system with N identical particles, each with generalised coordinates $q_i \in \mathcal{Q}$ and conjugate momenta $p_i \in \mathbb{R}$. We denote the combined locations and momenta by (p, q). The corresponding Hamiltonian function is given by

$$\mathcal{H}(q,p) := \mathcal{K}(p) + \mathcal{U}(q)$$

where $\mathcal{K}$ denotes the total kinetic energy of the system and $\mathcal{U}$ its potential energy. We can write the equations of time evolution of the system as

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p} \text{ and } \dot{p} = -\frac{\partial \mathcal{H}}{\partial q}.$$

The phase space corresponding to this system of equations is given by $\mathcal{Q}^{3N} \times \mathbb{R}^{3N} \subset \mathbb{R}^{6N}$, hence the space of all possible states is $6N$-dimensional. In order to consider all such states differing in their initial conditions, we are looking at many virtual copies of the same system which is called an ensemble. The distribution of such an ensemble of systems with a fixed number of particles is described by the probability distribution ρ which is given by

$$\rho(p, q) = \frac{1}{Z} e^{-\frac{1}{k_B T} \mathcal{H}(p,q)} \tag{2.1}$$

where

$$Z = \int_{\mathbb{R}^n \times \Omega} e^{-\frac{1}{k_B T} \mathcal{H}(p,q)} dp dq,$$

k_B denotes the Boltzmann constant and T the absolute temperature.

In thermodynamics, the Helmholtz free-energy is a thermodynamic potential which describes the amount of useful work contained in the system

$$\mathcal{F} = E - TS$$

where E is the average total energy of the system, T is the absolute temperature and S the entropy. At constant temperature and volume, the Helmholtz free-energy is a minimum at equilibrium because of the first and second laws of thermodynamics.

We rewrite Z as configurational quantity by integrating out the momenta component of $\mathcal{H}$. This is in fact equivalent to extracting a factor out of Z which in turn affects $\mathcal{F}$ only by an additive constant does not change minimisers. Overall, we obtain the following system of equations

$$Z_N := \frac{1}{N!} \int_{\mathcal{Q}^N} e^{-\frac{1}{k_B T} \mathcal{U}(q)} dq \text{ and } F_N := -k_B T \ln Z_N.$$

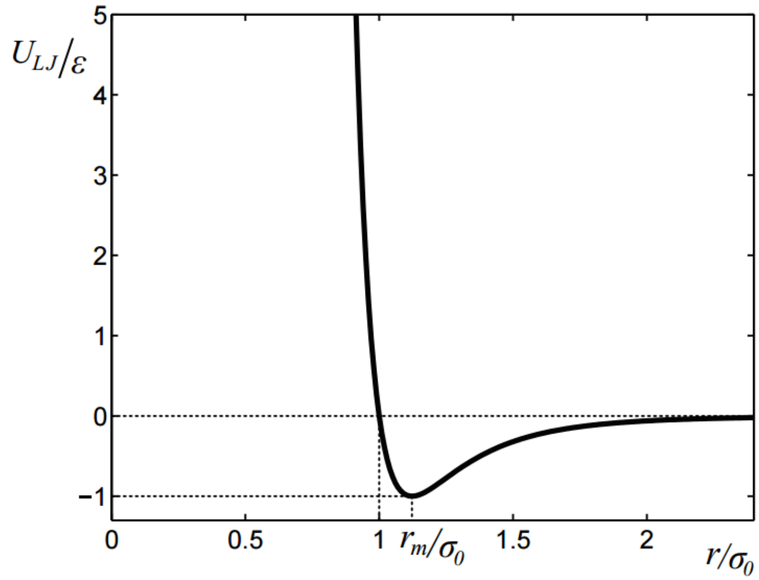


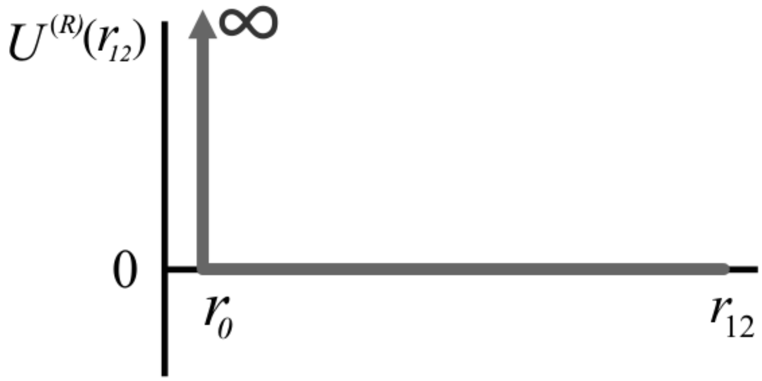
Figure 2.1: A schematic graph of the Lennard-Jones potential, one of the most popular two-body interaction potentials [?].

We now consider only the two-body interactions between the particles

$$\mathcal{U}(q) = \frac{1}{2}\sum_{i\neq j=1}^{N} U(q_i, q_j)$$

with $U(q_i, q_j) = U(q_j, q_i)$. These can be split into two different types of interactions, the slowly varying, long-range potentials and the rapidly varying, short range potentials. The former accounts for the attraction between particles and is called the soft component of U denoted by $U^{(A)}$ while the latter accounts for the repulsion between particles and is called the hard component of U which we denote by $U^{(R)}$. It follows that U can in general be decomposed as

$$U(q_i, q_j) = U^{(A)}(q_i, q_j) + U^{(R)}(q_i, q_j).$$



$$\Phi_{12}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \begin{cases} 0 & r_{12} > r_0 \\ -1 & r_{12} < r_0 \end{cases}$$

Figure 2.2: A schematic graph of the repulsive component of U in the idealised case [**?**].

The component $U^{(R)}$ is diverging abruptly when the particles are very close to each other. For definiteness, we assume that $U^{(R)}$ is arbitrarily close to zero when the interacting particles are not in contact and that it diverges to $+\infty$ when they touch (see Figure 2.2).

Taking all these assumptions into account, we can rewrite the Helmholtz free-energy as

$$\begin{aligned} \mathcal{F} = -\, k_B T \ln \Bigg(\frac{1}{N!} \int_{\Omega^N} & e^{-\frac{1}{2}\frac{1}{k_B T}\sum_{j=2}^{N} U^{(A)}(q_1, q_j)}\, dq_1 \times \dots \\ & \times e^{-\frac{1}{2}\frac{1}{k_B T}\sum_{j=1}^{N-1} U^{(A)}(q_N, q_j)}\, dq_N \Bigg). \end{aligned}$$

This expression can equivalently be written as

$$\mathcal{F} = -k_B T \ln \frac{1}{N!} \prod_{l=1}^{N} \int_{\mathcal{Q}^N} I_l dq_l \tag{2.2}$$

where

$$I_l := \exp\left(-\frac{1}{2} \frac{1}{k_B T} \sum_{j \neq l = 1}^{N} U^{(R)}(q_l, q_j) \right) \exp\left(-\frac{1}{2} \frac{1}{k_B T} \sum_{j=1, j \neq l}^{N} U^{(A)}(q_l, q_j) \right).$$

In general, there are two approaches to tackle this elaborate expression, one of which is a mean-field approximation which leads to the very successful Maier-Saupe interaction potential. The second approach has been chosen by Onsager himself in 1949 and is based on an excluded volume effect for rod-like molecules. The corresponding interaction potential has been named after him.

2.1 The mean-field approach

In 1958, Maier and Saupe's approach to tackle the expression in (2.2) was to concentrate only on attractive interactions $U^{(A)}$ while ignoring the repulsive part of the potential, that is

$$U^R(q_i, q_j) = 0 \text{ for all } i, j \in \mathbb{N}.$$

This approach leads to the Helmholtz free-energy

$$
\begin{aligned}
F_N = &- k_B T \ln \frac{1}{N!} \int_{\mathcal{Q}^N} \left(e^{-\frac{1}{2}\frac{1}{k_B T}\sum_{j=2}^{N} U^{(A)}(q_1,q_j)} \right) dq_1 \times \dots \\
&\qquad\qquad \times \left(e^{-\frac{1}{2}\frac{1}{k_B T}\sum_{j=1}^{N-1} U^{(A)}(q_N,q_j)} \right) dq_N \\
= &- k_B T \ln \frac{1}{N!} \int_{\mathcal{Q}^N} \prod_{l=1} I_l^{(A)} dq_1 \dots dq_N
\end{aligned}
$$

where

$$
I_l^{(A)} = \exp\left(-\frac{1}{2}\frac{1}{k_B T} \sum_{j=1, j\neq l}^{N} U^{(A)}(q_l, q_j) \right).
$$

The idea of Maier and Saupe was to apply a mean-field approach. That means that the individual interactions between all particles are viewed as interactions by a single effective particle. Hence the complicated expression above, which depends on N particles, is replaced by an approximative effective field that applies to every single one of them

$$
\frac{1}{2} \sum_{j=1, j\neq h}^{N} U^{(A)}(q_h, q_j) \approx \mathcal{E}(q_h).
$$

Thus, the mean-field free-energy is given by

$$
F_N^{mf} \approx -k_B T \ln \frac{1}{N!} \left(\int_{\mathcal{Q}} e^{-\frac{1}{k_B T}\mathcal{E}(q)} dq \right)^N .
$$

Within the canonical ensemble, we are now interested in rewriting the mean-field free energy as functional in terms of the probability distribution ρ in (2.1). Let

$f := \mathcal{Q} \mapsto \mathbb{R}^+$ denote the number density, that is

$$\int_{\mathcal{Q}} f(q)dq = N \text{ while } \rho(q) = \frac{f(q)}{N},$$

then we can rewrite the effective potential as

$$\mathcal{E}(p) := \int_{\mathcal{Q}} f(q)U^{(A)}(q,p)dq - \frac{1}{2}\int_{P} f(p)\int_{Q} f(q)U^{(A}(q,p)dqdp. \tag{2.3}$$

Let $\{\mathcal{Q}_i\}_{i=1}^{M}$ be a partition of $\mathcal{Q}$ into subsystems, each of which consists of N_i particles and whose cores are denoted by q_i. Further, let Δq_i be the measure of $\mathcal{Q}_i$ and

$$f_i := f(q_i)$$

be the discretisation of f with

$$N_i = f_i \Delta q_i \text{ and } \sum_{i=1}^{M} N_i = N.$$

Based on these definitions, the energy of each subsystem is given by

$$F_{N_i}^{(mf)} = -k_B T \ln \frac{1}{N_i!}\left(\int_{\mathcal{Q}_i} e^{-\frac{1}{k_B T}\mathcal{E}(q)}dq\right)^{N_i}$$

and thus the overall free-energy of all subsystems is

$$\begin{aligned} F_N^{(mf)} &= \sum_{i=1}^{M} F_{N_i}^{(mf)} \\ &= -\, k_B T \sum_{i=1}^{M} \ln \frac{1}{N_i!} \left(\frac{N_i}{f_i} e^{-\frac{1}{k_B T}\mathcal{E}^{(i)}(q)} \right)^{N_i} \end{aligned}$$

where $\mathcal{E}^i := \mathcal{E}(q_i)$. Using Stirling's approximation

$$\ln \left(\frac{1}{N-i!} N_i^{N_i} \right) \approx N_i$$

yields an expression of the mean-field energy

$$F_N^{(mf)} \approx -k_B T \sum_{i=1}^{M} N_i \left(\ln \frac{1}{f_i} - \frac{\mathcal{E}^{(i)}}{k_B T} \right) - k_B T N.$$

Dropping the last term because it is a constant and letting $N \to \infty$, we obtain the free-energy functional depending on the number density f

$$\mathcal{F}(f) := k_B T \int_{\mathcal{Q}} f(q) \ln f(q) dq + \frac{1}{2} \int_{\mathcal{Q}^2} U^{(A)}(q, q') f(q) f(q') dq dq'.$$

In order to obtain a meaningful free-energy functional, one needs to make assumptions on the type of long-range attractive interactions between the particles. The approach that has been undertaken by Maier and Saupe in 1959 was to derive an expression for $U^{(A)}$ based on London dispersion forces between non-polar molecules. The basic principle behind the London dispersion forces is that even though we assume that liquid crystal molecules do not have a permanent dipole, the interactions between all particles induce a dipole in the system. On average this dipole vanishes. However, the average energy induced by it does not. Based on these assumptions, Maier and Saupe defined $U^{(A)}$ as

$$U^{(A)}(q_i, q_j) := \begin{cases} U_{\text{disp}} & \text{if } r \geq R \\ 0 & \text{if } r < R \end{cases}$$

where U_{disp} denotes the London dispersion forces and r denotes the distance between the particles q and q'. In their celebrated paper from 1959 [**?**], Maier and Saupe impose further assumptions on the model in order to find an explicit expression for $U^{(A)}$. In fact they show that

$$U^{(A)}(q, q') = Ck_{\text{MS}}(q, q') = C\left(\frac{1}{3} - (q \cdot q')^2\right)$$

where C is a constant.

2.2 The Onsager interaction potential

In his enthusiastically received paper from 1949, Onsager presented an interaction potential which is only based on purely repulsive interactions between the particles. In particular,

$$U^{(A)}(q_i, q_j) = 0 \text{ for all } i, j \in \mathbb{N}$$

and thus the Helmholtz free-energy is given by

$$\mathcal{F} = -k_B T \ln \left(\frac{1}{N!} \int_{\Omega^N} e^{-\frac{1}{k_B T}\mathcal{U}^{(R)}(q)} dq_1 \dots dq_N \right)$$

where $\mathcal{U}^R$ denotes the repulsive part of all two body interactions of $\mathcal{U}(q) := \sum_{i<j}^N U(q_i, q_j)$. In case of the hard repulsive potential $\mathcal{U}^{(R)}$, we may now rewrite this expression in terms of Mayer functions, that is

$$e^{-\frac{1}{2k_B T}U^{(R)}(q_i,q_j)} = 1 + \Phi_{ij}$$

where

$$\Phi_{ij} = \begin{cases} 0 & \text{if the particles } i \text{ and } j \text{ are not in contact} \\ -1 & \text{if the particles } i \text{ and } j \text{ overlap} \end{cases} \tag{2.4}$$

(see Figure 2.2). It follows that the Helmholtz free-energy is given by

$$F = -k_B T \ln \left(\frac{1}{N!} \int_{\Omega^N} \prod_{i<j}^N (1 + \Phi_{ij}) dq_1 \dots dq_N \right).$$

Expanding this product yields

$$e^{-\frac{1}{k_B T}\mathcal{U}^{(R)}(q)} = \prod_{i<j}^N (1 + \Phi_{ij}) = 1 + \sum_{i>j} \Phi_{ij} + \sum_{i>j, i'>j'} \Phi_{ij}\Phi_{i'j'} + \dots$$

which is a sum of all possible products of Mayer functions which tend to lead to quite complicated expressions which are difficult to evaluate. Mayer and Mayer found a diagrammatic method to illustrate the particles and the interactions between them which gave them the name cluster integrals. Surprisingly, many of the terms cancel out so that one is left with the two dominant terms

$$\beta_1 = \frac{1}{V} \int_{Q^2} \Phi_{12} dq_1 dq_2 \tag{2.5}$$

$$\beta_2 = \frac{1}{V} \int_{Q^3} \Phi_{12} \Phi_{23} \Phi_{13} dq_1 dq_2 dq_3 \tag{2.6}$$

for the first and second cluster integral. For more details on higher order terms we refer the reader to [?]. In particular these terms constitute the first two correction terms to the ideal gas law

$$\ln Z_N = N \left(1 + \ln \frac{N}{V} + \frac{1}{2} \beta_1 \left(\frac{N}{V} \right) + \frac{1}{3} \beta_2 \left(\frac{N}{V} \right)^2 + \dots \right).$$

In case of lyotropic liquid crystals, when we are considering a solution rather than a gas, the cluster integrals β_1 and β_2 have to be averaged over all orientations in order to obtain the virial coefficients. In particular, the first and second virial coefficient are given by

$$B_2 = -\frac{1}{2} \int_{Q^2} \beta_1(q_1, q_2) \rho(q_1) \rho(q_2) dq_1 dq_2$$

$$B_3 = -\frac{1}{3} \int_{Q^3} \beta_2(q_1, q_2, q_3) \rho(q_1) \rho(q_2) \rho(q_3) dq_1 dq_2 dq_3$$

while the higher order virial coefficients have more complicated expressions.

Based on all of these considerations, we obtain a final expression for the Helmholtz free-energy functional

$$
\begin{aligned}
\frac{F}{Nk_BT} &= \ln\rho + B_2\rho + \frac{1}{2}B_3\rho^2 + \dots \\
&= \ln f + \int_Q \rho(q)\ln(4\pi\rho(q))dq - \frac{f}{2}\int_{Q^2}\beta_1(q_1,q_2)\rho(q_1)\rho(q_2)dq_1dq_2 \\
&\quad - \frac{f^2}{3}\int_{Q^3}\beta_2(q_1,q_2,q_3)\rho(q_1)\rho(q_2)\rho(q_3)dq_1dq_2dq_3 + \dots .
\end{aligned}
$$

In the case of long thin rods Onsager proved that the third virial coefficient β_2 in this expansion is in fact negligible compared to β_1. However, if the ratio of the length L and diameter D of the rods becomes smaller, the third virial coefficient gains importance over the first. In particular, if $L/D < 20$, then the second and third virial coefficients have similar weights while at $L/D \approx 100$ the contribution of the third virial coefficient β_2 is still around 10% of that of the second [**?**]. Only in the limit of $L/D \to \infty$ can we assume that all higher virial coefficients tend to zero. These facts illustrate the limitations of Onsager's theory.

We consider now the limit $L/D \to \infty$. Taking the exact form of the Mayer function and the form of the first cluster integral into account, see (2.4) and (2.5), we see that the first cluster integral can be computed as follows

$$
\beta_1(p,q) = \frac{1}{V}\int_{\substack{\text{if the particles}\\ p \text{ and } q \text{ overlap}}} (-1)dqdp.
$$

This integral constitutes the negative of the excluded volume of two particles with orientations p and q. Together with Onsager, we may now assume that

$$\frac{F}{Nk_BT} = \ln f + \int_{\mathcal{Q}} \rho(q) \ln(4\pi\rho(q)) dq - \frac{f}{2} \int_{\mathcal{Q}^2} V_{\text{excl}} \rho(q_1)\rho(q_2) dq_1 dq_2.$$

An extensive discussion of Onsager's derivation can be found in [**?**]. Excluded

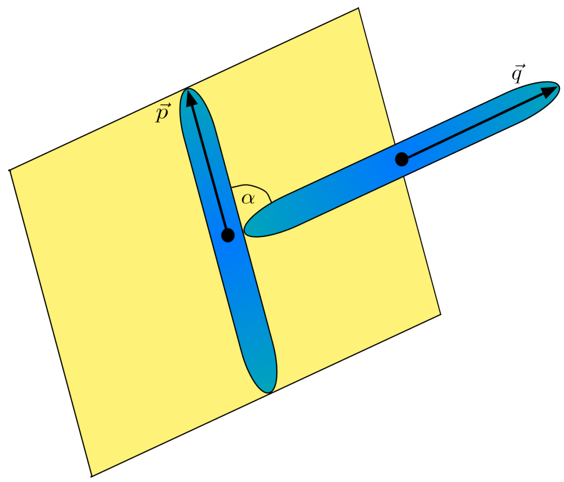


Figure 2.3: The excluded volume between two rod-like molecules whose orientations differ by an angle α.

volume effects arise in the system due to the impenetrability of the molecules. This means that the centre of mass of one molecule cannot move around freely without any constraints because it cannot enter the space that is already occupied by other molecules. Figure 2.3 illustrates schematically what the excluded volume looks like in case of rod-like molecules when two of them have an orientation differing by an angle α.

It is easy to see from Figure 2.3 that the excluded volume between these two molecules can be approximated by

$$V_{exc} \approx 2L^2D|\sin(\alpha)| = 2L^2D|p \times q|,$$

see also [?] for details. Observe that we do not consider any end effects in the above approximation. For a derivation of the excluded volume for other shapes of molecules, we recommend [?]. By the excluded volume argument,

$$K_O(p,q) = |\sin\alpha| = |p \times q| = \sqrt{1-(p\cdot q)^2}.$$

Especially from the third expression, we see that the Onsager interaction potential has a non-analytic structure due to its 'cusp' singularity occurring whenever p and q are orthogonal. Therefore it is not very convenient to work with and thus most of the literature is concerned with the Maier-Saupe interaction potential $K_{MS}(p,q) = \frac{1}{3} - (p\cdot q)^2$.

2.3 The dipolar interaction potential

The third very well-known interaction potential is the dipolar potential [?]

$$K_d(p,q) = -p \cdot q.$$

The major difference between the dipolar and the Maier-Saupe interaction potential is that the Maier-Saupe potential is invariant with respect to a change of sign in its argument and thus possesses a head-to-tail symmetry. To the contrary, the dipolar potential depends on the direction of the molecular vector of the molecules. From a physical perspective, the dipolar potential is used when the molecules possess a dipole moment parallel to their molecular axis.

Chapter 3

Existence and boundedness of minimisers

In order to keep the subsequent analysis as general as possible, we only impose the physically motivated assumptions listed in Assumption 1.3 on the two-body interaction kernel, that is that $k(\cdot)$ is rotationally symmetric and continuous in both variables. Based on these assumptions, we prove the existence of minimisers in Section 3.1 and we establish a lower and upper bound on the probability densities which are minimising the functional in Sections 3.2 and 3.3. Finally, we will reduce the minimisation problem to a certain class of probability densities in Section 3.4.

3.1 Existence of minimisers of the free-energy functional

In order to prove existence of minimisers of the Onsager free-energy functional given by

$$\mathcal{F}(\rho, \lambda) := \lambda \int_{\mathbb{S}^2} \rho(p) \ln \rho(p) \; dp + \frac{1}{2} \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} K(p, q) \rho(p) \rho(q) \; dp \; dq, \tag{3.1}$$

we apply the direct method of the calculus of variations [?]. We consider all probability densities

$$\mathcal{P}(\mathbb{S}^2) := \left\{ \rho \in L^1(\mathbb{S}^2) \Big| \int_{\mathbb{S}^2} \rho(p)\, dp = 1, \rho(p) \geq 0 \right\}.$$

Take a minimising sequence $\rho_n : \mathbb{S}^2 \to \mathbb{R}$ such that

$$\mathcal{F}(\rho_n) \to \inf\{\mathcal{F}(\rho) | \rho \in \mathcal{P}(\mathbb{S}^2)\}.$$

- Considering a minimising sequence ρ_n for $\mathcal{F}$, we have to show that there exists a subsequence ρ_{n_k} which converges to $\rho^\star$ weakly in $L^1(\mathbb{S}^2)$.
- We prove that the functional $\mathcal{F}(\rho)$ is weakly lower-semicontinuous, that is

  $$\liminf_{n\to\infty} \mathcal{F}(\rho_n) \geq \mathcal{F}(\rho^\star)$$

  for any $\rho_n \rightharpoonup \rho^\star$.

We may then conclude the existence of a minimiser because

$$\begin{aligned}\inf\{\mathcal{F}(\rho) | \rho \in \mathcal{P}(\mathbb{S}^2)\} &= \lim_{n\to\infty} \mathcal{F}(\rho_n) = \lim_{k\to\infty} \mathcal{F}(\rho_{n_k}) \\ &\geq \mathcal{F}(\rho^\star) \geq \inf\{\mathcal{F}(\rho) | \rho \in \mathcal{P}(\mathbb{S}^2)\}\end{aligned}$$

and thus,

$$\mathcal{F}(\rho^\star) = \inf\{\mathcal{F}(\rho) | \rho \in \mathcal{P}(\mathbb{S}^2)\}.$$

In the following, we make these steps rigorous for the Onsager free-energy functional.

Theorem 3.1. *Assume that the interaction potential $K(\cdot,\cdot) : \mathbb{S}^2 \times \mathbb{S}^2 \to \mathbb{R}$ is continuous. Then there exists a minimiser to the Onsager free-energy in* (3.1)*.*

Proof. First of all, let us show that the functional is bounded from below. It is straightforward to see that $\rho \ln \rho$ attains its minimum value at $\rho = e^{-1}$. Thus, $\min_\rho \rho \ln \rho = -e^{-1} > -1$ and hence we may conclude that the entropy part of the Onsager free-energy functional is bounded below by

$$\mathcal{F}_1(\rho) := \lambda \int_{\mathbb{S}^2} \rho(p) \ln \rho(p) \; dp \geq -\lambda |\mathbb{S}^2| = -4\pi\lambda.$$

Let us now consider the interaction term

$$\mathcal{F}_2(\rho) := \frac{1}{2} \int_{\mathbb{S}^2 \times \mathbb{S}^2} K(p,q)\rho(p)\rho(q) \; dp \; dq.$$

Assuming that the interaction potential $K(p,q)$ is continuous and defined on the compact set $\mathbb{S}^2 \times \mathbb{S}^2$, it follows that $K(p,q)$ is bounded. Hence there exists $M > 0$ such that $\big|K(p,q)\big| \leq M$ for all $p, q \in \mathbb{S}^2$. Therefore

$$\mathcal{F}_2(\rho) = \frac{1}{2} \int_{\mathbb{S}^2 \times \mathbb{S}^2} K(p,q)\rho(p)\rho(q) \; dp \; dq \geq -\frac{M}{2} \int_{\mathbb{S}^2 \times \mathbb{S}^2} \rho(p)\rho(q) \; dp \; dq \geq -\frac{M}{2},$$

proving that the Onsager free-energy is bounded from below. Hence there exists a minimising sequence $\rho_n : \mathbb{S}^2 \to \mathbb{R}$ such that

$$\mathcal{F}(\rho_n) \to \inf\{\mathcal{F}(\rho) | \rho \in \mathcal{P}(\mathbb{S}^2)\}.$$

Claim 1: Any minimising sequence admits a weakly convergent subsequence.

Let ρ_n be a minimising sequence of $\mathcal{F}$, that is

$$\mathcal{F}(\rho_n) \to \inf\{\mathcal{F}(\rho) | \rho \in \mathcal{P}(\mathbb{S}^2)\}.$$

Because every convergent sequence is bounded, it follows that $\mathcal{F}(\rho_n)$ is bounded. Following Theorem 13.6 in [?], we know that a subset F of $L^1(\mathbb{S}^2)$ is relatively weakly compact if and only if it is uniformly integrable, that is

$$\sup_{f \in F} \int_{\{|f|>a\}} |f(t)| \, dt \to 0 \text{ as } a \to \infty.$$

Hence it is enough to show that the minimising sequence ρ_n is uniformly integrable. Let us assume the contrary, that is

$$\exists \, \epsilon > 0 \; \forall \, A \; \exists \, a > A \text{ such that } \sup_{\{\rho_n | n \in \mathbb{N}\}} \int_{\{|\rho_n|>a\}} \rho_n(p) \, dp > \epsilon.$$

In particular, since the left hand side is decreasing in a, we may assume that

$$\exists \, \epsilon > 0 \text{ such that } \; \forall \, a \sup_{\{\rho_n | n \in \mathbb{N}\}} \int_{\{|\rho_n|>a\}} \rho_n(p) \, dp > \epsilon$$

and hence for any $a > 0$ there exists $m(a)$ such that

$$\int_{\rho_m > a} \rho_m(p)\ dp > \frac{\epsilon}{2}. \tag{3.2}$$

Let us now derive a contradiction from this assumption by showing that $\mathcal{F}(\rho_n)$ is not bounded if ρ_n is not uniformly integrable.

Fix $a > 0$ and let m be as in (3.2). We can make the following estimate for the first part of the Onsager free-energy functional

$$\begin{aligned}
\mathcal{F}_1(\rho_{m(a)}) &= \lambda \int_{\mathbb{S}^2} \rho_{m(a)}(p) \ln \rho_{m(a)}(p)\ dp \\
&\geq -\lambda \left(|\mathbb{S}^2| + \int_{\{\rho_{m(a)} > a\}} \rho_{m(a)}(p) \ln \rho_{m(a)}(p)\ dp \right) \\
&\geq -\lambda \left(|\mathbb{S}^2| + \ln a \int_{\{\rho_{m(a)} > a\}} \rho_{m(a)}(p)\ dp \right) \\
&\geq -\lambda \left(|\mathbb{S}^2| + \ln a \frac{\epsilon}{2} \right).
\end{aligned}$$

However, the sequence $\mathcal{F}(\rho_n)$ is bounded from above for all $n \in \mathbb{N}$ and thus choosing a to be very large, this lower bound exceeds the upper bound leading to a contradiction. Therefore the sequence ρ_n is relatively compact and thus ρ_n admits a weakly convergent subsequence.

Claim 2: The Onsager free-energy functional is weakly lower semi-continuous.

It follows directly from Theorem 3.2.5 in [**?**] that $\mathcal{F}_1$ is weakly lower semi-continuous. Hence it is enough to prove that $\mathcal{F}_2(\rho)$ is weakly continuous. Suppose that $\rho_n \rightharpoonup \rho$ in $L^1(\mathbb{S}^2)$. Then any integral functional in $L^\infty(\mathbb{S}^2)$ converges strongly and since

$K(\cdot,\cdot)$ is continuous, it is bounded on $\mathbb{S}^2$. Hence

$$\int_{\mathbb{S}^2} K(p,q)\rho_n(q)\, dq \to \int_{\mathbb{S}^2} K(p,q)\rho(q)\, dq \text{ for } p \in \mathbb{S}^2.$$

Fix $\epsilon > 0$. Since $K(\cdot,\cdot)$ is uniformly continuous, there exists $\delta > 0$ such that for all $|p_1 - p_2| < \delta$

$$|K(p_1,q) - K(p_2,q)| < \frac{\epsilon}{3}.$$

Moreover, there are $\{p_1, \ldots, p_m\} \subset \mathbb{S}^2$ such that for all $p \in \mathbb{S}^2$ there exists $i \in \{1, \ldots, m\}$ such that $|p_i - p| < \delta$. Hence there is an N_i corresponding to p_i such that

$$\left| \int_{\mathbb{S}^2} K(p_i,q)\rho_n(q)\, dq - \int_{\mathbb{S}^2} K(p,q)\rho(q)\, dq \right| < \frac{\epsilon}{3} \text{ for all } n \geq N_i.$$

Let $N = \max_i N_i$, then

$$\left| \int_{\mathbb{S}^2} K(p_i,q)\rho_n(q)\, dq - \int_{\mathbb{S}^2} K(p,q)\rho(q)\, dq \right| < \frac{\epsilon}{3} \text{ for all } n \geq N \text{ and } \forall i = 1, \ldots, m$$

and hence

$$\begin{aligned}
\Big| \int_{\mathbb{S}^2} & K(p,q)\rho_n(q)\, dq - \int_{\mathbb{S}^2} K(p,q)\rho(q)\, dq \Big| \\
&\leq \left| \int_{\mathbb{S}^2} (K(p_i,q) - K(p,q))\rho_n(q)\, dq \right| + \left| \int_{\mathbb{S}^2} (K(p_i,q) - K(p,q))\rho(q)\, dq \right| \\
&\quad + \left| \int_{\mathbb{S}^2} K(p_i,q)\rho_n(q)\, dq - \int_{\mathbb{S}^2} K(p_i,q)\rho(q)\, dq \right| \\
&< \frac{\epsilon}{3} + \frac{\epsilon}{3} + \frac{\epsilon}{3} = \epsilon. \qquad (3.3)
\end{aligned}$$

Thus, we have proven uniform convergence of $U(\rho_n, p)$ in $L^\infty(\mathbb{S}^2)$ since

$$\left| \int_{\mathbb{S}^2} K(p,q)\rho_n(q)\, dq \right| \leq \sup_{q \in \mathbb{S}^2} |K(p,q)| = M < \infty.$$

We are now able to deduce that if $\rho_n \rightharpoonup \rho$ in $L^1(\mathbb{S}^2)$, then

$$\begin{aligned}
&\int_{\mathbb{S}^2} \int_{\mathbb{S}^2} K(p,q)\rho_n(q)\rho_n(p)\, dq\, dp \\
&\qquad = \int_{\mathbb{S}^2} \underbrace{\int_{\mathbb{S}^2} K(p,q)\rho(q)\, dq}_{\in L^\infty(\mathbb{S}^2)} \rho_n(p)\, dp \\
&\qquad\quad + \int_{\mathbb{S}^2} \underbrace{\int_{\mathbb{S}^2} [K(p,q)\rho_n(q) - K(p,q)\rho(q)]\, dq}_{\to 0 \text{ by Equation (3.3)}} \rho_n(p)\, dp \\
&\qquad \to \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} K(p,q)\rho(q)\rho(p)\, dq\, dp,
\end{aligned}$$

thus proving that $\mathcal{F}_2$ is weakly continuous and therefore $\mathcal{F}$ is weakly lower semi continuous.

Putting all these steps together, we have verified the direct method of the calculus of variations proving existence of a minimiser to the Onsager free-energy functional. $\square$

3.2 Restriction to probability densities which are bounded from below

We prove that any admissible probability density that minimises the Onsager free-energy functional is bounded away from zero.

Lemma 3.2. *Assume that the kernel satisfies* $0 \leq K(p,q) \leq M$. *Let* $\rho \in L^1(\mathbb{S}^2)$ *be an arbitrary probability density. Suppose that there exists a set* $A \subset \mathbb{S}^2$ *of positive measure such that* $\rho(p) \leq \frac{1}{8\pi}\exp(-3M/\lambda)$. *Then there exists a modification of* ρ*, denoted by* $\rho^\star$*, such that* $\rho^\star$ *is bounded from below by* $\epsilon = \frac{1}{8\pi}\exp(-3M/\lambda)$ *and* $\mathcal{F}(\rho^\star) < \mathcal{F}(\rho)$.

Proof. Suppose that

$$\operatorname*{ess\,inf}_{p \in \mathbb{S}^2} \rho(p) = 0. \tag{3.4}$$

The idea of the proof is to construct a function $\rho^\star$ from ρ by lifting ρ at every point where it is less than ϵ to ϵ in order to obtain a function that is bounded away from zero. However, we also have to lower ρ on a different set because otherwise $\rho^\star$ is not a probability density as it does not integrate to one. Therefore we define $\rho^\star$ as

$$\rho^\star(p,\gamma) := \epsilon \mathbb{1}_{\{p|\rho(p)\leq\epsilon\}} + \rho(p)\mathbb{1}_{\{p|\epsilon\leq\rho(p)<\gamma\}} + \gamma\mathbb{1}_{\{p|\rho(p)\geq\gamma\}}$$

with $\epsilon := \frac{1}{8\pi}\exp(-3M/\lambda)$ where $M := \sup_{p,q\in\mathbb{S}^2} K(p,q)$. In order to keep our presentation simple in the subsequent analysis, we define

$$A := \{p|\rho(p) \leq \epsilon\}, \qquad B := \{p|\epsilon \leq \rho(p) < \gamma\} \qquad \text{and} \qquad C := \{p|\rho(p) \geq \gamma\}.$$

We choose γ such that $\rho^\star$ integrates to 1. This can be achieved by noting that the map $\gamma \mapsto \int \rho^\star(p,\gamma)$ is continuous by applying the monotone convergence theorem and then applying the intermediate value theorem (for $\gamma = \frac{1}{8\pi}$ the integral is less than 1 and bigger than 1 if γ is sufficiently large). Integrating $\rho^\star$, it is easy to see that γ has to be chosen such that

$$\delta := \frac{1}{|C|}\left(1 - \epsilon|A| - \int_B \rho(p)\, dp\right)$$

because then $\rho^\star \in \mathcal{P}(\mathbb{S}^2) := \{\rho \in L^1(\mathbb{S}^2) | \rho(p) \geq 0, \int_{S^2} \rho = 1\}$. It follows from the same reasoning that $\gamma \geq \frac{1}{4\pi}$ and therefore $|C| > 0$ as well as $|A| > 0$ by assumption. Therefore $\rho^\star$ is a well-defined probability density which is admissible for our minimisation problem. For details on this construction for a particular example it might be helpful for the reader to consider Figure 3.2.

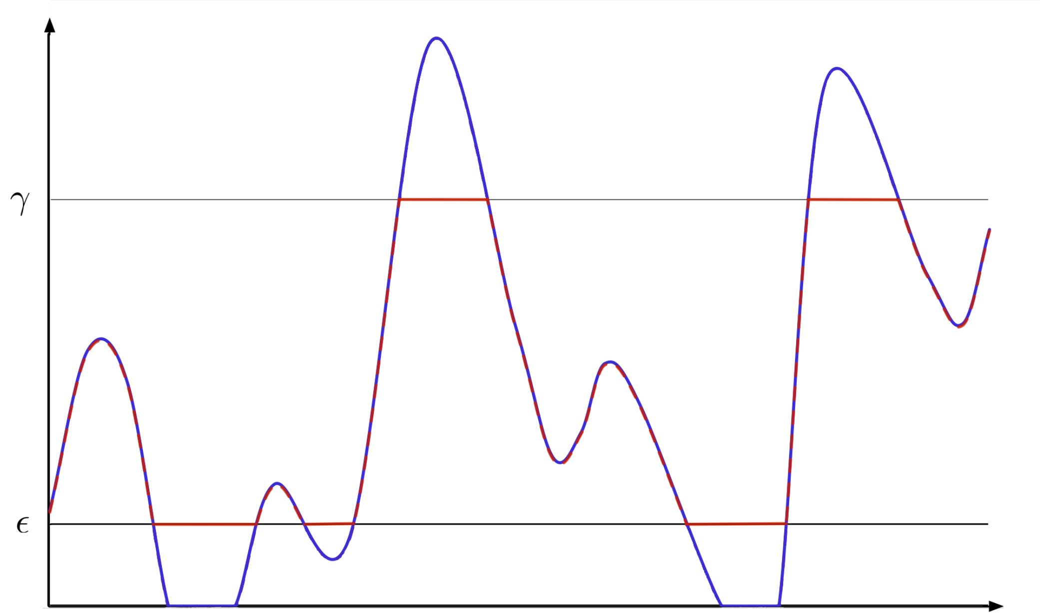


Figure 3.1: Schematic illustration of ρ (in blue) and its refinement $\rho^\star$ (in red)

In the following, we would like to show that $\mathcal{F}(\rho) - \mathcal{F}(\rho^\star) > 0$. Let us start with the entropic term. Let

$$f(x) := x \ln x, \quad g(p) := \epsilon - \rho(p) \quad \text{and} \quad h(p) := \rho(p) - \gamma,$$

then by an application of the mean value theorem it follows that

$$\begin{aligned}\mathcal{F}_1(\rho) - \mathcal{F}_1(\rho^\star) =& \lambda \int_A (\rho(p) \ln \rho(p) - \epsilon \ln \epsilon)\, dp + \lambda \int_C (\rho(p) \ln \rho(p) - \gamma \ln \gamma)\, dp \\ \geq& -\lambda(\ln(\epsilon) + 1) \int_A g(p)\ dp + \lambda(\ln(\gamma) + 1) \int_C h(p)\ dp.\end{aligned}$$

For the step above we used that for the convex function $f(x) = x \ln x$ it holds that $f(y) \geq f(x) + f'(x)(y - x)$. Moreover, we observe that $\int_A g(p)\ dp = \int_C h(p)\ dp$ and hence

$$\mathcal{F}_1(\rho) - \mathcal{F}_1(\rho^\star) \geq \lambda \ln \frac{\gamma}{\epsilon} \int_A g(p)\ dp.$$

Now let us turn to the interaction term $\mathcal{F}_2(\rho) = \frac{1}{2} \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} K(p, q)\rho(p)\rho(q)\ dq\ dp$. Plugging in $\rho^\star$ and ρ yields

$$\begin{aligned}&\mathcal{F}_2(\rho,\lambda) - \mathcal{F}_2(\rho^\star) = \\ &\quad \frac{1}{2} \int_{A\times A} K(p, q)(\rho(p)\rho(q) - \epsilon^2) dpdq + \frac{1}{2} \int_{C\times C} K(p, q)(\rho(p)\rho(q) - \gamma^2) dpdq \\ &\quad + \int_{A\times B} K(p, q)(\rho(p)\rho(q) - \epsilon\rho(q)) dpdq + \int_{A\times C} K(p, q)(\rho(p)\rho(q) - \epsilon\gamma) dpdq \\ &\quad + \int_{B\times C} K(p, q)(\rho(p)\rho(q) - \rho(p)\gamma) dpdq\end{aligned}$$

$$
\begin{aligned}
=&\frac{1}{2}\int_{A\times A} K(p,q)(\rho(p)\rho(q)-\epsilon\rho(q)+\epsilon\rho(q)-\epsilon^2)dpdq\\
&+\frac{1}{2}\int_{C\times C} K(p,q)\underbrace{(\rho(p)\rho(q)-\gamma^2)}_{\geq 0}dpdq+\int_{A\times B} K(p,q)\rho(q)(\rho(p)-\epsilon)dpdq\\
&+\int_{A\times C} K(p,q)(\rho(p)\rho(q)-\epsilon\rho(q)+\epsilon\rho(q)-\epsilon\gamma)dpdq\\
&+\int_{B\times C} K(p,q)\rho(p)(\rho(q)-\gamma)dpdq\\
\geq&\frac{1}{2}\int_{A\times A} K(p,q)\rho(q)(\rho(p)-\epsilon)dpdq+\frac{\epsilon}{2}\int_{A\times A} K(p,q)(\rho(q)-\epsilon)dpdq\\
&+\int_{A\times B} K(p,q)\rho(q)(\rho(p)-\epsilon)dpdq+\int_{A\times C} K(p,q)\rho(q)(\rho(p)-\epsilon)dpdq\\
&+\epsilon\int_{A\times C} K(p,q)(\rho(q)-\gamma)dpdq+\int_{B\times C} K(p,q)\rho(p)(\rho(q)-\gamma)dpdq\\
\geq&-\frac{M}{2}\int_A g(p)dp-\frac{4\pi\epsilon M}{2}\int_A g(p)dp-M\int_A g(p)dp-M\int_A g(p)dp\\
=&-M\left(\frac{5}{2}+2\pi\epsilon\right)\int_A g(p)dp.
\end{aligned}
$$

Putting both terms together yields

$$
\mathcal{F}(\rho)-\mathcal{F}(\rho^\star)\geq\int_A g(p)\,dp\left(\lambda\ln\frac{\gamma}{\epsilon}-M\left(\frac{5}{2}+2\pi\epsilon\right)\right).
$$

Hence using the facts that $\gamma\geq\frac{1}{4\pi}$ and $\epsilon\leq\frac{1}{4\pi}$, we may conclude that

$$
\begin{aligned}
\mathcal{F}(\rho)-\mathcal{F}(\rho^\star)>0 \quad &\Leftarrow \quad \lambda\ln\frac{\gamma}{\epsilon}>M\left(\frac{5}{2}+2\pi\epsilon\right)\\
&\Leftarrow \quad \lambda\ln\frac{1}{4\pi\epsilon}>M\left(\frac{5}{2}+2\pi\epsilon\right)\\
&\Leftarrow \quad \epsilon<\frac{1}{4\pi}\exp\left(-\frac{M\left(\frac{5}{2}+2\pi\epsilon\right)}{\lambda}\right)
\end{aligned}
$$

$$\Leftarrow \quad \epsilon < \frac{1}{4\pi}\exp\left(-\frac{3M}{\lambda}\right)$$

which we have assumed at the beginning of the proof. □

3.3 Restriction to probability densities which are bounded from above

By constructing a test function $\rho^\star$ that is bounded above by a constant $C^\star$, we prove that $\mathcal{F}(\rho) > \mathcal{F}(\rho^\star)$ for all admissible probability densities ρ and thus we show that we can restrict our attention to probability densities that are bounded above. This result holds for all continuous interaction kernels, see Assumption 1.3.

Lemma 3.3. *Assume that the kernel satisfies* $0 \le K(p,q) \le M$*. Let* $\rho \in L^1(\mathbb{S}^2)$ *be a probability density and suppose that there exists a set* $A \subset \mathbb{S}^2$ *of positive measure such that* $\rho(p) \ge C^\star := \exp(16M/\lambda)$ *for all* $p \in A$ *where* $M := \max_{p,q\in\mathbb{S}^2} K(p,q) > 0$ *and* $\lambda > 0$*. Then there exists a modification of* ρ*, denoted by* $\rho^\star$*, such that* $\rho^\star$ *is bounded from above by* $C^\star$ *and* $\mathcal{F}(\rho^\star) < \mathcal{F}(\rho)$*.*

Proof. Let

$$\rho^\star(p) := C^\star \mathbb{1}_{\{p|\rho(p)>C^\star\}} + \rho(p)\mathbb{1}_{\{p|C^\star\ge\rho(p)>\frac{1}{2\pi}\}} + (\rho(p)+\gamma)\mathbb{1}_{\{p|\rho(p)\le\frac{1}{2\pi}\}}$$

where $\gamma := \frac{\int_{\mathbb{S}^2}(\rho(p)-C^\star)\mathbb{1}_{\{\rho(p)>C^\star\}}\,dp}{|\{p|\frac{1}{2\pi}\ge\rho(p)\}|}$. Again, for ease of presentation, we use the

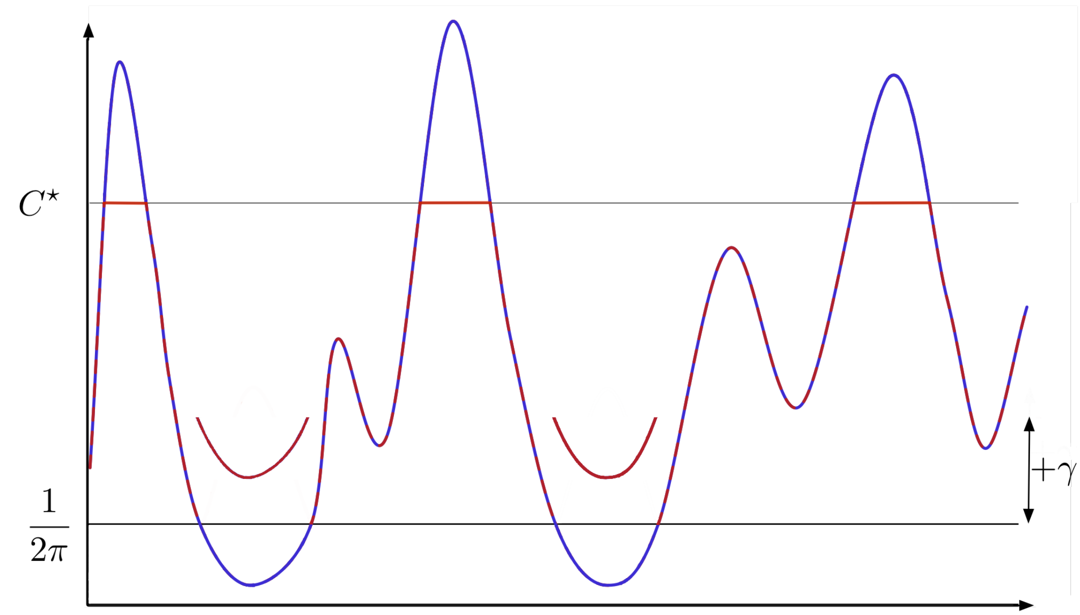


Figure 3.2: Schematic illustration of ρ (in blue) and its refinement $\rho^\star$ (in red)

following notation

$$A := \left\{ p \in \mathbb{S}^2 \middle| \rho(p) > C^\star \right\}, \quad B := \left\{ p \in \mathbb{S}^2 \middle| C^\star \geq \rho(p) > \frac{1}{2\pi} \right\} \text{ and}$$
$$C := \left\{ p \in \mathbb{S}^2 \middle| \frac{1}{2\pi} \geq \rho(p) \right\}.$$

It is easy to see that $|C| > 0$ since otherwise $\int_{\mathbb{S}^2} \rho(p)\ dp > 1$ contradicting the fact that ρ is a probability density. By the choice of γ, we make sure that $\rho^\star$ still integrates to one. Observe that $C^\star = \exp(16M/\lambda) \geq 1 > \frac{1}{2\pi}$ and hence that $A \cap C = \emptyset$. In order to ensure that $\rho^\star \leq C^\star$ on C, we claim that $\gamma < \frac{1}{2\pi}$. Since ρ

is a probability density, it follows that $\int_A (\rho(p) - C^\star)\, dp \leq 1$. Hence

$$\gamma := \frac{\int_{\mathbb{S}^2} (\rho(p) - C^\star) \mathbb{1}_{\{\rho(p) > C^\star\}}\, dp}{|\{p| \frac{1}{2\pi} \geq \rho(p)\}|} \leq \frac{1}{|\{p| \frac{1}{2\pi} \geq \rho(p)\}|}$$

and we only have to show that $|C| = |\{p| \frac{1}{2\pi} \geq \rho(p)\}| \geq 2\pi$. Suppose the contrary, that is $|C| < 2\pi$ and thus $|A \cup B| = |\{\rho(p) > \frac{1}{2\pi}\}| \geq 2\pi$ since the total measure of the unit sphere is given by 4π and thus $|A \cup B \cup C| = 4\pi$. Moreover, since ρ is non-negative,

$$\int_{\mathbb{S}^2} \rho(p)\, dp \geq \int_{C^c} \rho(p)\, dp \geq \frac{1}{2\pi} \int_{C^c} 1\, dp \geq \frac{1}{2\pi} 2\pi = 1$$

contradicting the fact that ρ integrates to one. Therefore $\gamma \leq \frac{1}{2\pi}$.

Having defined $\rho^\star$, we are now in a position to prove that

$$\mathcal{F}(\rho) - \mathcal{F}(\rho^\star) > 0.$$

In the following, we deal with the entropy and the interaction terms separately. We begin by deriving a lower bound on the entropy term. In particular,

$$\begin{aligned}
&\mathcal{F}_1(\rho) - \mathcal{F}_1(\rho^\star) \\
&\quad = \lambda \int_{\mathbb{S}^2} \rho(p) \ln(\rho(p))\, dp - \lambda \int_{\mathbb{S}^2} \rho^\star(p) \ln(\rho^\star(p))\, dp \\
&\quad = \lambda \int_A [f(\rho(p)) - f(C^\star)]\, dp + \lambda \int_C [f(\rho(p)) - f(\rho(p) + \gamma)]\, dp
\end{aligned}$$

where $f(x) := x \ln(x)$. Moreover, defining $g(p) := \rho(p) - C^\star$. Because of convexity, we have $f(y) \geq f(x) + f'(x)(y-x)$ implying that

$$\begin{aligned}
&\mathcal{F}_1(\rho) - \mathcal{F}_1(\rho^\star) \\
&\quad \geq \lambda(\ln C^\star + 1) \int_A g(p)\, dp - \gamma\lambda \int_C (\ln(\rho(p) + \gamma) + 1)\, dp \\
&\quad \geq \lambda(\ln C^\star + 1) \int_A g(p)\, dp - \gamma\lambda \int_C \left(\ln\left(\frac{1}{2\pi} + \gamma \right) + 1 \right)\, dp
\end{aligned}$$

where the last line results from the fact that $\rho \in C$ and hence $\rho(p) < \frac{1}{2\pi}$ for all $p \in C$. Observing that $g(p) \geq 0$ for all $p \in A$ and using the monotonicity of the logarithm as well as the facts that $\gamma < \frac{1}{2\pi}$, $\ln \frac{1}{\pi} < -1$ and $\lambda, \gamma, |C| > 0$, we deduce that

$$\begin{aligned}
&\mathcal{F}_1(\rho) - \mathcal{F}_1(\rho^\star) \\
&\quad \geq \lambda(\ln C^\star + 1) \int_A g(p)\, dp - \lambda \left(\ln\left(\frac{1}{2\pi} + \frac{1}{2\pi} \right) + 1 \right) \gamma |C| \\
&\quad \geq \lambda \ln(C^\star) \int_A g(p)\, dp. \qquad (3.5)
\end{aligned}$$

This gives us a lower bound on the entropic term and we can direct our attention to a lower bound on the interaction term. Using the definition of $\rho^\star$, it follows that

$$\begin{aligned}
\mathcal{F}_2(\rho) - \mathcal{F}_2(\rho^\star) =& \frac{1}{2} \int_{\mathbb{S}^2 \times \mathbb{S}^2} K(p,q)[\rho(p)\rho(q) - \rho^\star(p)\rho^\star(q)]\, dq\, dp \\
=& \frac{1}{2} \int_{A \times A} K(p,q) h(p,q)\, dq\, dp - \frac{\gamma^2}{2} \int_{C \times C} K(p,q)\, dq\, dp \\
&- \gamma \int_{C \times C} K(p,q)\rho(p)\, dq\, dp + \int_{A \times B} K(p,q)\rho(q) g(p)\, dp\, dq
\end{aligned}$$

$$
\begin{aligned}
&+ \int_{A\times C} K(p,q)\rho(q)g(p)\;dq\;dp - \gamma C^\star \int_{A\times C} K(p,q)\;dq\;dp \\
&- \gamma \int_{B\times C} K(p,q)\rho(q)\;dq\;dp
\end{aligned}
$$

where we used the symmetry of the kernel and again we defined $g(p) := \rho(p) - C^\star$ and $h(p,q) := \rho(p)\rho(q) - C^\star C^\star$ which are both non-negative for $p, q \in A$. Assuming without loss of generality that the interaction kernel is positive, we observe that all terms with a positive sign are positive while only those with a negative sign are negative. Neglecting the positive terms, we may therefore deduce that

$$
\begin{aligned}
&\mathcal{F}_2(\rho) - \mathcal{F}_2(\rho^\star) \\
&\quad \geq -\frac{\gamma^2}{2}\int_{C\times C} K(p,q)\;dq\;dp - \gamma \int_{C\times C} K(p,q)\rho(p)\;dq\;dp \\
&\qquad - \gamma \int_C \left(\int_A K(p,q)\rho(p)\;dp \right)\;dq - \gamma \int_{B\times C} K(p,q)\rho(q)\;dq\;dp \qquad (3.6) \\
&\quad \geq -\frac{\gamma^2}{2} M(4\pi)^2 - 4\pi\gamma M - 4\pi\gamma M - 4\pi M\gamma \\
&\quad \geq -\gamma^2 M 8\pi^2 - 12\pi\gamma M
\end{aligned}
$$

where we used the fact that $\rho(p) \geq C^\star$ for all $p \in A$ in (3.6). Since $\gamma < \frac{1}{2\pi}$

$$
\mathcal{F}_2(\rho) - \mathcal{F}_2(\rho^\star) > -4\pi\gamma M - 12\pi\gamma M = -16\pi\gamma M, \qquad (3.7)
$$

we obtain a lower bound on the interaction term.

We are now in the position to derive an overall bound on $\mathcal{F}$. Using (3.5), (3.7) and the definition of $\gamma := \frac{\int_A g(p)dp}{|C|}$, we obtain that

$$\begin{aligned}\mathcal{F}(\rho) - \mathcal{F}(\rho^\star) >& \lambda \ln(C^\star) \int_A g(p)\ dp - 16\pi\gamma M \\ =& \lambda \ln(C^\star)|C|\gamma - 16\pi\gamma M.\end{aligned}$$

Finally, making use of the assumption that $C^\star = \exp(16M/\lambda)$ and using the fact that $|C| \geq 2\pi$, the statement follows because

$$\mathcal{F}(\rho) - \mathcal{F}(\rho^\star) > \lambda \frac{16M}{\lambda}|C|\gamma - 16\pi\gamma M = 16M\gamma(|C| - \pi) > 0.$$

□

The following result is a straightforward consequence of Lemma 3.2 and 3.3.

Corollary 3.4. *Let two sets* $\mathcal{A}$ *and* $\mathcal{B}$ *be given by*

$$\mathcal{A} := \left\{\rho : \mathbb{S}^2 \to \mathbb{R} | \int_{\mathbb{S}^2} \rho(p)\ dp = 1, \rho \geq 0\right\}$$

and

$$\mathcal{B} := \left\{\rho : \mathbb{S}^2 \to \mathbb{R} | \int_{\mathbb{S}^2} \rho(p)\ dp = 1, \rho \geq 0, \rho \leq \exp(16M/\lambda)\right\}.$$

Then any solution of the minimisation problem $\min_{\mathcal{A}} \mathcal{F}(\rho)$ *is in fact a solution of the reduced minimisation problem* $\min_{\mathcal{B}} \mathcal{F}(\rho)$.

3.4 A reduction of the minimisation problem

Initially, we considered the problem of minimising the Onsager free-energy functional $\mathcal{F}$ among the set

$$\mathcal{P}(\mathbb{S}^2) := \left\{ \rho \in L^1(\mathbb{S}^2) \middle| \int_{\mathbb{S}^2} \rho(p)\, dp = 1, \rho(p) \geq 0 \right\}.$$

According to the results of Lemma 3.2 and Lemma 3.3, we observe that this original problem can be reduced to all probability densities of the set

$$\begin{aligned} \mathcal{S}(\mathbb{S}^2) := \Big\{ \rho \in L^1(\mathbb{S}^2) \Big| & \\ & \int_{\mathbb{S}^2} \rho(p)\, dp = 1, \rho(p) > \frac{1}{4\pi} \exp\Big(-\frac{2M}{\lambda} \Big) > 0 \ \forall p \in \mathbb{S}^2 \\ & \text{and } \rho(p) \leq \exp(4M/\lambda) \ \forall p \in \mathbb{S}^2 \Big\} \end{aligned}$$

because $\mathcal{P}(\mathbb{S}^2) \setminus \mathcal{S}(\mathbb{S}^2)$ does not contain a minimising sequence. In particular, since $\mathcal{S}(\mathbb{S}^2) \subset L^2(\mathbb{S}^2)$, we may use the Hilbert structure of $L^2(\mathbb{S}^2)$ in order to simplify our problem. The applicability of Lemma 3.2 and Lemma 3.3 is justified because $\|K\|_\infty < \infty$ so that K can be changed by an additive constant and made nonnegative.

Chapter 4

A complete description of all bifurcation points of the Onsager free-energy kernel along the isotropic state

The novel contribution of this chapter is the full characterisation of all bifurcation points of the Euler-Lagrange equation of the three-dimensional Onsager free-energy functional. In addition to writing the interaction potential in terms of associated Legendre polynomials, an idea that goes back to [?], we also use the Taylor expansion of the interaction kernel in three dimensions in order to generalise the applicability of this approach to a general class of two-body interaction potentials. The combination of these steps yields a direct relationship between the coefficients of the Taylor series and the eigenvalues of the interaction operator. This relationship will be made explicit in the case of the Onsager interaction potential.

The Euler-Lagrange equation of the free-energy functional in (1.2) is given by

$$\lambda \ln \rho(p) + \int_{\mathbb{S}^2} k(p \cdot q)\rho(q)\, dq = c.$$

Its derivation is well known and can for example be found in [**?**] or [**?**]. The constant c is obtained through rearranging the equation and imposing the constraint that the distribution function ρ of the orientation integrates to one, see the conditions in (1.1). In particular, c is given by

$$c = -\lambda \ln Z$$

where $Z = \int_{\mathbb{S}^2} \exp\left(-\frac{1}{\lambda}\int_{\mathbb{S}^2} k(p \cdot q)\rho(q)\, dq\right)\, dp$ denotes the partition function. Introducing the thermodynamic potential $\phi : \mathbb{S}^2 \to \mathbb{R}$

$$\phi(p) := \frac{1}{\lambda}\int_{\mathbb{S}^2} k(p \cdot q)\rho(q)\, dq,$$

it follows that $\rho(p) = Z^{-1}\exp(-\phi(p))$ and we can rewrite the Euler-Lagrange equation as

$$\lambda\phi(p) - \frac{1}{Z(\phi)}\int_{\mathbb{S}^2} k(p \cdot q)\exp(-\phi(q))\, dq = 0$$

for

$$Z(\phi) = \int_{\mathbb{S}^2} \exp(-\phi(q))\, dq.$$

Using the rotational symmetry of the interaction kernel, one can show that

$$\int_{\mathbb{S}^2} k(p \cdot q)\, dq = \int_{\mathbb{S}^2} k(p' \cdot q)\, dq$$

and thus we deduce that $\int_{\mathbb{S}^2} k(p \cdot q)\, dq = \text{const}$. The addition or subtraction of a constant to the free-energy functional in (1.2) does not change its critical points. Therefore we assume without loss of generality that

$$\int_{\mathbb{S}^2} k(p \cdot q)\, dq = 0, \tag{4.1}$$

see Remark 5.1 for details in the case of the Onsager interaction potential. Each minimiser of the Onsager free-energy functional must be a solution of the Euler-Lagrange equation. In particular, we prove in Proposition 4.4 that all critical points are elements of the space $C^\infty(\mathbb{S}^2)$. The trivial solution of the Euler-Lagrange equation is given by $\phi_0(p) = 0$ which corresponds to the uniform probability distribution $\rho_0(p) = \frac{1}{4\pi}$ and solves the Euler-Lagrange equation for all λ. It represents the isotropic phase and we are interested in analysing whether other solutions exist. Mathematically speaking, we are interested in those values of λ for which new solutions emerge. Locally, these are the values of λ for which the implicit function theorem is not applicable to the operator $E : H^2\left(\mathbb{S}^2\right) \to H^2\left(\mathbb{S}^2\right)$ given by

$$E(\phi, \lambda) := \lambda\phi(p) - \frac{1}{Z(\phi)} \int_{\mathbb{S}^2} k(p \cdot q) \exp(-\phi(q))\, dq. \tag{4.2}$$

More details about the space $H^2(\mathbb{S}^2)$ and different ways of defining a norm on $H^2(\mathbb{S}^2)$ can be found in Appendix A.

But before we will check the assumptions of the implicit function theorem, it is essential to make sure that the operator E is well-defined.

4.1 The Euler-Lagrange and the interaction operator for the Onsager kernel

In the following section we will step back for a moment and confirm the setting that we are working in. In particular we will show in Section 4.1.1 that the interaction operator U and the Euler-Lagrange operator E are actually acting on the space $H^2(\mathbb{S}^2)$ and that they map into the spaces $H^5(\mathbb{S}^2)$ and $H^2(\mathbb{S}^2)$, respectively. In Section 4.1.2 we prove that all solutions of E are smooth and that E is infinitely many times Fréchet differentiable.

4.1.1 Well-definedness of the Euler-Lagrange and the interaction operator with Onsager kernel

First of all, we will prove that the interaction operator U with Onsager kernel $k_O(\cdot,\cdot)$ is in fact an operator from $H^k(\mathbb{S}^2) \to H^{k+3}$. In particular we show that the operator norm is bounded.

Lemma 4.1. *Let U be the interaction operator corresponding to the Onsager kernel $k_O(p,q) = \sqrt{1-(p\cdot q)^2}$, that is*

$$U(\eta) = \int_{\mathbb{S}^2} k_O(p\cdot q)\eta(q)dq$$

acting on $\eta \in H^k(\mathbb{S}^2)$. *Then*

$$||U||_{H^k(\mathbb{S}^2)\to H^{k+3}(\mathbb{S}^2)} < \infty.$$

Proof. Suppose that $\eta \in H^k(\mathbb{S}^2) \subset L^2(\mathbb{S}^2)$. Expanding η in terms of spherical harmonics such that

$$\eta = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} b_{lm} Y_{lm},$$

we know from Corollary A.3 that the coefficients b_{lm} satisfy the following inequality [?]

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(l + \frac{1}{2}\right)^{2k} |b_{lm}|^2 < \infty. \tag{4.3}$$

Let U be the interaction operator with $UY_{lm} = \mu_l Y_{lm}$ where μ_l are the corresponding eigenvalues which are given by

$$\mu_l = \begin{cases} \frac{\pi\Gamma\left(\frac{l}{2}+\frac{1}{2}\right)\Gamma\left(\frac{l}{2}-\frac{1}{2}\right)}{2\Gamma\left(\frac{l}{2}+1\right)\Gamma\left(\frac{l}{2}+2\right)} & l \text{ even} \\ 0 & \text{otherwise} \end{cases}$$

(see Theorem 4.8 and Lemma 4.10 for details). Thus, for $\tilde{k} > k$

$$\|U\eta\|_{H^{\tilde{k}}} = \sqrt{\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(l + \frac{1}{2}\right)^{2\tilde{k}} |\mu_l|^2 |b_{lm}|^2}.$$

Rewriting the above yields

$$\|U\eta\|_{H^{\tilde{k}}(\mathbb{S}^2)} = \sqrt{\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(l+\frac{1}{2}\right)^{2k}|b_{lm}|^2\underbrace{\left(l+\frac{1}{2}\right)^{2(\tilde{k}-k)}|\mu_l|^2}_{\mathcal{A}_l}}.$$

Due to the fact that $\eta \in H^k(\mathbb{S}^2)$, we know that above bounded provided , see (4.3). Hence we are seeking a bound on the term $\mathcal{A}_l$ which depends on the rate of convergence of the eigenvalues μ_l.

Claim:

$$|\mu_l| \leq Cl^{-3}. \tag{4.4}$$

We know from Section 5.6 in [?] that for $b-a \geq 1$, $a \geq 0$ and $z = x+iy$ with $x > 0$,

$$\left|\frac{\Gamma(z+a)}{\Gamma(z+b)}\right| \leq \frac{1}{|z|^{b-a}} \tag{4.5}$$

and

$$\frac{\Gamma(x+s)}{\Gamma(x+1)} < x^{s-1} \tag{4.6}$$

for $0 < s < 1$. Using (4.5) and (4.6) with $x = \frac{l}{2}$, $s = \frac{1}{2}$, $z = \frac{l}{2} - \frac{1}{2}$, $a = 0$ and

$b = \frac{5}{2}$ yields

$$|\mu_l| = \frac{\pi\Gamma\left(\frac{l}{2}+\frac{1}{2}\right)\Gamma\left(\frac{l}{2}-\frac{1}{2}\right)}{2\Gamma\left(\frac{l}{2}+1\right)\Gamma\left(\frac{l}{2}+2\right)} < \frac{\pi}{2}\left(\frac{l}{2}\right)^{-\frac{1}{2}}\left(\frac{l}{2}-\frac{1}{2}\right)^{-2.5} \leq Cl^{-3}$$

for $l \geq 2$ even which therefore proves the claim.

Thus, if $\tilde{k} \leq k+3$, then

$$\mathcal{A}_l = \left(l+\frac{1}{2}\right)^{2(\tilde{k}-k)} |\mu_l|^2 \leq C\left(l+\frac{1}{2}\right)^6 l^{-6} < C^\star$$

for some constant $C^\star$. In particular,

$$\|U\eta\|_{H^{\tilde{k}}(\mathbb{S}^2)} \leq \sqrt{C\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left(l+\frac{1}{2}\right)^{2k}|b_{lm}|^2} = \sqrt{C}||\eta||_{H^k(\mathbb{S}^2)}$$

implying that

$$\|U\|_{H^k \to H^{k+3}} < \infty.$$

□

Based on this result, we can now prove that the operator T, which constitutes the second part of the Euler-Lagrange operator, E maps $H^2(\mathbb{S}^2)$ into $H^3(\mathbb{S}^2)$.

Lemma 4.2. *Let T be the operator*

$$T(\phi) := \int_{\mathbb{S}^2} k_O(p\cdot q)\exp(-\phi(q))dq$$

where k_O denotes the Onsager kernel. Then $T : H^2(\mathbb{S}^2) \to H^3(\mathbb{S}^2)$.

Proof. Let $\phi \in H^2(\mathbb{S}^2) \subset L^2(\mathbb{S}^2)$. Using Lemma 4.1, we know that $||U||_{H^k(\mathbb{S}^2)\to H^{k+3}(\mathbb{S}^2)} < \infty$. Hence

$$\begin{aligned}||T(\phi)||_{H^3(\mathbb{S}^2)} &= ||U||_{L^2(\mathbb{S}^2)\to H^3(\mathbb{S}^2)}||\exp(-\phi)||_{L^2(\mathbb{S}^2)}\\ &\leq 4\pi||U||_{L^2(\mathbb{S}^2)\to H^3(\mathbb{S}^2)}\exp(||\phi||_\infty)\\ &\leq 4\pi||U||_{L^2(\mathbb{S}^2)\to H^3(\mathbb{S}^2)}\exp C||\phi||_{H^2(\mathbb{S}^2)}\end{aligned}$$

where the last step follows from the Sobolev Embedding theorem

$$\|f\|_{C^0} \leq C\,\|f\|_{H^2(\mathbb{S}^2)}\,. \tag{4.7}$$

□

Finally, we are in a position to prove that E maps $H^2(\mathbb{S}^2)$ onto $H^2(\mathbb{S}^2)$.

Lemma 4.3. *The Euler-Lagrange operator corresponding to the Onsager kernel*

$$E(\phi)(p) = \lambda\phi(p) + \frac{1}{Z(\phi)}\int_{\mathbb{S}^2} k_O(p\cdot q)\exp(-\phi(q))dq$$

maps $\phi \in H^2(\mathbb{S}^2)$ onto $H^2(\mathbb{S}^2)$.

Proof. Again using the Sobolev Embedding theorem, we know that $||\phi||_{L^\infty} \leq C||\phi||_{H^2(\mathbb{S}^2)}$. Hence

$$Z(\phi) = \int_{\mathbb{S}^2}\exp(-\phi(q))dq \geq \exp(-||\phi||_\infty)\int_{\mathbb{S}^2} 1dq \geq 4\pi\exp(-||\phi||_\infty).$$

This fact together with the reasoning that we used in the proof of Lemma 4.2 yields

$$||E(\phi)||_{H^2(\mathbb{S}^2)} \leq |\lambda|||\phi||_{H^2(\mathbb{S}^2)} + \frac{1}{4\pi}e^{||\phi||_\infty}||U||_{L^2(\mathbb{S}^2)\to H^3(\mathbb{S}^2)}\exp(||\phi||_{H^2(\mathbb{S}^2)}).$$

$\square$

Hence we can in fact work under the assumptions we have imposed on the operator E at the beginning of this chapter.

4.1.2 Further properties of the Euler-Lagrange operator and its solutions

We will show that all solutions to $E(\phi, \lambda) = 0$ are smooth and that E is infinitely many times Fréchet differentiable as a mapping from $H^2(\mathbb{S}^2)$ to $H^2(\mathbb{S}^2)$.

Proposition 4.4. *Suppose that $\phi \in L^\infty(\mathbb{S}^2)$ satisfies*

$$E(\phi, \lambda + \lambda_s) = (\lambda_s + \lambda)\phi(p) - \frac{1}{Z(\phi)}\int_{\mathbb{S}^2} k(p \cdot q)e^{-\phi(q)}\,dq = 0.$$

and that k satisfies Assumption 1.3 and that it has a derivative in $L^1(\mathbb{S}^2)$. Then $\phi \in C^\infty(\mathbb{S}^2)$.

Proof. We rearrange the Euler-Lagrange equation as

$$(\lambda_s + \lambda)\phi(p) = \frac{1}{Z(\phi)}\int_{\mathbb{S}^2} k(p \cdot q)e^{-\phi(q)}\,dq.$$

Notice that ϕ is bounded, see Lemma 3.3. Thus, taking the limit for a sequence

$p_n \to p$ on the right hand side, we see that it is continuous due to the dominated convergence theorem and so is the left hand side. Because $k_O(p\cdot q)$ is differentiable almost everywhere, except for $|p \cdot q| = 1$ with an L^1-bounded derivative, we can swap integration and differentiation and conclude that ϕ is differentiable. Having proved that ϕ is continuous and differentiable, we want to show that the derivative of ϕ is continuous and differentiable as well. This will then allow us to proceed by an induction argument. By [**?**] one way to define the C^1-norm is

$$\|\phi\|_{C^1} := \|\phi\|_{C^0} + \max_{1\leq i<j\leq 3} |X_{ij}\phi|_{C^0}$$

where

$$X_{ij}\phi = \frac{d}{dt}\phi\Big(x_1, \ldots, x_{i-1},\\ x_i \cos t - x_j \sin t, x_{i+1}, \ldots, x_{j-1}, x_i \sin t + x_j \cos t, x_{j+1}, \ldots, x_n\Big)$$

are the intrinsic derivatives on $\mathbb{S}^{n-1}$. Here we consider the special case $n = 3$. An elementary calculation shows that

$$X_{ij} Y_l^m(p) Y_l^{m\star}(q) = -Y_l^m(p) X_{ij} Y_l^{m\star}(q).$$

Thus, using the expansion of $k(p, q) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c_l Y_l^m(p) Y_l^{m\star}(q)$, see (4.23), we can calculate

$$
\begin{aligned}
& X_{ij}\lambda\phi \\
&= \frac{1}{Z(\phi)} \int_{\mathbb{S}^2} X_{ij} k(p\cdot q) e^{-\phi(q)}\, dq \\
&= X_{ij} \frac{1}{Z(\phi)} \int_{\mathbb{S}^2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c_l Y_l^m(p) Y_l^{m\star}(q) e^{-\phi(q)}\, dq \\
&= \frac{1}{Z(\phi)} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c_l \int_{\mathbb{S}^2} X_{ij} Y_l^m(p) Y_l^{m\star}(q) e^{-\phi(q)}\, dq \\
&= \frac{1}{Z(\phi)} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c_l Y_l^m(p) \int_{\mathbb{S}^2} \left(- \left(X_{ij} Y_l^{m\star}(q)\right) e^{-\phi(q)} \right)\, dq \\
&= \frac{1}{Z(\phi)} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c_l Y_l^m(p) \int_{\mathbb{S}^2} Y_l^{m\star}(q) \left(X_{ij}\phi(q) e^{-\phi(q)} \right)\, dq \\
&= \frac{1}{Z(\phi)} \int_{\mathbb{S}^2} k_O(p\cdot q) \left(X_{ij}\phi(q) e^{-\phi(q)} \right)\, dq
\end{aligned}
$$

the second line shows that $X_{ij}\phi$ is bounded because the partial derivatives of k are in $L^1(\mathbb{S}^2)$, the step from the third to the second last line follows by applying integration by parts. In particular $(\lambda_s+\lambda)X_{ij}\phi(p)$ is continuous and differentiable. By iteration of this argument, the statement is proved. □

Lemma 4.5. *The Euler Lagrange Equation E corresponding to the Onsager kernel is infinitely many times Fréchet differentiable as a mapping from $H^2(\mathbb{S}^2) \to H^2(\mathbb{S}^2)$.*

Proof. In order to check Fréchet differentiability of E, we need to verify that there exist a linear operator DE satisfying

$$\lim_{\|\eta\|_{H^2(\mathbb{S}^2)}\to 0} \|E(\phi+\eta) - E(\phi) + DE(\phi)\eta\|_{H^2(\mathbb{S}^2)} \|\eta\|^{-1}_{H^2(\mathbb{S}^2)} = 0. \tag{4.8}$$

We take the first and second directional derivatives of

$$E(\phi)(p) = (\lambda_2 + \lambda)\,\phi(p) - \frac{1}{Z(\phi)} \int_{\mathbb{S}^2} k(p\cdot q) e^{-\phi(q)} dq.$$

These are given by

$$\begin{aligned}\partial_\epsilon E(\phi+\epsilon\eta)(p) = (\lambda_2+\lambda)\,\eta(p) &- \frac{\int e^{-\phi(q)-\epsilon\eta(q)}\eta(q)dq}{\left(\int e^{-\phi(q)-\epsilon\eta(q)}dq\right)^2} \int k(p\cdot q) e^{-\phi(q)-\epsilon\eta(q)} dq \\ &- \frac{1}{\int e^{-\phi(q)-\epsilon\eta(q)}dq} \int k(p\cdot q)\eta(q) e^{-\phi(q)-\epsilon\eta(q)} dq.\end{aligned}$$

This gives rise to the operator DE

$$\begin{aligned}DE(\phi)(\eta)(p) = (\lambda_2+\lambda)\,\eta(p) &- \frac{\int e^{-\phi(q)}\eta(q)dq}{\left(\int e^{-\phi(q)}dq\right)^2} \int k(p\cdot q) e^{-\phi(q)} dq \\ &- \frac{1}{\int e^{-\phi(q)-}dq} \int k(p\cdot q)\eta(q) e^{-\phi(q)} dq.\end{aligned}$$

The operator is linear by definition and also bounded which can be shown by a similar argument to the one used in Proposition 4.4. In particular,

$$
\begin{aligned}
&\partial_\epsilon^2 E\left(\phi+\epsilon\eta\right)(p) \\
&\quad= \underbrace{\frac{1}{\int e^{-\phi(q)-\epsilon\eta(q)}dq}\int k(p\cdot q)\eta^2(q)e^{-\phi(q)-\epsilon\eta(q)}dq}_{T_1} \\
&\qquad+ \underbrace{\frac{\int e^{-\phi(q)-\epsilon\eta(q)}\eta^2(q)dq\left(\int e^{-\phi(q)-\epsilon\eta(q)}dq\right)^2}{\left(\int e^{-\phi(q)-\epsilon\eta(q)}dq\right)^4}\int k(p\cdot q)e^{-\phi(q)-\epsilon\eta(q)}dq}_{T_2} \\
&\qquad- \underbrace{\frac{\left(\int e^{-\phi(q)-\epsilon\eta(q)}\eta(q)dq\right)^2 2\int e^{-\phi(q)-\epsilon\eta(q)}dq}{\left(\int e^{-\phi(q)-\epsilon\eta(q)}dq\right)^4}\int k(p\cdot q)e^{-\phi(q)-\epsilon\eta(q)}dq}_{T_3} \\
&\qquad- \underbrace{2\frac{\int e^{-\phi(q)-\epsilon\eta(q)}\eta(q)dq}{\left(\int e^{-\phi(q)-\epsilon\eta(q)}dq\right)^2}\int k(p\cdot q)\eta(q)e^{-\phi(q)-\epsilon\eta(q)}dq}_{T_4}\,.
\end{aligned}
\tag{4.9}
$$

Thus, by the integral form of the remainder in Taylor's theorem in ϵ, we have that

$$E\left(\phi+\eta\right)-\left(E\left(\phi\right)+D_\eta E(\phi)\right)=\int_0^1\left(\partial_\epsilon^2 E\right)\left(\phi+\epsilon\eta\right)(1-\epsilon)d\epsilon.$$

The $\|\cdot\|_{H^2(\mathbb{S}^2)}$-norm of the left hand side can be bounded by

$$\int_0^1\left\|\left(\partial_\epsilon^2 E\right)\left(\phi+\epsilon\eta\right)(1-\epsilon)\right\|_{H^2(\mathbb{S}^2)}d\epsilon$$

and our aim is now to establish an overall bound of the form

$$\left\|E\left(\phi+\eta\right)-\left(E\left(\phi\right)+D_\eta E(\phi)\right)\right\|_{H^2(\mathbb{S}^2)}\le b\left(\|\phi\|_{H^2(\mathbb{S}^2)},\|\eta\|_{H^2(\mathbb{S}^2)}\right)\|\eta\|^2_{H^2(\mathbb{S}^2)}$$

where $b : \mathbb{R}^2 \to \mathbb{R}$ is locally bounded. This would yield that E is Fréchet differentiable. In order to show this, we treat each of the four terms occurring in (4.9) separately using the triangle inequality and the same reasoning as in the proof of Lemma 4.1 and Lemma 4.2. In particular, using the Sobolev embedding theorem yields

$$\begin{aligned}
\|T_1\|_{H^2(\mathbb{S}^2)} &= \left\| \frac{1}{\int e^{-\phi(q)-\epsilon\eta(q)}dq} \int k(p\cdot q)\eta^2(q)e^{-\phi(q)-\epsilon\eta(q)}dq \right\|_{H^2(\mathbb{S}^2)} \\
&\leq \frac{\|U\|_{L^2(\mathbb{S}^2)\to H^2(\mathbb{S}^2)}}{4\pi} e^{2\|\phi\|_\infty + 2\epsilon\|\eta\|_\infty} \left\|\eta^2\right\|_{L^\infty(\mathbb{S}^2)} \\
&\leq C^2 \|U\|_{L^2(\mathbb{S}^2)\to H^2(\mathbb{S}^2)} 4\pi e^{2C\|\phi\|_{H^2(\mathbb{S}^2)} + 2C\epsilon\|\eta\|_{H^2(\mathbb{S}^2)}} \|\eta\|^2_{H^2(\mathbb{S}^2)} .
\end{aligned}$$

Bounds for all other terms and higher order derivatives can be obtained similarly and will be omitted. □

4.2 The eigenvalue problem for general interaction potentials

As mentioned in the beginning of this chapter, we are interested in all values of λ for which the implicit function theorem is not applicable. This is the case whenever the operator $\mathcal{L}_\lambda : H^2(\mathbb{S}^2) \times \mathbb{R} \to H^2(\mathbb{S}^2)$, given by

$$\mathcal{L}_\lambda \eta := \left. \frac{dE(\epsilon\eta, \lambda)}{d\epsilon} \right|_{\epsilon=0} = \lambda\eta(p) + \frac{1}{4\pi} \int_{\mathbb{S}^2} k(p\cdot q)\eta(q)\, dq,$$

is not invertible. Hence we are interested in all non-zero solutions (η, λ) of

$$\lambda\eta(p) + \frac{1}{4\pi}\int_{\mathbb{S}^2} k(p\cdot q)\eta(q)\,dq = 0 \tag{4.10}$$

and therefore in the nullspace of the operator $\mathcal{L}_\lambda$.

Remark 4.6. *Notice that the constraint that ρ integrates to one translates into the fact that the integration of η as in (4.10) yields*

$$\int_{\mathbb{S}^2} \eta(q)dq = 0$$

where we used (4.1).

Rearranging the equation $\mathcal{L}_\lambda\eta(p) = 0$, it becomes apparent that the problem is in fact equivalent to the eigenvalue problem for the interaction operator in (1.3)

$$U\eta(p) = \int_{\mathbb{S}^2} k(p\cdot q)\eta(q)\,dq.$$

In particular, we observe that for any eigenvalue μ of U, a solution to the Euler-Lagrange equation is given by the corresponding eigenvector of U and

$$\lambda = -\frac{\mu}{4\pi}. \tag{4.11}$$

Even though this eigenvalue problem involves only a linear interaction operator, it is not trivial. In the following theorem, we derive an explicit expression for all eigenvalues of U, and thus we find the set of all possible bifurcation points of the Onsager free-energy functional locally around $\phi_0 = 0$. In particular we make use of the fact that functions in $H^2(\mathbb{S}^2)$ can be expanded in terms of spherical harmonics, see Section 4.2.1 and Appendix A.

We solve the eigenvalue problem in (4.10) for all physically motivated interaction potentials satisfying Assumption 1.3, that means for all interaction potentials which are rotationally symmetric and continuous. The proofs rely heavily on the concept of spherical harmonics and Legendre polynomials which will be briefly introduced first.

4.2.1 Brief introduction to spherical harmonics and Legendre polynomials

The spherical harmonics are defined as

$$Y_l^m(\varphi, \theta) := N_{lm} e^{im\varphi} P_l^m(\cos\theta)$$

where $\varphi \in [0, 2\pi)$ is the polar angle and $\theta \in [0, \pi)$ the azimuthal angle. The subscript l denotes its degree while $-l \leq m \leq l$ denotes its order. N_{lm} is a normalisation constant given by

$$N_{lm} := (-1)^m \left(\frac{2l+1}{4\pi}\right)^{1/2} \left(\frac{(l-m)!}{(l+m)!}\right)^{1/2}.$$

We write P_l^m for the associated Legendre polynomials given by

$$P_l^m(\mu) := \frac{1}{2^l l!} \left(1-\mu^2\right)^{m/2} \frac{\partial^{l+m}}{\partial \mu^{l+m}} (\mu^2 - 1)^l.$$

The Legendre polynomials $P_n(x)$ are defined as

$$P_n(x) := \frac{1}{2^n n!} \frac{2^n}{dx^n} \left[(x^2-1)^n \right].$$

One of the most important facts about spherical harmonics is that they build an orthonormal basis of $L^2(\mathbb{S}^2)$. In general, spherical harmonics are known as eigenfunctions of the Laplacian. However, it seems that they can be understood in a much broader sense as eigenfunctions of rotationally symmetric operators. For more information on spherical harmonics, associated Legendre polynomials and Legendre polynomials we recommend [?], [?] and [?].

One of the main ingredients to write the interaction operator in terms of spherical harmonics is the following relationship between Legendre polynomials and monomials.

Lemma 4.7. *For $r \in \mathbb{N}$ and $x \in \mathbb{C}$*

$$x^r = \sum_{l=r,r-2,\dots} \frac{(2l+1)r!}{2^{(r-l)/2}(\frac{1}{2}(r-l))!(l+r+1)!!} P_l(x) \tag{4.12}$$

where P_l denotes the Legendre polynomial [?].

Even though this result seems to be known in the literature, we could not find a proof for it.

Proof. The claim follows from an induction based on the following reccurrence relation for Legendre polynomials

$$xP_l(x) = \frac{l+1}{2l+1}P_{l+1}(x) + \frac{l}{2l+1}P_{l-1}(x) \tag{4.13}$$

with the convention that $P_{-1} = 0$ [?]. The base case $r = 0$ is trivial because $P_0 = 1$, so let us move on to the actual induction step. Multiplying both sides of (4.12) by x and using (4.13) yields

$$x^{r+1} = \sum_{l=r,r-2,\dots} \frac{(2l+1)r!}{2^{(r-l)/2}(\frac{1}{2}(r-l))!(l+r+1)!!}\left(\frac{l+1}{2l+1}P_{l+1}(x) + \frac{l}{2l+1}P_{l-1}(x)\right).$$

We now change the indices in the two parts of the sum corresponding to P_{l+1} and P_{l-1} in order to create two sums with indices corresponding to P_l which can then be combined into one sum. Of course using such a procedure requires extra care when computing the border terms. Overall we obtain

$$\begin{aligned} x^{r+1} = &\sum_{l=r-1,r-3,\dots>1} \frac{lr!(l+r+2) + 2\frac{1}{2}(r+1-l)(l+1)r!}{2^{(r+1-l)/2}(\frac{1}{2}(r+1-l))!(l+r+2)!!}P_l(x) \\ &+ \frac{r!}{(l+1+r)!!}\frac{r+1}{1}P_{r+1}(x) + \begin{cases} \frac{3r!}{2^{(r-1)/2}(\frac{1}{2}(r-1))!(r+2)!!}\frac{1}{3}P_0(x) & \text{if } r \text{ is odd} \\ \frac{5r!}{2^{(r-2)/2}(\frac{1}{2}(r-2))!(r+3)!!}\frac{2}{5}P_1(x) & \text{if } r \text{ even} \end{cases}. \end{aligned}$$

Putting everything together yields

$$x^{r+1} = \sum_{l=r+1,r-1,\dots\geq 0} \frac{(2l+1)(r+1)!}{2^{(r+1-l)/2}(\frac{1}{2}(r+1-l))!(l+r+2)!!}P_l(x)$$

which concludes the induction step. □

This result can now be used in order to rewrite the interaction operator as multiplication operator acting on spherical harmonics.

4.2.2 Eigenvalues and eigenfunctions of interaction kernels

Theorem 4.8. *Let $K(\cdot,\cdot) : \mathbb{S}^2 \times \mathbb{S}^2 \to \mathbb{R}$ be an interaction kernel that satisfies Assumption 1.3 and assume that $k(\cdot)$ admits a Taylor expansion such that $k(p\cdot q) = \sum_{r=0}^{\infty} a_r (p \cdot q)^r$ converges for all $(p,q) \in \{p,q \in \mathbb{S}^2 || p \cdot q| < 1\}$ and a_r satisfy the condition that*

$$\sum_{l=0}^{\infty} \sum_{r=l,l+2,l+4,\ldots} \left| \frac{4\pi(4l+1)^{3/2} a_r r!}{2^{(r-l)/2}(\frac{1}{2}(r-l))!(l+r+1)!!} \right| < \infty. \tag{4.14}$$

Then the eigenfunctions of the corresponding interaction operator

$$U\eta(p) = \int_{\mathbb{S}^2} k(p\cdot q)\eta(q)\, dq$$

are given by the spherical harmonics $Y_l^m : \mathbb{S}^2 \to \mathbb{C}$. The corresponding eigenvalues are given by

$$\mu_s = \sum_{r=0}^{\infty} \frac{4\pi a_{s+2r}(s+2r)!}{2^r r!(2s+2r+1)!!} \tag{4.15}$$

where $s \in \mathbb{N}$.

Remark 4.9. *Notice that the dipolar kernel corresponds to $a_1 = 1$ while the Maier-Saupe kernel corresponds $a_2 = -1$ and all other coefficients set to 0.*

Proof. We denote by $P_l(x)$ the associated Legendre polynomials of order l (for more details see Section 4.2.1). Applying Lemma 4.7 to the kernel

$$k(p \cdot q) = \sum_{r=0}^{\infty} a_r (p \cdot q)^r,$$

it follows that

$$k(p \cdot q) = \sum_{r=0}^{\infty} \sum_{l=r,r-2,\ldots} a_r \frac{(2l+1)r!}{2^{(r-l)/2}(\frac{1}{2}(r-l))!(l+r+1)!!} P_l(p \cdot q).$$

Using the addition theorem for Legendre polynomials [?, page 395],

$$P_l(x \cdot x') = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_l^m(x) Y_l^{m\star}(x'), \tag{4.16}$$

we obtain that

$$k(p \cdot q) = \sum_{r=0}^{\infty} \sum_{l=r,r-2,\ldots} \sum_{m=-l}^{l} c_l^r Y_l^m(p) Y_l^{m\star}(q) \tag{4.17}$$

with

$$c_l^r := \frac{4\pi a_r r!}{2^{(r-l)/2}(\frac{1}{2}(r-l))!(l+r+1)!!}.$$

Integrating the interaction kernel against an arbitrary spherical harmonic $Y_s^n(q)$, swapping the order of the sum and the integral and using the orthogonality of spherical harmonics, it follows that

$$\begin{aligned}\int_{\mathbb{S}^2} k(p\cdot q)Y_s^n(q)\,dq &= \sum_{r=0}^{\infty}\sum_{l=r,r-2,\ldots}\sum_{m=-l}^{l} c_l^r Y_l^m(p)\int_{\mathbb{S}^2} Y_l^{m\star}(q)Y_s^n(q)\mathbb{1}_{|p\cdot q|<1}\,dq\\ &= \sum_{r=0}^{\infty}\sum_{l=r,r-2,\ldots}\sum_{m=-l}^{l} c_l^r Y_l^m(p)\delta_{sl}\delta_{mn}.\end{aligned} \tag{4.18}$$

Notice that the interchange of the infinite sum and the integral needs of course to be verified. Viewing the infinite sum as an integral with respect to the counting measure, Fubini's theorem applies if

$$\sum_{r=0}^{\infty}\int_{\mathbb{S}^2}\left|\sum_{l=r,r-2,\ldots}\sum_{m=-l}^{l} c_l^r Y_l^m(p)Y_l^{m\star}(q)Y_s^n(q)\right|\,dq<\infty. \tag{4.19}$$

In particular, using the Cauchy-Schwarz inequality and the fact that all spherical harmonics have unit mass with respect to the L^2-norm, we obtain

$$\begin{aligned}&\sum_{r=0}^{\infty}\int_{\mathbb{S}^2}\left|\sum_{l=r,r-2,\ldots}\sum_{m=-l}^{l} c_l^r Y_l^m(p)Y_l^{m\star}(q)Y_s^n(q)\mathbb{1}_{|p\cdot q|<1}\right|\,dq\\ &\qquad\le \sum_{r=0}^{\infty}\sum_{l=r,r-2,\ldots}\sum_{m=-l}^{l}|c_l^r||Y_l^m(p)|\int_{\mathbb{S}^2}\left|Y_l^{m\star}(q)Y_s^n(q)\mathbb{1}_{|p\cdot q|<1}\right|\,dq\\ &\qquad\le \sum_{r=0}^{\infty}\sum_{l=r,r-2,\ldots}\sum_{m=-l}^{l}|c_l^r||Y_l^m(p)|.\end{aligned}$$

Moreover, it follows from [?, Proposition 7.0.1] that any spherical harmonic Y_l^m is bounded by

$$||Y_l^m||_\infty \le \sqrt{\frac{2l+1}{\text{vol }(\mathbb{S}^2)}}.$$

Hence,

$$\sum_{r=0}^{\infty}\int_{\mathbb{S}^2}\left|\sum_{l=r,r-2,\ldots}\sum_{m=-l}^{l} c_l^r Y_l^m(p)Y_l^{m\star}(q)Y_s^n(q)\mathbb{1}_{|p\cdot q|<1}\right| dq$$
$$=\frac{1}{(4\pi)^{3/2}}\sum_{r=0}^{\infty}\sum_{\substack{l=0\\ l\leq r}}^{\infty}(2l+1)^{3/2}|c_l^r|. \tag{4.20}$$

Again we can view the two sums as integrals with respect to the counting measure and we may swap the order of summation according to Fubini's theorem if the absolute value of the underlying function is integrable with respect to any order of integration. Therefore the validity of swapping the order of summation in (4.20) is simultaneously proved when we establish our original claim in (4.19). Therefore a basic condition that suffices to be proved in order to guarantee the validity of the interchange of the integrals in (4.18) is given by

$$\sum_{l=0}^{\infty}\sum_{r=l,l+2,l+4,\ldots}(2l+1)^{3/2}|c_l^r|<\infty. \tag{4.21}$$

In particular, one needs to show on a case to case basis that the coefficients $|c_l^r|$ decay faster than $l^{3/2}$. In Lemma 4.11 we prove this condition in the case of the Onsager kernel. For all other cases this condition is assumed to hold (see the statement of the theorem).

Having established (4.18), we deduce that

$$\int_{\mathbb{S}^2} k(p\cdot q)Y_s^n(q)\, dq=\sum_{r=0}^{\infty}\frac{4\pi a_{s+2r}(s+2r)!}{2^r r!(2s+2r+1)!!}Y_s^n(p) \tag{4.22}$$

with

$$c_l^r = \sum_{r=s,s+2,\ldots}^{\infty} \frac{4\pi a_r r!}{2^{(r-s)/2}(\frac{1}{2}(r-s))!(s+r+1)!!} \qquad = \sum_{r=0}^{\infty} \frac{4\pi a_{s+r}(s+2r)!}{2^r(r)!(2s+2r+1)!!}.$$

From the last equation we may conclude that the eigenfunctions of the interaction operator $U\eta(p) = \int_{\mathbb{S}^2} k(p\cdot q)\eta(q)\, dq$ associated to the class of two-body interaction potentials $k(p \cdot q)$ described in the statement of this theorem are given by the spherical harmonics Y_s^n and that their corresponding eigenvalues are given by

$$\mu_s = \sum_{r=0}^{\infty} \frac{4\pi a_{s+2r}(s+2r)!}{2^r r!(2s+2r+1)!!}$$

with $s \in \mathbb{N}$. $\square$

4.3 Bifurcation points of the Onsager free-energy functional with Maier-Saupe and Onsager kernel

Recall that the Maier-Saupe interaction potential is given by

$$k_{MS}(p \cdot q) = \frac{1}{3} - (p \cdot q)^2. \qquad \text{(see 1.5)}$$

In terms of Legendre polynomials, the Maier-Saupe kernel can also be written as

$$k_{MS}(p \cdot q) = -\frac{2}{3} P_2(p \cdot q)$$

where P_2 denotes the second Legendre polynomial. Using (4.16), we have that

$$k_{MS}(p \cdot q) = -\frac{8\pi}{15} \sum_{m=-2}^{2} Y_l^m(p) Y_l^m(q).$$

Following the reasoning in the proof of Theorem 4.8, we may conclude that there is only one non-zero eigenvalue in the case of the Maier-Saupe interaction kernel which is given by

$$\mu_{MS} = -\frac{8\pi}{15}$$

(notice that the verification of (4.21) is trivial in this case). The only other eigenvalue is zero with infinite multiplicity. Thus, the only bifurcation from the isotropic state occurs at $\lambda_{MS} = \frac{2}{15}$.

Due to its singular nature, the Onsager kernel is a little bit more complex. In fact, we will see that we have got infinitely many eigenvalues corresponding to the interaction operator U. By the help of the following lemma all eigenvalues can be written as single expressions of closed form. For ease of presentation we will state the result now and leave the proof until the end of the section.

Lemma 4.10. *Let $s \in 2\mathbb{N}$. Then*

$$\sum_{r=s/2}^{\infty} \frac{4\pi (2r)!^2}{(1-2r)(r!)^2 (4^r) 2^{r-s/2} (r-s/2)!(s+2r+1)!!} = -\frac{\pi \Gamma(s/2+\frac{1}{2})\Gamma(s/2-1/2)}{2\Gamma(s/2+1)\Gamma(s/2+2)}$$

where $\Gamma(\cdot)$ *denotes the gamma function, see* [**?**, page 1137] *for details.*

Based on this result, we are now in the position to verify condition (4.21) allowing us to interchange the order of integration and the infinite sum in Theorem 4.8.

Lemma 4.11. *The change of integral and infinite sum in* (4.18) *is valid in the case of the Onsager kernel. In other words, we can verify condition* (4.21)*, stating that*

$$\sum_{l=0}^{\infty}\sum_{r=l}^{\infty}(2l+1)^{3/2}|c_l^r| < \infty,$$

for

$$c_l^r := \begin{cases} \frac{4\pi(2r)!^2}{(1-2r)(r!)^2(4^r)2^{r-l}(r-l)!(2l+2r+1)!!} & \text{if } l \leq r \\ 0 & \text{if } l > r \end{cases}.$$

Moreover, the eigenvalues of the interaction operator equipped with the Onsager kernel decrease faster than l^{-3}*.*

Proof. Based on the Taylor expansion of the square root function $\sqrt{1-x}$ for all $x \in (-1, 1)$, the Taylor expansion of the Onsager kernel is given by

$$k_O(p \cdot q) = \sum_{r=0}^{\infty} \frac{(2r)!}{(1-2r)(r!)^2(4^r)}(p \cdot q)^{2r}$$

for all $p, q \in \mathbb{S}^2$ such that $|p \cdot q| < 1$. We deduce that

$$k_O(p \cdot q) = \sum_{r=0}^{\infty} a_r (p \cdot q)^r \text{ with } a_r = \begin{cases} \frac{r!}{(1-r)(\frac{r}{2}!)^2(2^r)} & \text{if } r \text{ is even} \\ 0 & \text{if } r \text{ is odd} \end{cases}$$

and thus using (4.17)

$$\begin{aligned} k_O(p \cdot q) &= \sum_{r=0}^{\infty} \sum_{l=2r,2(r-1),\ldots} \sum_{m=-l}^{l} \frac{4\pi(2r)!^2 Y_l^m(p) Y_l^{m\star}(q)}{(1-2r)(r!)^2(4^r)2^{r-l/2}(r-l/2)!(l+2r+1)!!} \\ &= \sum_{r=0}^{\infty} \sum_{l=0}^{r} \sum_{m=-2l}^{2l} \frac{4\pi(2r)!^2 Y_{2l}^m(p) Y_{2l}^{m\star}(q)}{(1-2r)(r!)^2(4^r)2^{r-l}(r-l)!(2l+2r+1)!!}. \end{aligned} \tag{4.23}$$

With regard to (4.23), the Onsager kernel is given by

$$K_O(p, q) = \sum_{r=0}^{\infty} \sum_{l=0}^{r} \sum_{m=-2l}^{2l} \underbrace{\frac{4\pi(2r)!^2}{(1-2r)(r!)^2(4^r)2^{r-l}(r-l)!(2l+2r+1)!!}}_{=:c_l^r} Y_{2l}^m(p) Y_{2l}^{m\star}(q). \tag{4.24}$$

Due to the fact that the first factor in the denominator is the only negative factor in the whole product, all coefficients c_l^r are negative except for $c_0^0 = 4\pi$. Taking this into account and applying Lemma 4.10, we know that

$$\begin{aligned} &\sum_{l=0}^{\infty} \sum_{r=l}^{\infty} (2l+1)^{3/2} |c_l^r| \\ &\qquad = \sum_{l=1}^{\infty} (2l+1)^{3/2} \sum_{r=l}^{\infty} |c_l^r| + \sum_{r=0}^{\infty} |c_0^r| \end{aligned}$$

$$
\begin{aligned}
&= -\sum_{l=1}^{\infty}(2l+1)^{3/2}\sum_{r=l}^{\infty} c_l^r + \left(-\sum_{r=0}^{\infty} c_0^r + 2c_0^0\right) \\
&= \frac{\pi}{2}\sum_{l=1}^{\infty}(2l+1)^{3/2}\frac{\Gamma(l+\frac{1}{2})\Gamma(l-1/2)}{\Gamma(l+1)\Gamma(l+2)} + \left(\frac{\pi\Gamma(\frac{1}{2})\Gamma(-1/2)}{2\Gamma(1)\Gamma(2)} + 8\pi\right) \\
&= \frac{\pi}{2}\sum_{l=1}^{\infty}(2l+1)^{3/2}\frac{\Gamma(l+\frac{1}{2})\Gamma(l-1/2)}{\Gamma(l+1)\Gamma(l+2)} + \left(-\pi^2 + 8\pi\right). \qquad (4.25)
\end{aligned}
$$

Using the claim in (4.4) yields

$$
\frac{\Gamma(l+\frac{1}{2})\Gamma(l-1/2)}{\Gamma(l+1)\Gamma(l+2)} < \frac{C}{l^3}
$$

for some constant C. Inserting this inequality into (4.25) yields

$$
\sum_{l=0}^{\infty}\sum_{r=l}^{\infty}(2l+1)^{3/2}|c_l^r| < \frac{C\pi}{2}\sum_{l=1}^{\infty}\frac{(2l+1)^{3/2}}{l^3} + \left(-\pi^2+8\pi\right).
$$

Comparing this with the harmonic p-series, we observe that

$$
\frac{C\pi}{2}\sum_{l=1}^{\infty}\frac{(2l+1)^{3/2}}{l^3} + \left(-\pi^2+8\pi\right) \sim C_1\sum_{l=1}^{\infty}\frac{1}{l^{3/2}} + C_2 < \infty
$$

for some constants C_1 and C_2 which therefore proves the first part of the claim. The second part follows easily from (4.4). □

With Lemma 4.10 and Lemma 4.11 at hand, we are now ready to prove the main result of this section.

Theorem 4.12. *The eigenfunctions and eigenvalues of the interaction operator U associated with the Onsager kernel $k_O(p \cdot q) = \sqrt{1-(p\cdot q)^2}$ are given by the* *spherical harmonics*

$$\{Y_s^n \in L^2(\mathbb{S}^2) : s \in \mathbb{N} \textit{ even }, -s \leq n \leq s\}$$

and

$$\mu_O(s) := \begin{cases} -\frac{\pi\Gamma(s/2+\frac{1}{2})\Gamma(s/2-1/2)}{2\Gamma(s/2+1)\Gamma(s/2+2)} & \textit{if } s \textit{ is even} \\ 0 & \textit{if } s \textit{ is odd} \end{cases}.$$

Each eigenvalue $\mu_O(s)$ for $s > 0$ even has multiplicity $2s+1$. The eigenvalue zero has infinite multiplicity.

Proof. First of all we recall from (4.24) that the series expansion of the Onsager interaction potential in terms of spherical harmonics is given by

$$K_O(p,q) = \sum_{r=0}^{\infty}\sum_{l=0}^{r}\sum_{m=-2l}^{2l} \underbrace{\frac{4\pi(2r)!^2}{(1-2r)(r!)^2(4^r)2^{r-l}(r-l)!(2l+2r+1)!!}}_{=:c_l^r} Y_{2l}^m(p)Y_{2l}^{m\star}(q).$$

Based on this expansion, it follows that

$$\begin{aligned}
&\int_{\mathbb{S}^2} k_O(p\cdot q)Y_s^n(q)\,dq \\
&\quad = \int_{\mathbb{S}^2}\left(\sum_{r=0}^{\infty}\sum_{l=0}^{r}\sum_{m=-2l}^{2l}\frac{4\pi(2r)!^2 Y_{2l}^m(p)Y_{2l}^{m\star}(q)Y_s^n(q)\mathbb{1}_{|p\cdot q|<1}}{(1-2r)(r!)^2(4^r)2^{r-l}(r-l)!(2l+2r+1)!!}\right)dq \\
&\quad = \sum_{l=0}^{\infty}\sum_{r=l}^{\infty}\frac{4\pi(2r)!^2}{(1-2r)(r!)^2(4^r)2^{r-l}(r-l)!(2l+2r+1)!!}\sum_{m=-2l}^{2l}Y_{2l}^m(p)\delta_{mn}\delta_{(2l)s}
\end{aligned}$$

$$= \begin{cases} \sum_{r=s/2}^{\infty} \frac{4\pi(2r)!^2}{(1-2r)(r!)^2(4^r)2^{r-s/2}(r-s/2)!(s+2r+1)!!} Y_s^n(p) & \text{if } s \text{ is even} \\ 0 & \text{if } s \text{ is odd} \end{cases}$$

where we used the orthogonality of the spherical harmonics and Lemma 4.11 which allows us to change the order of integration and summation. An application of Lemma 4.10 yields the result. □

Based on Theorem 4.12 and (4.11), we therefore conclude that a set of all possible bifurcation points is given by

$$\lambda_O(s) = \begin{cases} \frac{\Gamma(s/2+\frac{1}{2})\Gamma(s/2-1/2)}{8\Gamma(s/2+1)\Gamma(s/2+2)} & \text{if } s \text{ is even} \\ 0 & \text{if } s \text{ is odd} \end{cases}.$$

Remark 4.13. *We will show in Section 7.5 that in fact any point $\lambda_O(s)$ is a bifurcation point.*

In order to conclude this section, it is left to prove the statement of Lemma 4.10.

Proof of Lemma 4.10. First of all, we translate the sum by $s/2$. This yields

$$\sum_{r=s/2}^{\infty} \frac{4\pi(2r)!^2}{(1-2r)(r!)^2(4^r)2^{r-s/2}(r-s/2)!(s+2r+1)!!}$$
$$= \sum_{r=0}^{\infty} \frac{\pi((2r+s)!)^2}{(1-2r-s)((r+s/2)!)^2 2^{3r+s-2} r!(2s+2r+1)!!}.$$

In the case of odd integers $n = 2k-1$ for $k \geq 1$, the double factorial $n!!$ can be replaced by the expression $n!! = \frac{(2k)!}{2^k k!}$ [**?**, page 823]. Hence we can rewrite the terms such that

$$
\begin{aligned}
&\sum_{r=0}^{\infty} \frac{\pi((2r+s)!)^2}{(1-2r-s)((r+s/2)!)^2(2^{3r+s-2})r!(2(r+s+1)-1)!!} \\
&\quad = \sum_{r=0}^{\infty} \frac{\pi((2r+s)!)^2 2^{-2r+3}(r+s+1)!}{(1-2r-s)((r+s/2)!)^2 r!(2(r+s+1))!} \\
&\quad = -\pi \sum_{r=0}^{\infty} \left(\frac{(2r+s)!}{(r+s/2)!}\right)^2 \frac{(r+s+1)!}{(2(r+s+1))!} \frac{(2r+s-2)!}{(2r+s-1)!} \frac{2^{-2r+3}}{r!}.
\end{aligned}
$$

Notice that we also expressed the first factor in the denominator as fraction of two factorials. This sum can now further be manipulated by rewriting it in terms of gamma functions [**?**, page 1137], $\Gamma(s+1) = s!$. It follows that

$$
\begin{aligned}
&-\pi \sum_{r=0}^{\infty} \left(\frac{(2r+s)!}{(r+s/2)!}\right)^2 \frac{(r+s+1)!}{(2(r+s+1))!} \frac{(2r+s-2)!}{(2r+s-1)!} \frac{2^{-2r+3}}{r!} \\
&\quad = -\pi \sum_{r=0}^{\infty} \left(\frac{\Gamma(2r+s+1)}{\Gamma(r+s/2+1)}\right)^2 \frac{\Gamma(r+s+2)}{\Gamma(2(r+s)+3))} \frac{\Gamma(2r+s-1)}{\Gamma(2r+s)} \frac{2^{-2r+3}}{r!} \\
&\quad = -\pi \sum_{r=0}^{\infty} \left(\frac{(2r+s)\Gamma(2r+s)}{(r+s/2)\Gamma(r+s/2)}\right)^2 \frac{(r+s+1)\Gamma(r+s+1)\Gamma(2r+s-1)2^{-2r+3}}{(2(r+s+1))\Gamma(2(r+s+1))\Gamma(2r+s)r!} \\
&\quad = -\pi \sum_{r=0}^{\infty} \left(\frac{\Gamma(2r+s)}{\Gamma(r+s/2)}\right)^2 \frac{\Gamma(r+s+1)}{\Gamma(2(r+s+1))} \frac{\Gamma(2r+s-1)}{\Gamma(2r+s)} \frac{2^{-2r+4}}{r!}.
\end{aligned}
$$

Applying the duplication formula for the gamma function [**?**, page 1139]

$$
\frac{\Gamma(2z)}{\Gamma(z)} = \frac{2^{2z-1}\Gamma(z+\frac{1}{2})}{\sqrt{\pi}}
$$

to the first two factors and its rearranged form

$$\Gamma(z) = \frac{2^{z-1}\Gamma(z/2+\frac{1}{2})\Gamma(z/2)}{\sqrt{\pi}},]$$

to the two terms forming the third factor, we deduce that

$$\begin{aligned}
&-\pi\sum_{r=0}^{\infty}\left(\frac{\Gamma(2r+s)}{\Gamma(r+s/2)}\right)^2\frac{\Gamma(r+s+1)}{\Gamma(2(r+s+1))}\frac{\Gamma(2r+s-1)}{\Gamma(2r+s)}\frac{2^{-2r+4}}{r!}\\
&\quad=-\pi\sum_{r=0}^{\infty}\left(\frac{2^{2r+s-1}\Gamma(r+s/2+\frac{1}{2})}{\sqrt{\pi}}\right)^2\frac{2^{1-2(r+s+1)}\sqrt{\pi}}{\Gamma(r+s+3/2)}\\
&\qquad\qquad\cdot\frac{2^{2r+s-2}\Gamma(r+s/2)\Gamma(r+s/2-1/2)}{2^{2r+s-1}\Gamma(r+s/2+1/2)\Gamma(r+s/2)}\frac{2^{-2r+4}}{r!}\\
&\quad=-\sqrt{\pi}\sum_{r=0}^{\infty}\frac{\Gamma(r+s/2+\frac{1}{2})\Gamma(r+s/2-1/2)}{\Gamma(r+s+3/2)}\frac{1}{r!}.
\end{aligned}$$

Let $(x)_r$ denote the Pochhammer symbols which are given by

$$\begin{aligned}
(x)_0 &= 1\\
(x)_r &= \frac{\Gamma(x+r)}{\Gamma(x)}
\end{aligned}$$

for any $x \in \mathbb{C}$ and $r \in \mathbb{R}$. Rewriting our expression in terms of Pochhammer symbols [**?**], we obtain

$$\begin{aligned}
&-\sqrt{\pi}\sum_{r=0}^{\infty}\frac{\Gamma(r+s/2+\frac{1}{2})\Gamma(r+s/2-1/2)}{\Gamma(r+s+3/2)}\frac{1}{r!}\\
&\quad=-\frac{\sqrt{\pi}\Gamma(s/2+\frac{1}{2})\Gamma(s/2-1/2)}{\Gamma(s+3/2)}\sum_{r=0}^{\infty}\frac{(s/2+\frac{1}{2})_r(s/2-1/2)_r}{(s+3/2)_r}\frac{1}{r!}.
\end{aligned}$$

This sum can now easily be evaluated using generalised hypergeometric functions [?].

Definition 4.14. *The generalised hypergeometric function ${}_pF_q$ is defined as*

$$ {}_pF_q(x_1, x_2, \ldots, x_p; y_1, y_2, \ldots, y_q; z) = \sum_{r=0}^{\infty} \frac{(x_1)_r (x_2)_r \ldots (x_p)_r}{(y_1)_r (y_2)_r \ldots (y_q)_r} \frac{z^r}{r!} $$

for $x_i, y_i, z \in \mathbb{C}$ and where $(x)_r$ denote the Pochhammer symbols.

In particular, we are now in the position to use Gauss's Hypergeometric Theorem which states that

Theorem 4.15 (Gauss's Hypergeometric Theorem, [?, page 1438])**.** *For $a, b, c \in \mathbb{C}$*

$$ {}_2F_1(a, b, c; 1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} $$

for $Re(c - a - b) > 0$ where $Re(z)$ denotes the real part of a complex number.

An application of Gauss's Hypergeometric Theorem yields

$$ \begin{aligned} & -\frac{\sqrt{\pi}\Gamma(s/2+\frac{1}{2})\Gamma(s/2-1/2)}{\Gamma(s+3/2)} \sum_{r=0}^{\infty} \frac{(s/2+\frac{1}{2})_r (s/2-1/2)_r}{(s+3/2)_r} \frac{1}{r!} \\ &= -\frac{\sqrt{\pi}\Gamma(s/2+\frac{1}{2})\Gamma(s/2-1/2)}{\Gamma(s+3/2)} {}_2F_1(s/2+1/2, s/2-1/2; s+3/2, 1) \\ &= -\frac{\sqrt{\pi}\Gamma(s/2+\frac{1}{2})\Gamma(s/2-1/2)}{\Gamma(s+3/2)} \frac{\Gamma(s+3/2)\Gamma(3/2)}{\Gamma(s/2+1)\Gamma(s/2+2)} \\ &= -\frac{\sqrt{\pi}\Gamma(s/2+\frac{1}{2})\Gamma(s/2-1/2)\Gamma(3/2)}{\Gamma(s/2+1)\Gamma(s/2+2)}. \end{aligned} $$

Using the fact that $\Gamma(3/2) = \frac{\sqrt{\pi}}{2}$, it follows that for all $s \in 2\mathbb{N}$

$$\sum_{r=s/2}^{\infty} \frac{4\pi (2r)!^2}{(1-2r)(r!)^2(4^r)2^{r-s/2}(r-s/2)!(s+2r+1)!!}$$
$$= -\frac{\pi\Gamma(s/2+\frac{1}{2})\Gamma(s/2-1/2)}{2\Gamma(s/2+1)\Gamma(s/2+2)}.$$

$\square$

Chapter 5

Bifurcations of the Onsager free-energy functional

The Onsager free-energy functional

$$\mathcal{F}(\rho, \lambda) := \lambda \int_{\mathbb{S}^2} \rho(p) \ln \rho(p) \; dp + \frac{1}{2} \int_{\mathbb{S}^2} \int_{\mathbb{S}^2} K(p, q)\rho(p)\rho(q) \; dp \; dq$$

consists of two terms, each of which resembles the orientational and the translational entropy of the system, respectively. Due to the interplay between these two entropies, there exist critical values of λ at which the system undergoes a phase transition. In this chapter, we show that for all interaction potentials satisfying Assumption 1.3 for large values of λ the unique minimiser is given by the uniform probability density $\rho_0 = \frac{1}{4\pi}$ and that new bifurcation branches form as λ decreases. In particular we will show analytically that a transcritical bifurcation arises in case of the Onsager potential at the value $\lambda_2 = \frac{\pi}{32}$. This fact has been proven numerically by Kayser and Raveché [?]. Their result is shown in Figure 5.1.

Our aim is to understand better how many different branches of solutions (up

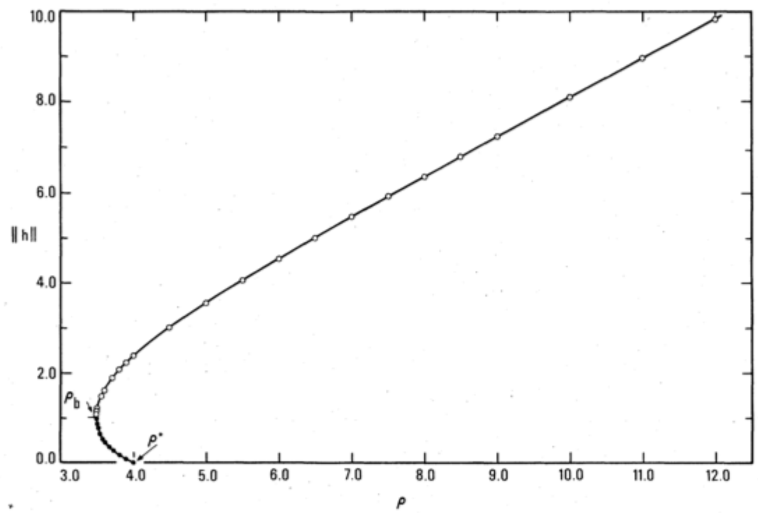


Figure 5.1: Numerical calculation of the bifurcation diagram of $\mathcal{F}$ with Onsager interaction potential [?]. Notice that the value at which the transcritical bifurcation occurs differs from the value $\lambda_2 = \frac{\pi}{32} \approx 0.1$ which we found in Chapter 4. This is due to a difference in constants that have been taken into account.

to rotational symmetry) arise for different interaction potentials so we will keep most of our analysis quite general.

Having found all bifurcation points from the isotropic state of the Onsager free-energy functional equipped with a general class of interaction operators in Chapter 4, we are now in the position to direct our attention to the corresponding bifurcation equations. The presentation of our results is divided into two parts. We begin by giving a brief introduction to the Lyapunov-Schmidt decomposition, which is our main tool for computing the bifurcation equation, see Section 5.1. In Section 5.2 we focus on the practicalities that are involved when we apply the Lyapunov-Schmidt decomposition to the Euler-Lagrange operator given in (4.2). In particular, Section 5.2 is divided into four parts: a reformulation of the problem in the language of Section 5.1, see Section 5.2.1, an algorithmic procedure that allows us to fulfil the decomposition, see Sections 5.2.2 and 5.2.4, and the presentation of an algorithm that allows the fast computation of products of spherical harmonics in terms of spherical harmonics, see Section 5.2.3.

5.1 The theory: The Lyapunov-Schmidt decomposition

This brief introduction to the Lyapunov-Schmidt decomposition is based on [?]. The main idea of the Lyapunov-Schmidt decomposition is the reduction of a possibly infinite-dimensional bifurcation problem to a finite-dimensional one. Let

$$F(w, \lambda) = 0 \tag{5.1}$$

be the equation of interest with $w \in X$, $\lambda \in \mathbb{R}$ and $F : X \times \mathbb{R} \to \mathbb{R}$ where X denotes a Banach space. Without loss of generality we assume that

$$F(0, 0) = 0.$$

The linear and non-linear parts of (5.1) decompose as

$$F(w, \lambda) = \mathcal{L}(w) + \mathcal{R}(w, \lambda), \text{ where } \mathcal{L}(\eta) := \left.\frac{\partial F(0 + \epsilon\eta, 0)}{\partial \epsilon}\right|_{\epsilon=0} \tag{5.2}$$

and where $\mathcal{R}$ denotes its remainder. We assume that $\mathcal{L}$ is a Fredholm operator of index zero, which means that the kernel $N(\mathcal{L})$ has finite dimension d, the range

$R(\mathcal{L})$ has finite codimension r and that the dimensions d and r agree.

The idea of the Lyapunov-Schmidt decomposition is to reduce the dimension of the equation and its solution by projecting it onto the kernel of $\mathcal{L}$ which is, due to the assumptions on $\mathcal{L}$, finite-dimensional. Let $P : X \to N(\mathcal{L})$ denote the projection onto the nullspace of $\mathcal{L}$ and let Q be the projection onto its complement $\mathcal{R}(\mathcal{L})$. Then (5.1) is equivalent to the system of equations

$$(1 - Q)F(u + v, \lambda) = 0 \tag{5.3a}$$

$$QF(u + v, \lambda) = 0 \tag{5.3b}$$

where $u := Pw$ denotes the projection of the solution onto $N(\mathcal{L})$ and $v := (1-P)w$ its projection onto the complement.

. The second of these equations can uniquely be solved for v using the implicit function theorem and the solution $v(u, \lambda)$ can then be plugged back into the first equation, which yields the bifurcation equation

$$f(u, \lambda) := (1 - Q)\mathcal{R}(u + v(u, \lambda), \lambda) = 0. \tag{5.4}$$

Note that we dropped the first term appearing in (5.3a) because $(1 - Q)\mathcal{L}(u + v, \lambda) = \mathcal{L}v - Q\mathcal{L}v = 0$. The solutions of (5.4) are equivalent to the solutions of our original problem in (5.1), see [?], because it only depends on u, which is an element of the finite-dimensional kernel of $\mathcal{L}$, and thus reduces the possibly infinite-dimensional problem to a finite-dimensional one.

5.2 Practicalities: An algorithmic procedure to derive the bifurcation equation

According to the previous section, the computations for the derivation of the bifurcation equation in (5.4) are divided into two parts:

Step A. An application of the implicit function theorem to (5.3b) that gives us an explicit expression of v in terms of u and λ.

Step B. Plugging v back into (5.3a) which results in the bifurcation equation.

By using the implicit function theorem in the first of these two steps, it is often not possible to derive an expression in closed form. Instead, we obtain a Taylor expansion of $v(u, \lambda)$ (which is justified by the implicit function theorem [**?**, Theorem 2.3]) and its coefficients are obtained by matching those of the same order that occur in (5.3a).

More concretely, u and v are expanded in series expansions of complementary sets of basis elements. For the problem at hand this is done in Equation (5.9). The implicit function theorem then relates the series coefficients of v in terms of those of u. The resulting expression for $v(u, \lambda)$ can then be plugged into the expansion of $\mathcal{R}$. An application of the projection P finally yields an expansion of the bifurcation equation in (5.4).

In order to characterise the bifurcation occurring at λ_s, it is often sufficient to obtain an expansion of (5.4) up to a particular order. We know that a certain order is sufficient by looking at the so-called recognition problem that corresponds to the problem at hand. More details on the particular recognition problem that we need to apply in order to solve the bifurcation equation can be found in Section 6.3, where we will show that it suffices to compute the bifurcation equation up to third order for λ_2.

In the following, we will first restate the problem in the language of Section 5.1 before directing our attention to the first of the two main steps mentioned above in Section 5.2.2. In order to make all computations tractable, we write all expressions in terms of spherical harmonics. An essential tool for the comparison of coefficients with matching order is an algorithmic procedure that allows us the fast computation of products of spherical harmonics with a computer. This will be the subject of Section 5.2.3. We conclude this section by performing Step B above which yields the bifurcation equation in five dimensions.

5.2.1 Reformulation of the problem

In order to find the minimisers of the free-energy functional, we consider its Euler-Lagrange equation and thus the corresponding Euler-Lagrange operator

$$E(\phi, \lambda) = (\lambda_s + \lambda)\phi(p) - \frac{1}{Z(\phi)} \int_{\mathbb{S}^2} k(p \cdot q) \exp(-\phi(q)) \, dq. \tag{5.5}$$

By Lemma 4.3 we can view this as an operator on $H^2(\mathbb{S}^2)$ which is the function space we are working in.

Remark 5.1. *Notice that* (5.5) *is an additive translation of the Euler-Lagrange operator in* (4.2). *In order to ensure that the assumption* $E(0,0) = 0$ *holds, see* *also* (4.1)*, the interaction operator* $k(\cdot)$ *had to be translated by the constant*

$$c = \int_{\mathbb{S}^2} k(p \cdot q)\, dq$$

(in the case of the Onsager interaction potential, this value is given by $c = \pi^2$*). Moreover, we translated the operator in* λ *by the value* λ_s *which is the bifurcation point we are interested in.*

According to (4.11), the bifurcation point is given by $\lambda_s = -\frac{\mu_s}{4\pi}$, where μ_s denotes the eigenvalue of order s of the interaction operator associated to the Onsager kernel, see Theorem 4.12 for details. The variable λ denotes the deviation from this bifurcation point and will act as bifurcation parameter. Having this translation of the problem in mind, we are interested in bifurcations around the point $(\phi_0, \lambda) = (0, 0)$. In particular, we are looking for the first phase transformation that occurs when the bifurcation parameter is descending. Hence we consider the largest bifurcation point which is, in the case of the Onsager kernel and according to the result of Theorem 4.12, given by

$$\lambda_2 = -\frac{\mu_2}{4\pi} = \frac{\pi}{32}.$$

In order to derive the decomposition of the above functional into its linear and non-linear part, we consider its Taylor expansion $\hat{E}$ up to fourth order in both variables ϕ and λ around the point $(0,0)$, namely

$$
\begin{aligned}
&\hat{E}(\phi,\lambda) \\
&:=(\lambda_2+\lambda)\phi(p) + \frac{1}{4\pi}\int_{\mathbb{S}^2} k(p\cdot q)\phi(q)\;dq + \frac{\int_{\mathbb{S}^2}\phi(q)\;dq}{16\pi^2}\int_{\mathbb{S}^2} k(p\cdot q)\phi(q)\;dq \\
&\quad - \frac{1}{8\pi}\int_{\mathbb{S}^2} k(p\cdot q)\phi^2(q)\;dq + \frac{\left(\int_{\mathbb{S}^2}\phi(q)\;dq\right)^2}{64\pi^3}\int_{\mathbb{S}^2} k(p\cdot q)\phi(q)\;dq \\
&\quad - \frac{\int_{\mathbb{S}^2}\phi^2(q)\;dq}{32\pi^2}\int_{\mathbb{S}^2} k(p\cdot q)\phi(q)\;dq - \frac{\int_{\mathbb{S}^2}\phi(q)\;dq}{32\phi^2}\int_{\mathbb{S}^2} k(p\cdot q)\phi^2(q)\;dq \\
&\quad + \frac{1}{24\pi}\int_{\mathbb{S}^2} k(p\cdot q)\phi^3(q)\;dq + \frac{\left(\int_{\mathbb{S}^2}\phi(q)\;dq\right)^3}{256\pi^4}\int_{\mathbb{S}^2} k(p\cdot q)\phi(q)\;dq \qquad (5.6)\\
&\quad - \frac{\int_{\mathbb{S}^2}\phi(q)\;dq}{64\pi^3}\int_{\mathbb{S}^2}\phi^2(q)\;dq\int_{\mathbb{S}^2} k(p\cdot q)\phi(q)\;dq \\
&\quad + \frac{\int_{\mathbb{S}^2}\phi^3(q)\;dq}{96\pi^2}\int_{\mathbb{S}^2} k(p\cdot q)\phi(q)\;dq - \frac{\left(\int_{\mathbb{S}^2}\phi(q)\;dq\right)^2}{128\pi^3}\int_{\mathbb{S}^2} k(p\cdot q)\phi^2(q)\;dq \\
&\quad + \frac{\int_{\mathbb{S}^2}\phi^2(q)\;dq}{64\pi^2}\int_{\mathbb{S}^2} k(p\cdot q)\phi^2(q)\;dq + \frac{\int_{\mathbb{S}^2}\phi(q)\;dq}{96\pi^4}\int_{\mathbb{S}^2} k(p\cdot q)\phi^3(q)\;dq \\
&\quad - \frac{1}{96\pi}\int_{\mathbb{S}^2} k(p\cdot q)\phi^4(q)\;dq.
\end{aligned}
$$

According to (5.2), its linear and non-linear parts therefore decompose as

$$
\mathcal{L}(\phi) = \lambda_2\phi(p) + \frac{1}{4\pi}\int_{\mathbb{S}^2} k(p\cdot q)\phi(q)\;dq
$$

and

$$
\hat{\mathcal{R}}(\phi,\lambda) := \hat{E}(\phi,\lambda) - \mathcal{L}(\phi), \tag{5.7}
$$

respectively. The fact that $\mathcal{L}$ is a Fredholm operator of index zero is a consequence of the following corollary in [**?**].

Corollary 5.2 ([**?**, Corollary 4.47])**.** *Let $\mathcal{X}$ and $\mathcal{Y}$ be Banach spaces and let $S, K : \mathcal{X} \to \mathcal{Y}$ be linear operators. Assume in addition that S is a Fredholm operator and that K is compact. Then $S + K$ is also a Fredholm operator with* $\text{index}(S + K) = \text{index}(S)$.

Schematically, $\mathcal{L}$ can be written as

$$\mathcal{L} = C \text{ Id} + U.$$

Hence in order to apply Corollary 5.2, we have to show that the operator

$$U(\phi)(p) := \int_{\mathbb{S}^2} k(p \cdot q)\phi(q) \; dq$$

is compact for all continuous interaction kernels and that the identity is a Fredholm operator of index zero. The compactness in H^2 has been proved in Lemma 4.2 of Section 4.1. The following computation shows compactness in $L^1(\mathbb{S}^2)$.

Lemma 5.3. *Let $U : L^1(\mathbb{S}^2) \to L^1(\mathbb{S}^2)$ be the interaction operator*

$$(U\rho)(q) := \int_{\mathbb{S}^2} k(p \cdot q)\rho(p) \; dp \tag{5.8}$$

with continuous interaction kernel $k(\cdot)$. Then U is compact, that is for any bounded sequence $\rho_n \in L^1(\mathbb{S}^2)$ such that $||\rho_n||_{L^1(\mathbb{S}^2)} \leq M$ for all $n \in \mathbb{N}$ the sequence $U\rho_n$ has a convergent subsequence $(U\rho_{n_k}) \to U\rho$ for some $\rho \in L^1(\mathbb{S}^2)$.

Proof. The statement follows by an application of the Arzelá-Ascoli Theorem. In particular, the following two claims hold.

U is uniformly bounded:

Using the fact that $k(\cdot)$ is continuous on $[-1, 1]$, we know that $k(\cdot)$ is bounded. Hence

$$\left| \int_{\mathbb{S}^2} k(p \cdot q)\rho(q)\ dq \right| \leq M \left| \int_{\mathbb{S}^2} \rho(q)\ dq \right| = M.$$

U is uniformly equicontinuous:

Pick $\epsilon > 0$. Since $k(\cdot)$ is continuous on the compact set $[-1, 1]$, it is uniformly continuous and therefore there exists a $\delta > 0$, so that for all $p_1, p_2 \in \mathbb{S}^2$ such that $|p_1 - p_2| \leq \delta$,

$$|k(p_1 \cdot q) - k(p_2 \cdot q)| < \epsilon$$

for all $q \in \mathbb{S}^2$. Hence for the same δ it follows that

$$\begin{aligned}
\big|(U\rho)(p_1) - (U\rho)(p_2)\big| &= \Big| \int_{\mathbb{S}^2} [k(p_1 \cdot q) - k(p_2 \cdot q)]\rho(q)\ dq \Big| \\
&\leq \int_{\mathbb{S}^2} \big|k(p_1 \cdot q) - k(p_2 \cdot q)\big|\rho(q)\ dq \\
&\leq \epsilon \int_{\mathbb{S}^2} \rho(q)\ dq \\
&\leq \epsilon.
\end{aligned}$$

Hence the operator U is equicontinuous and it follows from the Arzelá-Ascoli theorem that every convergent sequence $U\rho_n$ admits a convergent subsequence $(U\rho_{n_k}) \to U\rho$. Thus, U is a compact operator. $\square$

Having proved the compactness of U, it is left to show that the identity is a Fredholm operator. Let us make the following observations

(a) Id is bounded and linear

(b) $\mathcal{N}(\mathrm{Id}) = \{0\}$ and $\mathrm{coker}(\mathrm{Id}) = \{0\}$.

Hence the identity is a Fredholm operator of index zero and thus so is $\mathcal{L}$ as claimed.

In view of the results of Section 4.3, it is easy to conclude that the kernel of the operator $\mathcal{L}$, denoted by $N(\mathcal{L})$, is the eigenspace of the spherical harmonics corresponding to the degree of the bifurcation point of interest, which is in our case λ_2. Thus,

$$N(\mathcal{L}) = \{Y_2^m : -2 \leq m \leq 2\}$$

which is a five-dimensional space. It follows that the projection P onto $N(\mathcal{L})$ is given by

$$P : L^2(\mathbb{S}^2) \to L^2(\mathbb{S}^2) \text{ where } Pw := \sum_{m=-2}^{2} (w, Y_2^m)_{L^2} Y_2^m \text{ for all } w \in L^2(\mathbb{S}^2).$$

Since the set of all spherical harmonics $\{Y_l^m\}_{l=0,\dots,\infty}^{m=-l,\dots,l}$ is an orthonormal basis for the space $L^2(\mathbb{S}^2)$ and orthogonal for $H^2(\mathbb{S}^2)$. This naturally induces $P : H^2(\mathbb{S}^2) \to H^2(\mathbb{S}^2)$ as projection. The interaction operator in these operators in fact diagonalises over the set of spherical harmonics. This fact leads to an enormous simplification of our subsequent computations. Let $u(p) := P\phi(p)$ and

$v(p) := (1-P)\phi(p)$ such that $u(p) + v(p) = \phi(p)$ and let us further define u_m and $v_{l,m}$ such that

$$u(p) := \sum_{m=-2}^{2} u_m Y_2^m(p) \quad \text{and} \quad v(p) := \sum_{\substack{l=0 \\ l\neq 2}}^{\infty} \sum_{m=-l}^{l} v_{l,m} Y_l^m(p), \tag{5.9}$$

respectively. We will see that it will be an essential step to write all expressions in terms of spherical harmonics as this simplifies the actions of all operators. In particular, we may deduce from Theorem 4.8 that

$$U(Y_l^m) = \int_{\mathbb{S}^2} k(p\cdot q) Y_l^m(q)\, dq = \mu_l Y_l^m(p).$$

Accordingly, we conclude that

$$\mathcal{L}(Y_l^m) = \left(\lambda_2 + \frac{\mu_l}{4\pi}\right) Y_l^m$$

and similarly,

$$\mathcal{L}^{-1}(Y_l^m) = \frac{4\pi}{4\pi\lambda_2 + \mu_l} Y_l^m. \tag{5.10}$$

5.2.2 Step A: An application of the implicit function theorem

It is relatively straightforward to show that the implicit function theorem is applicable to

$$\mathcal{L}v + (1 - P)\mathcal{R}(u + v, \lambda) = 0. \tag{5.3b}$$

The operator $\mathcal{L}$ is invertible in $R(\mathcal{L})$, its inverse is bounded and $D_u\mathcal{R}(0, 0) = 0$. Moreover, based on Lemma 4.5, one can show that the Euler-Lagrange operator E is sufficiently smooth.

Lemma 5.4. *The bifurcation equation $f(u, \lambda)$ associated to the Euler-Lagrange equation for the Onsager free-energy functional is infinitely many times differentiable .*

Proof. The bifurcation equation is defined by

$$P\mathcal{R}(u + v(u, \lambda)) = f(u, \lambda)$$

where $\mathcal{R}$ is given by

$$E(\rho, \lambda) = \mathcal{L}(\rho, \lambda) + \mathcal{R}(\rho, \lambda).$$

Since $\mathcal{L}$ is a linear operator, the smoothness of E and $\mathcal{R}$ is the same. Moreover, the implicit function theorem tells us, that the smoothness of $\mathcal{R}$ and v is the same. Since the smoothness of the bifurcation equation is given by the minimal number of derivatives of $\mathcal{R}$ and v (using the chain rule) which are then equal, we conclude that the smoothness of f is the same as the smoothness of E (the Euler-Lagrange equation). The Euler-Lagrange operator is infinitely many times differentiable, see Proposition 4.5. □

Hence we may conclude that the implicit function theorem is applicable. However, writing down the exact solution $v(u, \lambda)$ is not possible in practice. Instead, an algorithmic procedure is required which has been presented in [**?**]. It is mainly based on writing v as a Taylor expansion in terms of both variables u and λ which is justified by the differentiability of the implicit function $v(u, \lambda)$, see the implicit function theorem [**?**, Theorem 2.3]. In particular, we expand $v = (1 - P)\phi$ up to fourth order by

$$\hat{v}(u, \lambda)(p) := \sum_{0 \leq i+j \leq 4} \frac{1}{i!j!} \hat{v}_{i,j}(u, \lambda)(p)$$

where the terms $\hat{v}_{i,j}$ denote terms of i^{th} order in u and of j^{th} order in λ. Furthermore, we identify u as before with

$$u(p) = \sum_{m=-2}^{2} u_m Y_2^m(p).$$

By definition $v \in N(\mathcal{L})^{\perp}$ and thus, without loss of generality, we assume that $\hat{v}_{i,j} \in N(\mathcal{L})^{\perp}$ for all i, j. Plugging this expression into (5.3b)

$$\mathcal{L}(v) = -(1 - P)\mathcal{R}(u + v, \lambda)$$

and matching the terms of the right order on both sides of the equation, we obtain expressions for each of the $\hat{v}_{ij}$. In the following we will execute this calculation for the first couple of terms.

Remark 5.5. *Because the spherical harmonics form an orthonormal basis for $L^2(\mathbb{S}^2)$, the $v_{i,j}$ can be written as an infinite series expansion. In fact, when considering the first few steps of the procedure, we will see that this expansion is finite.*

Since there does not exist any term that is constant in both variables, we conclude that

$$\hat{v}_{0,0} = 0.$$

As a second step, we consider $\hat{v}_{1,0}$ which only depends on u. Hence we only consider terms of order one in u on both sides of (5.3b) taking the expansion of $\hat{E}$ in (5.6) and the definition of $\mathcal{R}$ in (5.7) into account. All terms on the right hand side depend on λ or on higher order terms of u, so they can be neglected when we match the coefficients. Thus, we obtain

$$\lambda \hat{v}_{1,0}(p) + \frac{1}{4\pi} \int_{\mathbb{S}^2} k(p \cdot q) \hat{v}_{1,0}(q) \; dq = 0.$$

This is equivalent to solving $\mathcal{L}\hat{v}_{1,0} = 0$. Because we are assuming that $\hat{v}_{i,j} \in N(\mathcal{L})^{\perp}$, we conclude that $\hat{v}_{1,0} = 0$. Similarly, one can deduce that

$$\hat{v}_{0,1} = 0.$$

As the first non-zero term, we consider $\frac{1}{2}\hat{v}_{2,0}$. Matching the order of terms on the two sides of (5.3b), we obtain

$$\begin{aligned}
&\frac{\lambda}{2}\hat{v}_{2,0}(p) + \frac{1}{8\pi}\int_{\mathbb{S}^2} k(p\cdot q)\hat{v}_{2,0}(q)\,dq \\
&\quad = -(1-P)\left(\frac{\int_{\mathbb{S}^2} u(q)\,dq}{16\pi^2}\int_{\mathbb{S}^2} k(p\cdot q)u(q)\,dq - \frac{1}{8\pi}\int_{\mathbb{S}^2} k(p\cdot q)u^2(q)\,dq\right).
\end{aligned}$$

This yields an explicit expression for $\hat{v}_{2,0}$ if we bear in mind that the operator $\mathcal{L}$ and its inverse $\mathcal{L}^{-1}$ can actually be interpreted as simple multiplications, see (5.10). However, in order to be able to apply this multiplication to the right hand side, we need to write it in terms of spherical harmonics. Recall that u itself is already given as an expansion in terms of spherical harmonics, see (5.9),

$$u(p) = \sum_{m=-2}^{2} u_m Y_2^m(p).$$

Hence we only have to expand the terms

$$\int_{\mathbb{S}^2} k(p\cdot q)u(q)\,dq \int_{\mathbb{S}^2} u(q)\,dq \quad \text{and} \quad \int_{\mathbb{S}^2} k(p\cdot q)u^2(q)\,dq.$$

In fact,

$$\int_{\mathbb{S}^2} k(p\cdot q)u(q)\,dq \int_{\mathbb{S}^2} u(q)\,dq = 0$$

because the second factor, being the sum of integrals of spherical harmonics of degree $l = 2$, is zero. In the case of the second term, we observe that we have to compute u^2 which is based on computing products of spherical harmonics. In order to fulfil this task, we have developed an algorithm that is presented in

Section 5.2.3. Applying it to the case above yields an expansion of u^2 in terms of spherical harmonics and we are thus in the position to apply the interaction operator U, the projection $1-P$ and the operator $\mathcal{L}^{-1}$ which, according to (5.10), reduces to a simple multiplication in this case. We obtain

$$\begin{aligned}\hat{v}_{2,0}(p) =& -\mathcal{L}^{-1}\left((1-P)\int_{\mathbb{S}^2} k(p\cdot q)u^2(q)\,dq)\right)\\ =&\frac{\sqrt{\frac{5}{14}\pi^3}}{64}u_{-2}^2Y_4^{-4}(p)+\frac{\sqrt{\frac{5}{7}\pi^3}}{64}u_{-1}u_{-2}Y_4^{-3}(p)+\frac{\sqrt{15\pi^3}}{448}u_0u_{-2}Y_4^{-2}(p)\\ &+\frac{\sqrt{5\pi^3}}{448}u_1u_{-2}Y_4^{-1}(p)+\frac{\pi^{3/2}}{448}u_2u_{-2}Y_4^0(p)+\frac{\sqrt{\frac{5}{2}\pi^3}}{224}u_{-1}^2Y_4^{-2}(p)\\ &+\frac{\sqrt{\frac{15}{2}\pi^3}}{224}u_{-1}u_0Y_4^{-1}(p)+\frac{3\pi^{3/2}}{448}u_0^2Y_4^0+\frac{\pi^{3/2}}{112}u_{-1}u_1Y_4^0(p)\\ &+\frac{\sqrt{\frac{15}{2}\pi^3}}{224}u_0u_1Y_4^1(p)+\frac{\sqrt{5\pi^3}}{448}u_{-1}u_2Y_4^1(p)+\frac{\sqrt{\frac{5}{2}\pi^3}}{224}u_1^2Y_4^2(p)\\ &+\frac{\sqrt{15\pi^3}}{448}u_0u_2Y_4^2(p)+\frac{\sqrt{\frac{5}{7}\pi^3}}{64}u_1u_2Y_4^3(p)+\frac{\sqrt{\frac{5}{14}\pi^3}}{64}u_2^2Y_4^4(p).\end{aligned}$$

This concludes the computation of $\hat{v}_{2,0}$. The computation of the other terms follows the same pattern. However, because they are more complex and tedious, we will omit them. In order to give a good overview of the individual steps for each case, we present a summary of the procedure in form of a general algorithm. We would like to conclude this section by remarking that the expansion of $\hat{v}$ resulting from this procedure is in fact finite and that this is always the case when considering a finite expansion of an equation. The reason for this is that u is a linear combination of spherical harmonics that span the kernel of $\mathcal{L}$ which is itself

Algorithm 1: Matching the terms in Equation (5.3b)

1. Input: Fix $\hat{v}_{i,j}$ such that $0 \leq i + j \leq 4$.
2. Write down $\mathcal{R}(u + \hat{v})$ keeping only terms in u and all terms in $\hat{v}_{i,j}$ up to i'th order and in λ up to j'th order.
3. Expand $\mathcal{R}(u + \hat{v})$ in terms of spherical harmonics using the results of Section 5.2.3.
4. Apply the projection $(1 - P)$ by dropping all spherical harmonics of degree $l = 2$.
5. Apply $-\mathcal{L}^{-1}$ by multiplying $\mathcal{R}(u + \hat{v})$ by $\frac{-4\pi}{4\pi\lambda_2+\mu_l}$.
6. Output: $\hat{v}_{i,j} = \frac{-4\pi}{4\pi\lambda_2+\mu_l}\mathcal{R}(u + \hat{v})$.

finite. Considering products of up to four terms in u and $\hat{v}_{i,j}$, we can therefore only reach spherical harmonics up to degree $l = 8^4$ since the highest degree for $\hat{v}_{i,j}$ with $i + j = 4$ can only be $l = 8$.

Remark 5.6. *The operator $\mathcal{L}$ depends on the bifurcation parameter and the eigenvalues of the interaction operator U. For any kernel satisfying Assumption 1.3 the expansion of v would only depend on finitely many eigenvalues corresponding to spherical harmonics of low order. That means the resulting bifurcation can then be studied using the combination of methods presented here.*

5.2.3 Products of spherical harmonics

The crucial step in matching the coefficients in (5.3b) is to expand products of spherical harmonics again in terms of spherical harmonics. It is known that this can be achieved using Clebsch-Gordan coefficients which arise in angular momentum coupling [?]. However, it is very hard to compute them explicitly because it takes too much computing time. Therefore we devised an algorithm for the computation of products of spherical harmonics with short run time on the computer. The exact algorithm that we implemented on the computer is given at the end of this section while we present its crucial ideas first.

We recall the definition of spherical harmonics, see Section 4.2.1 for details,

$$Y_l^m(\varphi, \theta) = N_{lm} e^{im\theta} P_l^m(\cos\varphi), \qquad -l \leq m \leq l,$$

where φ and θ denote the polar and the azimuthal angle corresponding to the unit vector $p \in \mathbb{S}^2$. The functions P_l^m are called associated Legendre polynomials and their exact definition is also given in Section 4.2.1. Thus, a product of two spherical harmonics is given by

$$Y_l^m(\varphi, \theta) Y_p^q(\varphi, \theta) = N_{lm} N_{pq} e^{i(m+q)\theta} P_l^m(\cos(\varphi)) P_p^q(\cos(\varphi)). \tag{5.11}$$

Notice that we will abuse the notation and drop the (ϕ, θ) or p dependence in due course. Due to the factor $e^{i(m+q)}$, we observe that the order of each spherical harmonic occurring in an expansion of the product in (5.11) has to be of order $m + q$ while its degree may be arbitrary. On the basis of this observation, we would like to investigate products of associated Legendre polynomials. In fact, we use the following recurrence formula from [?]

$$(l - m + 1) P_{l+1}^m = (2l + 1) x P_l^m - (l + m) P_{l-1}^m. \tag{5.12}$$

Rearranging it gives

$$P_l^m = \frac{2l-1}{l-m} x P_{l-1}^m - \frac{l-1+m}{l-m} P_{l-2}^m$$

and thus,

$$P_l^m P_p^q = \frac{2l-1}{l-m} x P_{l-1}^m P_p^q - \frac{l-1+m}{l-m} P_{l-2}^m P_p^q.$$

Applying the original recurrence rule in (5.12) again, but this time to the product $xP_{p,q}$, yields

$$P_l^m P_p^q = \frac{2l-1}{l-m}\left(\frac{p-q+1}{2p+1} P_{p+1}^q P_{l-1}^m + \frac{p+q}{2p+1} P_{p-1}^q P_{l-1}^m\right) - \frac{l-1+m}{l-m} P_{l-2}^m P_p^q.$$

Using the definition of spherical harmonics, we deduce that

$$\begin{aligned} Y_l^m Y_p^q = & \frac{2l-1}{l-m} \frac{p-q+1}{2p+1} \frac{N_{l,m}}{N_{(l-1),m}} \frac{N_{p,q}}{N_{(p+1),q}} Y_{l-1}^m Y_{p+1}^q \\ & + \frac{2l-1}{l-m} \frac{p+q}{2p+1} \frac{N_{l,m}}{N_{(l-1),m}} \frac{N_{p,q}}{N_{(p-1),q}} Y_{l-1}^m Y_{p-1}^q \\ & - \frac{l-1+m}{l-m} \frac{N_{l,m}}{N_{(l-2),m}} Y_{l-2}^m Y_p^q \end{aligned}$$

and thus, we observe that we reduced the degree of the spherical harmonics Y_l^m with index l by one or two. We repeat this procedure until we reach either a term of the form Y_{s+1}^s or Y_s^s (which has to happen eventually). Hitting Y_{s+1}^s first, we use another recurrence rule from [**?**], namely

$$P_{s+1}^s = (2s+1) x P_s^s \quad \text{leading to} \quad Y_{s+1}^s Y_p^q = \frac{N_{(s+1),s}}{N_{s,s}} (2s+1) x Y_s^s Y_p^q,$$

so that we obtain $Y_s^s Y_p^q$ in any case. Again we apply a recurrence rule

$$P_s^s = (-1)^s (2s-1)!!(1-x^2)^{s/2}$$

which yields

$$Y_s^s Y_p^q = (-1)^s (2s-1)!!(1-x^2)^{s/2} N_{s,s} Y_p^q.$$

This last product can then be resolved by using

$$\sqrt{1-x^2} Y_p^q = \frac{1}{2p+1} \left(\frac{N_{p,q}}{N_{(p-1),(q+1)}} Y_{p-1}^{q+1} - \frac{N_{p,q}}{N_{(p+1),(q+1)}} Y_{p+1}^{q+1} \right)$$

repeatedly if necessary. Again this recurrence formula arises from using recurrence formulae for associated Legendre polynomials.

The computation of the first couple of steps of the algorithmic procedure above illustrates how an expansion of a product of two spherical harmonics in terms of spherical harmonics can be obtained. The general method involves a couple of other cases to start with, such as spherical harmonics of negative order for example which also have to be taken into account and for which special rules need to be defined. The whole algorithm is stated subsequently.

Algorithm 2: Rules for the computation of products of spherical harmonics

Require: a polynomial f of spherical harmonics of arbitrary degree.
Ensure: an expansion in terms of spherical harmonics.

If a is a constant, **then define** $S[a] := a$ and $T[a] := a$.

Define $N_{l,m} := \sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}}$.

Define $S\left[Y_l^m\right] := Y_l^m$ and $T\left[Y_l^m\right] := Y_l^m$.

If a is a constant, **then define** $S[ay] := aS\left[y\right]$ and $T[ay] := aT\left[y\right]$.

Define $S\left[x+y\right] := S\left[x\right] + S\left[y\right]$.

Define $S\left[aY_l^m Y_p^q\right] := S\left[aS\left[Y_l^m Y_p^q\right]\right]$.

If $p > q$ and $l - 2 \geq |m|$, **then define**

$$\begin{aligned} S\left[Y_l^m Y_p^q\right] :=& \frac{2l-1}{l-m}\frac{p-q+1}{2p+1}\frac{N_{l,m}}{N_{(l-1),m}}\frac{N_{p,q}}{N_{(p+1),q}}S\left[Y_{p+1}^q Y_{l-1}^m\right] \\ &+ \frac{2l-1}{l-m}\frac{p+q}{2p+1}\frac{N_{l,m}}{N_{(l-1),m}}\frac{N_{p,q}}{N_{(p-1),q}}S\left[Y_{p-1}^q Y_{l-1}^m\right] \\ &- \frac{l-1+m}{l-m}\frac{N_{l,m}}{N_{(l-2),m}}S\left[Y_{l-2}^m Y_p^q\right]. \end{aligned}$$

If $l = m$, **then define**

$$S\left[Y_l^m Y_p^q\right] := (-1)^l N_{l,m}(2l-1)!!S\left[(1-x^2)^{l/2}Y_p^q\right].$$

If $l = m+1$, **then define**

$$S\left[Y_l^m Y_p^q\right] := N_{l,m}(2l-1)(-1)^{l-1}(2l-3)!!S\left[(1-x^2)^{\frac{l-1}{2}}xY_p^q\right].$$

If $l = -m$, **then define**

$$S\left[Y_l^m Y_p^q\right] := \frac{N_{l,m}}{(2l)!}(2l-1)!!T\left[(1-x^2)^{l/2}Y_p^q\right].$$

If $l = -m+1$, **then define**

$$S\left[Y_l^m Y_p^q\right] := \frac{N_{l,m}}{(2l-2)!}(-1)^{m+l-1}(2l-3)!!T\left[(1-x^2)^{\frac{l-1}{2}}xY_p^q\right].$$

If $l > |m|$, **then define**

$$S\left[a \cdot x Y_l^m\right] := \frac{N_{l,m}}{N_{(l+1),m}} S\left[a \frac{l-m+1}{2l+1} Y_{l+1}^m\right] + \frac{N_{l,m}}{N_{(l-1),m}} S\left[a \frac{l+m}{2l+1} Y_{l-1}^m\right].$$

If $l = |m|$, **then define**

$$S\left[a \cdot x Y_l^m\right] := \frac{N_{l,m}}{N_{(l+1),m}} S\left[a \frac{l-m+1}{2l+1} Y_{l+1}^m\right].$$

If $l > m+2$, **then define**

$$\begin{aligned} S\left[(1-x^2)^s Y_l^m\right] :=& \frac{1}{2l+1} \frac{N_{l,m}}{N_{(l-1),(m+1)}} S\left[(1-x^2)^{s-1/2} Y_{l-1}^{m+1}\right] \\ &- \frac{1}{2l+1} \frac{N_{l,m}}{N_{(l+1),(m+1)}} S\left[(1-x^2)^{s-1/2} Y_{l+1}^{m+1}\right]. \end{aligned}$$

If $l = m$ or $l = m+1$, **then define**

$$S\left[(1-x^2)^s Y_l^m\right] := -\frac{1}{2l+1} \frac{N_{l,m}}{N_{(l+1),(m+1)}} S\left[(1-x^2)^{s-1/2} Y_{l+1}^{m+1}\right].$$

Define $S\left[a (Y_l^m)^s\right] := S\left[a (Y_l^m)^{s-2} S\left[(Y_l^m)^2\right]\right]$.

If $l - 2 > |m|$, **then define**

$$\begin{aligned} S\left[(Y_l^m)^2\right] :=& \frac{2l-1}{l-m} \frac{l-m+1}{2l+1} \frac{N_{l,m}}{N_{(l-1),m}} \frac{N_{l,m}}{N_{(l+1),m}} S\left[Y_{l-1}^m Y_{l+1}^m\right] \\ &+ \frac{2l-1}{l-m} \frac{l+m}{2l+1} \left(\frac{N_{l,m}}{N_{(l-1),m}}\right)^2 S\left[Y_{l-1}^m Y_{l-1}^m\right] \\ &- \frac{l+m-1}{l-m} \frac{N_{l,m}}{N_{(l-2),m}} S\left[Y_{l-2}^m Y_l^m\right]. \end{aligned}$$

If $l = m$, **then define**

$$S\left[(Y_l^m)^2\right] := N_{l,m}(-1)^l(2l-1)!!S\left[(1-x^2)^{l/2}Y_l^m\right].$$

If $l = -m$, **then define**

$$S\left[(Y_l^m)^2\right] := N_{l,-l}((2l)!)^{-1}(2l-1)!!T\left[(1-x^2)^{l/2}Y_l^m\right].$$

If $l = m+1$, **then define**

$$S\left[(Y_l^m)^2\right] := N_{l,m}(-1)^{l-1}(2l-1)(2l-3)!!S\left[(1-x^2)^{\frac{l-1}{2}}xY_l^m\right].$$

If $l = -m+1$, **then define**

$$\begin{aligned}S\left[(Y_l^m)^2\right] := N_{l,m}(-1)^{m+l-1}((2l-1)!)^{-1}(2l-1)(2l-3)!!\\ \cdot T\left[(1-x^2)^{\frac{l-1}{2}}xY_l^m\right].\end{aligned}$$

If $l > |m|$, **then define**

$$\begin{aligned}S\left[a\cdot xY_l^m\right] :=& \frac{N_{l,m}}{N_{(l+1),m}}\frac{l-m+1}{2l+1}T\left[aY_{l+1}^m\right]\\ &+\frac{N_{l,m}}{N_{(l-1),m}}\frac{l+m}{2l+1}T\left[aY_{l-1}^m\right].\end{aligned}$$

If $l = |m|$, **then define**

$$S\left[a\cdot xY_l^m\right] := \frac{N_{l,m}}{N_{(l+1),m}}\frac{l-m+1}{2l+1}T\left[aY_{l+1}^m\right].$$

If $l \geq -m+2$, **then define**

$$\begin{aligned}&T\left[(1-x^2)^sY_l^m\right]\\ &\quad=\frac{(l-m+1)(l-m+2)N_{l,m}}{(2l+1)N_{(l+1),(m-1)}}T\left[(1-x^2)^{s-1/2}Y_{l+1}^{m-1}\right]\\ &\quad\quad-\frac{(l+m-1)(l+m)N_{l,m}}{(2l+1)N_{(l-1),(m-1)}}T\left[(1-x^2)^{s-1/2}Y_{l-1}^{m-1}\right].\end{aligned}$$

25: **If** $l = -m+1$ or $l = -m$, **then define**

$$T\Big[(1-x^2)^s Y_l^m\Big] := \frac{(l-m+1)(l-m+2)N_{l,m}}{(2l+1)N_{(l+1),(m-1)}} T\left[(1-x^2)^{s-1/2} Y_{l+1}^{m-1}\right].$$

In order to implement this algorithm, it is important to use a conditioned replacement rule that makes it faster. This means that the algorithm itself remembers cases that it has computed already so that it will stop once it hits a known target.

5.2.4 Step B: Derivation of the bifurcation equation

Having found an explicit expression for $\hat{v}(u,\lambda)$ in Section 5.2.2, we are now in the position to plug this expression into (5.3a) which finally gives us an approximation of the bifurcation equation up to fourth order

$$\hat{f}(u,\lambda) := P\hat{\mathcal{R}}(u+\hat{v}(u,\lambda),\lambda).$$

Remark 5.7. *One can show that the bifurcation equation corresponding to the Onsager free-energy functional is smooth, see Lemma 5.4.*

Remark 5.8. *In fact, we used a fourth order Taylor approximation of the Euler-Lagrange operator and a Taylor approximation of $v(u,\lambda)$ up to a joint fourth order in both variables. Thus, we obtained an approximation of the bifurcation equation of at least fourth order. More precisely, the bifurcation equation $\hat{f} =$*

$\hat{\mathcal{R}}(u + \hat{v}(u, \lambda), \lambda) = 0$ *is approximated based on the following expansions of* v *and* $\mathcal{R}$

$$
\begin{aligned}
v(u, \lambda) &= \hat{v}(u, \lambda) + O\left(\sum_{i=1}^{5} ||u||^{i}_{H^2(\mathbb{S}^2)} |\lambda|^{5-i} \right) \\
\mathcal{R}(\phi, \lambda) &= \hat{\mathcal{R}}(\phi, \lambda) + O\left(\sum_{i=1}^{5} ||\phi||^{i}_{H^2(\mathbb{S}^2)} |\lambda|^{5-i} \right).
\end{aligned}
$$

The following calculation shows that $\hat{f}$ *agrees with* f *up to fourth order*

$$
\begin{aligned}
f =& \mathcal{R}(u + v(u, \lambda), \lambda) \\
=& \hat{R}(u + v(u, \lambda), \lambda) + O\left(\sum_{i=1}^{5} ||u + v(u, \lambda)||^{i}_{H^2(\mathbb{S}^2)} |\lambda|^{5-i} \right) \\
=& \hat{\mathcal{R}}(u + \hat{v}(u, \lambda), \lambda) + O\left(\sum_{i=1}^{6} ||u||^{i}_{H^2(\mathbb{S}^2)} |\lambda|^{6-i} \right) \\
&+ O\left(\sum_{i=1}^{5} ||u||^{i}_{H^2(\mathbb{S}^2)} |\lambda|^{5-i} \right) \\
f(u, \lambda) =& \hat{f}(u, \lambda) + O\left(\sum_{i=1}^{5} ||\phi||^{i}_{H^2(\mathbb{S}^2)} |\lambda|^{5-i} \right).
\end{aligned}
$$

The bifurcation equation can also be written as an expansion in spherical harmonics of degree $l = 2$, and therefore admits the form

$$
\hat{f}(u,\lambda)(p) = \sum_{m=-2}^{2} \hat{f}_m(u, \lambda) Y_2^m(p). \tag{5.13}
$$

The solutions of this equation are equivariantly equivalent to the solutions of the Euler-Lagrange equation of the Onsager free-energy functional in (1.2). In order to find the zeroes of (5.13), each of the coefficients $\hat{f}_i$ for $-2 \leq i \leq 2$ needs to be zero. Therefore we seek the solutions to a system of five polynomials, each depending on the six variables $u_{-2}, u_{-1}, u_0, u_1, u_2$ and λ reducing the infinite-dimensional state space $H^2(\mathbb{S}^2)$ to the ten-dimensional one i.e. $\mathbb{C}^5$.

However, we are only interested in real solutions to this equation, so we can reduce the dimension further by restricting the equation onto the space of real spherical harmonics with real coefficients. In particular, the real spherical harmonics are defined as

$$Y_{l,m} := \begin{cases} \frac{i}{\sqrt{2}}(Y_l^m - (-1)^m Y_l^{-m}) & \text{if } m < 0 \\ Y_l^0 & \text{if } m = 0 \cdot \\ \frac{1}{\sqrt{2}}(Y_l^{-m} + (-1)^m Y_l^m) & \text{if } m > 0 \end{cases}$$

Thus, if the function $u(p)$ in (5.9) is real-valued, its coefficients

$$\mathbf{u} := (u_{-2}, u_{-1}, u_0, u_1, u_2)$$

can be written as

$$\mathbf{u} = T(\mathbf{a}) := \begin{pmatrix} \frac{i}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & \frac{i}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\ -\frac{i}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} a_{-2} \\ a_{-1} \\ a_0 \\ a_1 \\ a_2 \end{pmatrix} \tag{5.14}$$

where $T : \mathbb{R}^5 \to \mathbb{C}^5$ for some $\mathbf{a} := (a_{-2}, \dots, a_2) \in \mathbb{R}^5$. Using this transformation, we define the following real version of the bifurcation equation which corresponds to the set of real spherical harmonics $\{Y_{2,m} : -2 \leq m \leq 2\}$

$$f_{\mathrm{real}}(\mathbf{a}, \lambda) := T^{-1} f(T\mathbf{a}, \lambda).$$

Equivalently, we will use the expression

$$\hat{f}_{\mathrm{real}}(\mathbf{a}, \lambda) := T^{-1} \hat{f}(T\mathbf{a}, \lambda) \tag{5.15}$$

in order to denote its approximation up to fourth order. Due to its complicated form, we will not state the bifurcation equation in terms of real spherical harmonics explicitly in this section. Instead it can be found in Appendix B.

Chapter 6

Solutions of the bifurcation equation of the Onsager free-energy functional

The most common approach to investigate the local structure of a system of polynomial equations at a given solution point is to use its Groebner basis. A Groebner basis is the generating set of an ideal in a polynomial ring over a field $K[x_1, x_2, \ldots, x_n]$. The advantage of this method is that it can be used in order to find the dimensionality of the solution set at a given point. However, due to the lengthy form of the bifurcation equation in (5.15), this method is not directly applicable. Instead, we make use of the symmetries of our problem in order to reduce its dimensionality. In particular we consider the Onsager free-energy functional with a rotationally symmetric intermolecular two-body potential. This means that if we can find a rotation that maps one solution of the bifurcation Equation (5.15) onto another, we can consider the two solutions to be equivalent. This chapter is organised as follows. In Section 6.1 we will describe the symmetry properties inherent to the problem in terms of a group action acting on the state space of the bifurcation equation. We will then find invariant polynomials that separate the orbits of this group action and we will reduce the dimension of the state space of the bifurcation equation in Section 6.2. Finally, we derive non-degeneracy conditions which guarantee the existence of solutions in Section 6.3.

6.1 The symmetry properties of the bifurcation equation

In order to represent an arbitrary rotation matrix $R(\varphi_R, \psi_R, \theta_R)$ with respect to the Euler angles φ_R, ψ_R and θ_R, we use the so-called y-convention. In this convention, a rotation $R(\varphi_R, \psi_R, \theta_R)$ is given by the product

$$R(\varphi_R,\psi_R, \theta_R) = R_z \cdot R_x \cdot R_y$$

where the first rotation is by an angle φ_R around the z-axis, the second rotation is by an angle θ_R around the y-axis and the third rotation is by an angle ψ_R around the z-axis. In particular, the three matrices are given by

$$R_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta_R) & \sin(\theta_R) \\ 0 & -\sin(\theta_R) & \cos(\theta_R) \end{pmatrix}, R_y = \begin{pmatrix} -\sin(\varphi_R) & \cos(\varphi_R) & 0 \\ -\cos(\varphi_R) & -\sin(\varphi_R) & 0 \\ 0 & 0 & 1 \end{pmatrix},$$
$$R_z = \begin{pmatrix} \sin(\psi_R) & -\cos(\psi_R) & 0 \\ \cos(\psi_R) & \sin(\psi_R) & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

In contrast to the rotation of points in the state space, the rotation of a function $u(p)$ written in terms of complex spherical harmonics of order $l = 2$ corresponds to a linear transformation of its coefficients $\mathbf{u} = (u_{-2}, \ldots, u_2)$. This transformation is given by the 5×5 Wigner matrix $D(\varphi_R, \psi_R, \theta_R)$ for complex spherical harmonics of degree $l = 2$ which is given by

$$D(\phi_R, \psi_R, \theta_R) = \begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} \\ d_{41} & d_{42} & d_{43} & d_{44} & d_{45} \\ d_{51} & d_{52} & d_{53} & d_{54} & d_{55} \end{pmatrix} \tag{6.1}$$

with

$$\begin{aligned}
d_{11} &= e^{-2i\phi_R - 2i\psi_R} \cos^4\left(\tfrac{\theta_R}{2}\right), \\
d_{12} &= 2e^{-2i\phi_R - i\psi_R} \cos^3\left(\tfrac{\theta_R}{2}\right) \sin\left(\tfrac{\theta_R}{2}\right), \\
d_{13} &= \sqrt{6} e^{-2i\phi_R} \cos^2\left(\tfrac{\theta_R}{2}\right) \sin^2\left(\tfrac{\theta_R}{2}\right), \\
d_{14} &= 2e^{i\psi_R - 2i\phi_R} \cos\left(\tfrac{\theta_R}{2}\right) \sin^3\left(\tfrac{\theta_R}{2}\right), \\
d_{15} &= e^{2i\psi_R - 2i\phi_R} \sin^4\left(\tfrac{\theta_R}{2}\right), \\
d_{21} &= -2e^{-i\phi_R - 2i\psi_R} \cos^3\left(\tfrac{\theta_R}{2}\right) \sin\left(\tfrac{\theta_R}{2}\right), \\
d_{22} &= e^{-i\phi_R - i\psi_R} \cos^2\left(\tfrac{\theta_R}{2}\right) (2\cos(\theta_R) - 1), \\
d_{23} &= \sqrt{6} e^{-i\phi_R} \cos\left(\tfrac{\theta_R}{2}\right) \cos(\theta_R) \sin\left(\tfrac{\theta_R}{2}\right), \\
d_{24} &= e^{i\psi_R - i\phi_R} (2\cos(\theta_R) + 1) \sin^2\left(\tfrac{\theta_R}{2}\right), \\
d_{25} &= 2e^{2i\psi_R - i\phi_R} \cos\left(\tfrac{\theta_R}{2}\right) \sin^3\left(\tfrac{\theta_R}{2}\right),
\end{aligned}$$

$$
\begin{aligned}
d_{31} &= \sqrt{6}e^{-2i\psi_R}\cos^2\left(\tfrac{\theta_R}{2}\right)\sin^2\left(\tfrac{\theta_R}{2}\right), \\
d_{32} &= -\sqrt{6}e^{-i\psi_R}\cos\left(\tfrac{\theta_R}{2}\right)\cos(\theta_R)\sin\left(\tfrac{\theta_R}{2}\right), \\
d_{33} &= \left(\tfrac{3}{2}\cos^2(\theta_R)-\tfrac{1}{2}\right), \\
d_{34} &= \sqrt{6}e^{i\psi_R}\cos\left(\tfrac{\theta_R}{2}\right)\cos(\theta_R)\sin\left(\tfrac{\theta_R}{2}\right), \\
d_{35} &= \sqrt{6}e^{2i\psi_R}\cos^2\left(\tfrac{\theta_R}{2}\right)\sin^2\left(\tfrac{\theta_R}{2}\right), \\
d_{41} &= -2e^{i\phi_R-2i\psi_R}\cos\left(\tfrac{\theta_R}{2}\right)\sin^3\left(\tfrac{\theta_R}{2}\right), \\
d_{42} &= e^{i\phi_R-i\psi_R}(2\cos(\theta_R)+1)\sin^2\left(\tfrac{\theta_R}{2}\right), \\
d_{43} &= -\sqrt{6}e^{i\phi_R}\cos\left(\tfrac{\theta_R}{2}\right)\cos(\theta_R)\sin\left(\tfrac{\theta_R}{2}\right), \\
d_{44} &= e^{i\phi_R+i\psi_R}\cos^2\left(\tfrac{\theta_R}{2}\right)(2\cos(\theta_R)-1), \\
d_{45} &= 2e^{i\phi_R+2i\psi_R}\cos^3\left(\tfrac{\theta_R}{2}\right)\sin\left(\tfrac{\theta_R}{2}\right), \\
d_{51} &= e^{2i\phi_R-2i\psi_R}\sin^4\left(\tfrac{\theta_R}{2}\right), \\
d_{52} &= -2e^{2i\phi_R-i\psi_R}\cos\left(\tfrac{\theta_R}{2}\right)\sin^3\left(\tfrac{\theta_R}{2}\right), \\
d_{53} &= \sqrt{6}e^{2i\phi_R}\cos^2\left(\tfrac{\theta_R}{2}\right)\sin^2\left(\tfrac{\theta_R}{2}\right), \\
d_{54} &= -2e^{2i\phi_R+i\psi_R}\cos^3\left(\tfrac{\theta_R}{2}\right)\sin\left(\tfrac{\theta_R}{2}\right), \\
d_{55} &= e^{2i\phi_R+2i\psi_R}\cos^4\left(\tfrac{\theta_R}{2}\right)
\end{aligned}
$$

where ϕ_R, ψ_R and θ_R denote the Euler angles corresponding to a rotation.

In particular, this relationship is formulated as

$$
\left(\sum_{m=-2}^{2} u_m Y_2^m\right)(R(\varphi_R,\psi_R,\theta_R)\cdot p) = \left(\sum_{m=-2}^{2}(D(\varphi_R,\psi_R,\theta_R)u)_m Y_2^m\right)(p) \quad (6.2)
$$

for all $p \in \mathbb{S}^2$ [**?**]. If we are given two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^5$ each representing the five coefficients of a real-valued solution written in terms of real spherical harmonics, then we say that $\mathbf{a} \sim \mathbf{b}$ if and only if there exists a triple of rotation angles

$(\varphi_R, \psi_R, \theta_R)$ such that

$$M(\varphi_R, \psi_R, \theta_R)\mathbf{a} := T^{-1} D(\varphi_R, \psi_R, \theta_R) \cdot T\mathbf{a} = \mathbf{b} \tag{6.3}$$

where T denotes the transformation onto the real spherical harmonics given in (5.14). In other words, M is the real version corresponding to the complex Wigner matrix $D(\varphi_R, \psi_R, \theta_R)$ given in (6.1). The explicit form of the representation of the group action of $SO(3)$ acting on $\mathbb{R}^5$ is given by

$$M(\phi_R, \psi_R, \theta_R) = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} & M_{15} \\ M_{21} & M_{22} & M_{23} & M_{24} & M_{25} \\ M_{31} & M_{32} & M_{33} & M_{34} & M_{35} \\ M_{41} & M_{42} & M_{43} & M_{44} & M_{45} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} \end{pmatrix} \tag{6.4}$$

with

$$\begin{aligned}
M_{11} = &\ \cos(\theta_R)\cos(2\psi_R)\cos(2\phi_R) - \tfrac{1}{4}(\cos(2\theta_R)+3)\sin(2\psi_R)\sin(2\phi_R), \\
M_{12} = &\ \sin(\theta_R)(\cos(\theta_R)\sin(2\psi_R)\sin(\phi_R) - \cos(2\psi_R)\cos(\phi_R)), \\
M_{13} = &\ -\sqrt{3}\sin^2(\theta_R)\sin(\psi_R)\cos(\psi_R), \\
M_{14} = &\ \sin(\theta_R)(\cos(\theta_R)\sin(2\psi_R)\cos(\phi_R) + \cos(2\psi_R)\sin(\phi_R)), \\
M_{15} = &\ -\cos(\theta_R)\cos(2\psi_R)\sin(2\phi_R) - \tfrac{1}{4}(\cos(2\theta_R)+3)\sin(2\psi_R)\cos(2\phi_R), \\
M_{21} = &\ \sin(\theta_R)(\cos(\psi_R)\cos(2\phi_R) - 2\cos(\theta_R)\sin(\psi_R)\sin(\phi_R)\cos(\phi_R)), \\
M_{22} = &\ \cos(\theta_R)\cos(\psi_R)\cos(\phi_R) - \cos(2\theta_R)\sin(\psi_R)\sin(\phi_R),
\end{aligned}$$

$$
\begin{aligned}
M_{23} = &\ \sqrt{3}\sin(\theta_R)\cos(\theta_R)\sin(\psi_R),\\
M_{24} = &\ -\cos(\theta_R)\cos(\psi_R)\sin(\phi_R) - \cos(2\theta_R)\sin(\psi_R)\cos(\phi_R),\\
M_{25} = &\ \sin(\theta_R)(-\cos(\psi_R))\sin(2\phi_R) - \tfrac{1}{2}\sin(2\theta_R)\sin(\psi_R)\cos(2\phi_R),\\
M_{31} = &\ \sqrt{3}\sin^2(\theta_R)\sin(\phi_R)\cos(\phi_R),\\
M_{32} = &\ \sqrt{3}\sin(\theta_R)\cos(\theta_R)\sin(\phi_R),\\
M_{33} = &\ \tfrac{1}{4}(3\cos(2\theta_R)+1),\\
M_{34} = &\ \sqrt{3}\sin(\theta_R)\cos(\theta_R)\cos(\phi_R),\\
M_{35} = &\ \tfrac{1}{2}\sqrt{3}\sin^2(\theta_R)\cos(2\phi_R),\\
M_{41} = &\ \sin(\theta_R)(\cos(\theta_R)\cos(\psi_R)\sin(2\phi_R) + \sin(\psi_R)\cos(2\phi_R)),\\
M_{42} = &\ \cos(2\theta_R)\cos(\psi_R)\sin(\phi_R) + \cos(\theta_R)\sin(\psi_R)\cos(\phi_R),\\
M_{43} = &\ -\sqrt{3}\sin(\theta_R)\cos(\theta_R)\cos(\psi_R)\\
M_{44} = &\ \cos(2\theta_R)\cos(\psi_R)\cos(\phi_R) - \cos(\theta_R)\sin(\psi_R)\sin(\phi_R),\\
M_{45} = &\ \tfrac{1}{2}\sin(2\theta_R)\cos(\psi_R)\cos(2\phi_R) - \sin(\theta_R)\sin(\psi_R)\sin(2\phi_R),\\
M_{51} = &\ \tfrac{1}{4}(\cos(2\theta_R)+3)\cos(2\psi_R)\sin(2\phi_R) + \cos(\theta_R)\sin(2\psi_R)\cos(2\phi_R),\\
M_{52} = &\ -\tfrac{1}{2}\sin(2\theta_R)\cos(2\psi_R)\sin(\phi_R) - \sin(\theta_R)\sin(2\psi_R)\cos(\phi_R),\\
M_{53} = &\ \tfrac{1}{2}\sqrt{3}\sin^2(\theta_R)\cos(2\psi_R),\\
M_{54} = &\ \sin(\theta_R)\sin(2\psi_R)\sin(\phi_R) - \tfrac{1}{2}\sin(2\theta_R)\cos(2\psi_R)\cos(\phi_R),\\
M_{55} = &\ \tfrac{1}{4}(\cos(2\theta_R)+3)\cos(2\psi_R)\cos(2\phi_R) - \cos(\theta_R)\sin(2\psi_R)\sin(2\phi_R).
\end{aligned}
$$

Having introduced these concepts, we are now in the position to establish symmetry properties of our bifurcation equation.

Proposition 6.1. *The bifurcation equation $\hat{f}_{\text{real}}$ is equivariant with respect to the Wigner matrices $M(\varphi_R, \psi_R, \theta_R)$, which means that for all $M(\varphi_R, \psi_R, \theta_R)$ and* *every* $\mathbf{a} \in \mathbb{R}^5$,

$$\hat{f}_{\text{real}}(M(\varphi_R, \psi_R, \theta_R)\mathbf{a}, \lambda) = M(\varphi_R, \psi_R, \theta_R)\hat{f}_{\text{real}}(\mathbf{a}, \lambda).$$

Proof. Let $R(\varphi_R, \psi_R, \theta_R)$ be the rotation matrix with associated Wigner matrix $M(\varphi_R, \psi_R, \theta_R)$. For ease of notation, we drop the dependence of R on the Euler angles φ_R, ψ_R and θ_R. Defining $R\phi(p) := \phi(Rp)$, we see that

$$\begin{aligned}
E(R\phi, \lambda) =& \lambda\phi(Rp) - \frac{1}{Z(R\phi)} \int_{\mathbb{S}^2} k(p \cdot q) \exp(-\phi(Rq))\, dq \\
=& \lambda\phi(Rp) - \frac{1}{\int_{\mathbb{S}^2} \exp(-\phi(Rs))\, ds} \int_{\mathbb{S}^2} k(p \cdot q) \exp(-\phi(Rq))\, dq \\
=& \lambda\phi(Rp) - \frac{1}{\int_{\mathbb{S}^2} \exp(-\phi(s))\, ds} \int_{\mathbb{S}^2} k(p \cdot R^t q) \exp(-\phi(q))\, dq \\
=& \lambda\phi(Rp) - \frac{1}{\int_{\mathbb{S}^2} \exp(-\phi(s))\, ds} \int_{\mathbb{S}^2} k(Rp \cdot q) \exp(-\phi(q))\, dq \\
=& RE(\phi, \lambda).
\end{aligned}$$

Hence the operator E is equivariant with respect to the Wigner matrices. By definition, see Section 5.2.2,

$$f := P\mathcal{R}(\mathbf{u} + \mathbf{v}(\mathbf{u}, \lambda), \lambda)$$

where $\mathcal{R}$ denotes the non-linear part of E and is therefore also equivariant. The projection P maps all terms onto the spherical harmonics of degree $l = 2$ and therefore also preserves the equivariance as well as the approximation of the equation up to fourth order. The restriction to the subspace of real solutions is also a linear transformation and therefore we can deduce that $\hat{f}_{\text{real}}$ is equivariant with respect to the Wigner matrices $M(\varphi_R, \psi_R, \theta_R)$. □

Knowing that f is in fact equivariant with respect to rotations, we can restrict our attention to one representative of each class of solutions that can be turned into each other by a rotation. In other words we are interested in the orbit space that corresponds to the action of $SO(3)$ on the space $\mathbb{R}^5$. To illustrate this idea, consider the example of $SO(2)$ acting on $\mathbb{R}^2$. The orbit space in this case can then be taken to be the non-negative part of the x-axis and is therefore one-dimensional.

6.2 Reducing the dimension of the orbit space of $SO(3)$ acting on $\mathbb{R}^5$

The aim of this section is to show that the orbit space of $SO(3)$ acting on $\mathbb{R}^5$ can in fact be reduced to two dimensions. In particular, using invariant theory for groups, we can prove that the space

$$\mathcal{S} := \{(0, 0, x, 0, y) | x, y \in \mathbb{R}\} \tag{6.5}$$

contains at least one representative of every orbit.

One can show that the generators of the ring of G-invariant polynomials for any compact Lie-group G separate the orbits; thus for any two distinct orbits Γ and Γ', there exists at least one of the generators taking different values on Γ and Γ' [?, Appendix C]. In the case of the group action given in (6.3) there exist two invariant polynomials I_1 and I_2 generating the ring. The fact that these generators separate the orbits can be reformulated as follows. If

$$(I_1(\mathbf{a}), I_2(\mathbf{a})) = (I_1(\mathbf{b}), I_2(\mathbf{b})),$$

then there exist rotation angles φ_R, ψ_R and θ_R such that $M(\varphi_R, \psi_R, \theta_R)\mathbf{a} = \mathbf{b}$ and hence $\mathbf{a} \sim \mathbf{b}$. This allows us to check that $\mathcal{S}$ contains at least one representative for every orbit by verifying that

$$\left\{I_1(\mathbf{a}), I_2(\mathbf{a}) \mid \mathbf{a} \in \mathbb{R}^5\right\} = \left\{I_1(\mathbf{a}), I_2(\mathbf{a}) \mid \mathbf{a} \in \mathcal{S}\right\}. \tag{6.6}$$

In other words, we show that the state space can in fact be reduced to two dimensions.

In [?] Wachsmuth achieves a similar two-dimensional reduction by the interesting device of considering the set of homogeneous polynomials restricted to the sphere, which is an equivalent description of the set of spherical harmonics. A more detailed account can be found in Appendix C.

This section is structured as follows. In Section 6.2.1 we find an isomorphic representation of the group action, called the Cartan representation, and we derive an explicit way to separate its orbits. Using the isomorphism between the Cartan representation and the group action given in (6.3), which is based on the Wigner matrix, see (6.9), we obtain similar expressions for the invariant polynomials with respect to the group action in (6.3). We conclude this section by proving that the reduced state space $\mathcal{S}$ contains a representative of every orbit, see Section 6.2.2.

6.2.1 The separation of orbits of the group action $SO(3)$ acting on $\mathbb{R}^5$

There exists a unique irreducible representation of the group action of $SO(3)$ acting on $\mathbb{R}^5$ [?]. Since both the complex and real representation based on the Wigner matrix given in (6.1) and (6.4) are irreducible, the real representation is isomorphic to any other irreducible representation of $SO(3)$ acting on the five-dimensional real space. One of these isomorphic representations is called the Cartan representation.

The Cartan representation can be expressed as

$$\rho : SO(3) \times \mathfrak{su}(3)/\mathfrak{so}(3), \quad (S, X + \mathfrak{so}(3)) \to SXS^{-1} + \mathfrak{so}(3)$$

where $\mathfrak{su}(3)$ and $\mathfrak{so}(3)$ denote the Lie-algebras associated with the Lie groups $SU(3)$ and $SO(3)$, respectively. The representation above then arises as the adjoint representation of $\mathfrak{so}(3)$ [?]. In this setting the matrix $X \in \mathfrak{su}(3)/\mathfrak{so}(3)$ is a traceless skew-Hermitian matrix, that is $X^\star = -X$. In particular, if we write $X = U + iV$, with U and V both being real 3×3 matrices, then we can make the following observation

$$X^\star = U^\star + (iV)^\star = U^t - iV^t.$$

Thus, in order for X to be skew-Hermitian, U needs to be a traceless skew-symmetric matrix, thus $U \in \mathfrak{so}(3)$, and V needs to be traceless and symmetric.

It follows that

$$\begin{aligned}\mathfrak{su}(3)/\mathfrak{so}(3) &= \{X + \mathfrak{so}(3) | X \in \mathfrak{su}(3)\} \\ &= \{iV + \mathfrak{so}(3) | \mathrm{tr}(V) = 0 \text{ and } V^t = V\}.\end{aligned}$$

The following set of matrices is a basis for this space

$$\begin{aligned}E = \Bigg\{ e_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, e_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, e_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ e_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, e_5 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \Bigg\}.\end{aligned} \tag{6.7}$$

Thus, any element in $\mathfrak{su}(3)/\mathfrak{so}(3)$ can be written as a linear combination of these matrices, that is for any $X \in \mathfrak{su}(3)/\mathfrak{so}(3)$ there exist $(x_1, \ldots, x_5)$ such that

$$X = \sum_{n=1}^{5} x_5 e_n.$$

In particular, we say that any two elements X and $Y \in \mathfrak{su}(3)/\mathfrak{so}(3)$ are equivalent, and thus are elements of the same orbit, if there exists a matrix $S(\varphi_R, \psi_R, \theta_R) \in SO(3)$ such that

$$S(\varphi_R, \psi_R, \theta_R) \left(\sum_{n=1}^{5} x_n e_n \right) S^{-1}(\varphi_R, \psi_R, \theta_R) = \sum_{n=1}^{5} y_n e_n$$

where $\mathbf{x} := (x_1, \ldots, x_5)$ and $\mathbf{y} := (y_1, \ldots, y_5)$ correspond to X and Y, respectively. Similarly, this relationship can also be represented by a 5×5 matrix mapping of $\mathbf{x}$ onto $\mathbf{y}$. In particular, $\mathbf{x} \sim \mathbf{y}$ if and only if there exist φ_R, ψ_R and θ_R such that

$$M_C(\varphi_R, \psi_R, \theta_R)\mathbf{x} = \mathbf{y}$$

where

$$M_C(\phi_R, \psi_R, \theta_R) = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} \end{pmatrix} \tag{6.8}$$

with

$$\begin{aligned}
C_{11} = \; & \tfrac{1}{4}\left(-4\cos^2(\phi_R)\cos^2(\psi_R)\sin^2(\theta_R) + (\cos(2\theta_R) + 2\cos(2\phi_R) - 1)\cos(2\psi_R)\right) \\
& +2\cos(\theta_R)(\cos(\theta_R) - 4\cos(\phi_R)\cos(\psi_R)\sin(\phi_R)\sin(\psi_R)), \\
C_{12} = \; & 2\cos(\theta_R)\cos(\psi_R)\sin(\phi_R)\sin(\psi_R)\cos(\phi_R) + \cos(2\theta_R)\cos^2(\psi_R)\sin^2(\phi_R) \\
& + \left(\sin^2(\psi_R) - \cos^2(\psi_R)\sin^2(\theta_R)\right)\cos^2(\phi_R), \\
C_{13} = \; & \tfrac{1}{4}\left((\cos(2\theta_R) + 3)\cos(2\psi_R) - 2\sin^2(\theta_R)\right)\sin(2\phi_R) \\
& + \cos(\theta_R)\cos(2\phi_R)\sin(2\psi_R), \\
C_{14} = \; & 2\cos(\psi_R)\sin(\theta_R)(\sin(\phi_R)\sin(\psi_R) - \cos(\theta_R)\cos(\phi_R)\cos(\psi_R)), \\
C_{15} = \; & -2\cos(\psi_R)\sin(\theta_R)(\cos(\theta_R)\cos(\psi_R)\sin(\phi_R) + \cos(\phi_R)\sin(\psi_R)), \\
C_{21} = \; & \cos^2(\psi_R)\sin^2(\theta_R)\sin^2(\phi_R) + \tfrac{1}{2}\cos(\theta_R)\sin(2\phi_R)\sin(2\psi_R)
\end{aligned}$$

$$
\begin{aligned}
& +\tfrac{1}{2}\left(\cos(2\theta_R)+\cos(2\psi_R)\left(\sin^2(\theta_R)-\cos^2(\theta_R)\cos(2\phi_R)\right)\right), \\
C_{22} = \;& -\cos(\phi_R)\cos(\psi_R)\sin(\phi_R)\sin(\psi_R)\cos^3(\theta_R) \\
& +\tfrac{1}{2}(\cos(2\phi_R)\cos(2\psi_R)+1)\cos^2(\theta_R) \\
& +\tfrac{1}{8}(\cos(2\theta_R)-3)\sin(2\phi_R)\sin(2\psi_R)\cos(\theta_R) \\
& +\sin^2(\theta_R)\left(\cos^2(\phi_R)\cos(2\psi_R)-\sin^2(\phi_R)\sin^2(\psi_R)\right), \\
C_{23} = \;& -2\cos(\phi_R)\cos^2(\psi_R)\sin(\phi_R)\sin^2(\theta_R) \\
& -\cos(\theta_R)(\cos(\theta_R)\cos(2\psi_R)\sin(2\phi_R)+\cos(2\phi_R)\sin(2\psi_R)), \\
C_{24} = \;& -2\sin(\theta_R)\sin(\psi_R)(\cos(\psi_R)\sin(\phi_R)+\cos(\theta_R)\cos(\phi_R)\sin(\psi_R)), \\
C_{25} = \;& 2\sin(\theta_R)\sin(\psi_R)(\cos(\phi_R)\cos(\psi_R)-\cos(\theta_R)\sin(\phi_R)\sin(\psi_R)), \\
C_{31} = \;& \tfrac{1}{8}\Big(-4\cos(\theta_R)\cos(2\psi_R)\sin(2\phi_R) \\
& -\left((\cos(2\theta_R)+3)\cos(2\phi_R)-6\sin^2(\theta_R)\right)\sin(2\psi_R)\Big), \\
C_{32} = \;& \tfrac{1}{8}\Big(4\cos(\theta_R)\cos(2\psi_R)\sin(2\phi_R) \\
& +\left(6\sin^2(\theta_R)+(\cos(2\theta_R)+3)\cos(2\phi_R)\right)\sin(2\psi_R)\Big), \\
C_{33} = \;& \cos(\theta_R)\cos(2\phi_R)\cos(2\psi_R)-\tfrac{1}{4}(\cos(2\theta_R)+3)\sin(2\phi_R)\sin(2\psi_R), \\
C_{34} = \;& \sin(\theta_R)(\cos(2\psi_R)\sin(\phi_R)+\cos(\theta_R)\cos(\phi_R)\sin(2\psi_R)), \\
C_{35} = \;& \sin(\theta_R)(\cos(\theta_R)\sin(\phi_R)\sin(2\psi_R)-\cos(\phi_R)\cos(2\psi_R)), \\
C_{41} = \;& \tfrac{1}{2}\sin(\theta_R)(\cos(\theta_R)(\cos(2\phi_R)+3)\cos(\psi_R)-2\cos(\phi_R)\sin(\phi_R)\sin(\psi_R)), \\
C_{42} = \;& \tfrac{1}{2}\sin(\theta_R)(\sin(2\phi_R)\sin(\psi_R)-\cos(\theta_R)(\cos(2\phi_R)-3)\cos(\psi_R)), \\
C_{43} = \;& \sin(\theta_R)(\cos(\theta_R)\cos(\psi_R)\sin(2\phi_R)+\cos(2\phi_R)\sin(\psi_R)), \\
C_{44} = \;& \cos(2\theta_R)\cos(\phi_R)\cos(\psi_R)-\cos(\theta_R)\sin(\phi_R)\sin(\psi_R), \\
C_{45} = \;& \cos(2\theta_R)\cos(\psi_R)\sin(\phi_R)+\cos(\theta_R)\cos(\phi_R)\sin(\psi_R), \\
C_{51} = \;& -\tfrac{1}{2}\sin(\theta_R)(\cos(\psi_R)\sin(2\phi_R)+\cos(\theta_R)(\cos(2\phi_R)+3)\sin(\psi_R)), \\
C_{52} = \;& \tfrac{1}{2}\sin(\theta_R)(\cos(\psi_R)\sin(2\phi_R)+\cos(\theta_R)(\cos(2\phi_R)-3)\sin(\psi_R)),
\end{aligned}
$$

$$
\begin{aligned}
C_{53} = &\ \sin(\theta_R)(\cos(2\phi_R)\cos(\psi_R) - 2\cos(\theta_R)\cos(\phi_R)\sin(\phi_R)\sin(\psi_R)),\\
C_{54} = &\ -\cos(\theta_R)\cos(\psi_R)\sin(\phi_R) - \cos(2\theta_R)\cos(\phi_R)\sin(\psi_R),\\
C_{55} = &\ \cos(\theta_R)\cos(\phi_R)\cos(\psi_R) - \cos(2\theta_R)\sin(\phi_R)\sin(\psi_R).
\end{aligned}
$$

The following lemma shows that the Cartan representation and the representation based on the Wigner rotation matrix for real spherical harmonics in (6.4) are in fact isomorphic to each other.

Lemma 6.2. *An isomorphism between the two representations of the group action is given by*

$$
\Phi = \begin{pmatrix} 0 & 0 & -\frac{1}{\sqrt{3}} & 0 & 1 \\ 0 & 0 & -\frac{1}{\sqrt{3}} & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}. \tag{6.9}
$$

In particular $M_C = \Phi M \Phi^{-1}$.

Proof. Omitted. □

Having established an equivalence relation that describes the orbits in the case of the Cartan representation, we are now in the position to describe its orbit space.

We recall that for any two real symmetric matrices X and Y, there exists a matrix $S \in SO(3)$ such that

$$SXS^{-1} = Y, \tag{6.10}$$

if and only if the characteristic polynomials of X and Y agree, that is $\chi(X) = \chi(Y)$.

We deduce that the orbits described by the Cartan representation are separated by the coefficients of the characteristic polynomials of the corresponding matrix. In particular, the characteristic polynomial $\chi(X)$ of a matrix $X \in \mathfrak{su}(3)/\mathfrak{so}(3)$ written in terms of the basis E in (6.7) is given by

$$\begin{aligned}\chi(X)(k) = &- k^3 + k\left(x_1^2 + x_1x_2 + x_2^2 + x_3^2 + x_4^2 + x_5^2\right) \\ &- x_1^2x_2 - x_1x_2^2 + x_1x_3^2 - x_1x_5^2 + x_2x_3^2 - x_2x_4^2 + 2x_3x_4x_5.\end{aligned}$$

Thus, the two invariant polynomials for the group action written in terms of the Cartan representation are

$$\begin{aligned}I_{C1} :=& x_1^2 + x_1x_2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 \text{ and} \\ I_{C2} :=& - x_1^2x_2 - x_1x_2^2 + x_1x_3^2 - x_1x_5^2 + x_2x_3^2 - x_2x_4^2 + 2x_3x_4x_5.\end{aligned}$$

In particular, both of these polynomials satisfy the relationship

$$I_{Cj}(M_C(\varphi_R, \psi_R, \theta_R)\mathbf{x}) = I_{Cj}(\mathbf{x})$$

for $j = 1, 2$, respectively, and for all $(\varphi_R, \psi_R, \theta_R) \in [0, \pi)^2 \times [0, 2\pi)$.

Using the explicit isomorphism in Lemma 6.2, the invariant polynomials that correspond to the group representation based on the Wigner rotation matrix in (6.4) are given by

$$
\begin{aligned}
I_1 &= x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 \text{ and} \\
I_2 &= -\frac{2x_1^2 x_3}{\sqrt{3}} + 2x_1x_2x_4 + \frac{x_2^2 x_3}{\sqrt{3}} - x_2^2 x_5 + \frac{2x_3^3}{3\sqrt{3}} + \frac{x_3 x_4^2}{\sqrt{3}} - \frac{2x_3 x_5^2}{\sqrt{3}} + x_4^2 x_5.
\end{aligned}
$$

In order to follow the programme outlined at the beginning of this section, it would now only be left to show that I_1 and I_2 are generators of the ring of invariant polynomials. However, in this case, we already know that both polynomials separate the orbits by using the explicit isomorphism and the fact stated in (6.10).

6.2.2 Reduction to a two-dimensional orbit space

Having found the fundamental invariants corresponding to the group action of $SO(3)$ acting on $\mathbb{R}^5$, we have an explicit description of all orbits as each orbit corresponds to exactly one constant value in the image of the two invariants. In order to reduce the state space to $\mathcal{S}$, we need to verify that

$$
\left\{I_1(\mathbf{a}), I_2(\mathbf{a}) \mid \mathbf{a} \in \mathbb{R}^5\right\} = \left\{I_1(\mathbf{a}), I_2(\mathbf{a}) \mid \mathbf{a} \in \mathcal{S}\right\}. \tag{6.6}
$$

In particular, we can express the left hand side and the right hand side as

$$
\left\{I_1(\mathbf{a}), I_2(\mathbf{a}) \mid \mathbf{a} \in \mathbb{R}^5\right\} = \bigcup_{r=0}^{\infty} \left\{\{r, I_2(\mathbf{a})\} \mid \mathbf{a} \in \mathbb{R}^5 \text{ and } I_1(\mathbf{a}) = r\right\}
$$

$$= \bigcup_{r=0}^{\infty} \{r\} \times \left[\min_{\substack{I_1(\mathbf{a})=r \\ \mathbf{a}\in\mathbb{R}^5}} I_2(\mathbf{a}), \max_{\substack{I_1(\mathbf{a})=r \\ \mathbf{a}\in\mathbb{R}^5}} I_2(\mathbf{a}) \right]$$

and

$$\begin{aligned} \{I_1(\mathbf{a}), I_2(\mathbf{a}) \mid \mathbf{a} \in \mathcal{S}\} &= \bigcup_{r=0}^{\infty} \{\{r, I_2(\mathbf{a})\} \mid \mathbf{a} \in \mathcal{S} \text{ and } I_1(\mathbf{a}) = r\} \\ &= \bigcup_{r=0}^{\infty} \{r\} \times \left[\min_{\substack{I_1(\mathbf{a})=r \\ \mathbf{a}\in\mathcal{S}}} I_2(\mathbf{a}), \max_{\substack{I_1(\mathbf{a})=r \\ \mathbf{a}\in\mathcal{S}}} I_2(\mathbf{a}) \right], \end{aligned}$$

respectively. Moreover, we observe that $\{I_1(\mathbf{a}) = r\}$ is a five-dimensional sphere which is connected and compact. Rewriting the problem like this, we observe that we are interested in the extrema of I_2 for points on the sphere with radius r. Since the sphere is compact, we know that these extrema are attained and an application of the intermediate value theorem gives us that I_2 attains in fact all values in between its extrema. Taking these arguments into account, the verification of (6.6) has thus been reduced to checking that the extrema defining the intervals agree for all $r > 0$. Because both invariant polynomials I_1 and I_2 are homogeneous, it actually suffices to verify this condition for the case $r = 1$. Moreover, since $-I_2(\mathbf{a}) = I_2(-\mathbf{a})$ and $\mathbf{a} \in \mathbb{S}^2$ if and only if $-\mathbf{a} \in \mathbb{S}^2$, it is enough to prove the equality of the maxima. Hence, we only need to show that the following relationship holds

$$\max_{\mathbf{a}\in\mathbb{R}^5, I_1(\mathbf{a})=1} I_2(\mathbf{a}) = \max_{\mathbf{a}\in\mathcal{S}, I_1(\mathbf{a})=1} I_2(\mathbf{a}).$$

A direct calculation shows that in both cases

$$\max_{\mathbf{a}\in\mathbb{R}^5} I_2(\mathbf{a}) = \max_{\mathbf{a}\in\mathcal{S}} I_2(\mathbf{a}) = \frac{2}{3\sqrt{3}}$$

if $I_1(\mathbf{a}) = 1$, which thus proves the claim, and we conclude that the state space can be reduced to the two-dimensional space $\mathcal{S}$.

It follows that at least one point of each orbit is an element of the set $\mathcal{S}$. However, there might in fact be several points representing one orbit which are elements of $\mathcal{S}$ which is why additional symmetry considerations might need to be taken, see Section 6.3 for details.

6.3 Solving the reduced bifurcation equation

Having shown that the equivariant state space of the bifurcation equation can in fact be restricted to the two-dimensional space $\mathcal{S}$ in (6.5), we are now in the position to solve this reduced problem. We denote the reduced form of the real bifurcation equation by $\hat{f}^{\mathcal{S}}_{\text{real}}$ which only depends on the two state variables a_0 and a_2. Its approximation up to fourth order is given by

$$\hat{f}^{\mathcal{S}}_{\text{real}}(\mathbf{a},\lambda)(p) = \sum_{m=-2}^{2} \hat{f}^{\mathcal{S}}_{\text{real}_m}(\mathbf{a},\lambda) Y_{2,m}(p) \tag{6.11}$$

with

$$\hat{f}^{\mathcal{S}}_{\text{real}_{-2}}(\mathbf{a},\lambda) = \hat{f}^{\mathcal{S}}_{\text{real}_{-1}}(\mathbf{a},\lambda) = \hat{f}^{\mathcal{S}}_{\text{real}_{1}}(\mathbf{a},\lambda) = 0,$$

$$
\begin{aligned}
\hat{f}^{\mathcal{S}}_{\text{real}_0}(\mathbf{a},\lambda) =& \lambda a_0 + \frac{18(\lambda a_0^3 + \lambda a_2^2 a_0)}{49\pi(1+32\pi)^2} + \frac{\sqrt{5}(448\pi(13+2800\pi)+577)a_0^4}{\sqrt{\pi}5795328(1+32\pi)^2} \\
&+ \left(\frac{9}{3136(1+32\pi)} - \frac{5}{1792}\right)(a_0^3 + a_2^2 a_0) + \frac{\sqrt{5\pi}}{448}(a_0^2 - a_2^2) \\
&- \frac{(224\pi(5+224\pi)+31)a_2^2 a_0^2}{5^{-\frac{3}{2}}965888\sqrt{\pi}(1+32\pi)^2} + \frac{(1792(1-140\pi)\pi - 89)a_2^4}{5^{-\frac{1}{2}}1931776\sqrt{\pi}(1+32\pi)^2}, \\
\hat{f}^{\mathcal{S}}_{\text{real}_2}(\mathbf{a},\lambda) =& \lambda a_2 + \frac{18(\lambda a_2 a_0^2 + \lambda a_2^3)}{49\pi(1+32\pi)^2} + \frac{\sqrt{\frac{5}{\pi}}(14(7-320\pi)\pi - 1)a_2 a_0^3}{25872(1+32\pi)^2} \\
&+ \left(\frac{9}{3136(1+32\pi)} - \frac{5}{1792}\right)(a_2 a_0^2 + a_2^3) - \frac{\sqrt{5\pi}}{224} a_2 a_0 \\
&- \frac{\sqrt{\frac{5}{\pi}}(56\pi(17+2240\pi)+61)a_2^3 a_0}{241472(1+32\pi)^2}.
\end{aligned}
$$

In particular, we observe that this equation can also be rewritten up to third order in a_i for $i \in \{0,2\}$ and λ as

$$
\hat{f}^{\mathcal{S}}_{\text{real}}(\mathbf{a},\lambda) = (\lambda + d(a_0^2 + a_2^2)) \begin{pmatrix} a_0 \\ a_2 \end{pmatrix} + c \begin{pmatrix} a_0^2 - a_2^2 \\ -2a_0 a_2 \end{pmatrix} \tag{6.12}
$$

where $c := \frac{\sqrt{5\pi}}{448}$ and $d := \left(\frac{9}{3136(1+32\pi)} - \frac{5}{1792}\right)$. However, we need to find conditions ensuring that we consider the equation up to a sufficiently high order to guarantee that the characteristics of the bifurcation do not change. Such a problem is called recognition problem and it will be presented both theoretically in Section 6.3.1 and in the context of the two-dimensional bifurcation equation in (6.12), see Section 6.3.2.

6.3.1 The recognition problem in two dimensions

The aim of this section is to derive non-degeneracy conditions which ensure a one-to-one correspondence between the solutions of the two-dimensional reduced bifurcation equation and the algebraic equation of a simple form of lower order. This problem is called recognition problem. In our presentation we follow [**?**, Chapter 9].

A one-to-one correspondence between the sets of solutions of two functions $f(\mathbf{u}, \lambda) = 0$ and $g(\mathbf{u}, \lambda) = 0$ for $\mathbf{u} \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$ exists if f and g are strongly equivalent.

Definition 6.3. *Two C^∞-functions f and g are strongly equivalent, denoted by $f \sim g$ if there exist $S : \mathbb{R}^n \times \mathbb{R} \to L(\mathbb{R}^n, \mathbb{R}^n)$ and $U : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ such that*

$$\begin{aligned} &\det S(\mathbf{u}, \lambda) > 0, \\ &\quad U(0,0) = 0, \frac{\partial U}{\partial \mathbf{u}}(\mathbf{u}, \lambda) \text{ is positive definite} \\ &\quad f(\mathbf{u}, \lambda) = S(\mathbf{u}, \lambda) g(U(\mathbf{u}, \lambda), \lambda). \end{aligned}$$

However, often it is not straightforward to verify strong equivalence for particular cases. Instead, it is easier if the problem inherits certain symmetry properties that can be taken into account. In the case of the reduced bifurcation equation in (6.12), the problem is symmetric with respect to the group action of S_3 acting on the space $\mathbb{R}^2$. In particular, S_3 acts on any element $\mathbf{u} \in \mathbb{R}^2$ by

$$g_i \mathbf{u} = \mathbf{u}' \text{ for all } i \in \{1, \ldots, 6\},$$

where g_i are defined as

$$\begin{aligned} S_3 =& \{g_i \in \mathbb{R}^{2\times 2}, i = 1, \ldots, 6\} \\ =& \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}, \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}, \right. \\ & \left. \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix} \right\}. \end{aligned}$$

Moreover, it is easy to show that the group action is generated by the elements

$$g_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ and } g_4 = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}. \tag{6.13}$$

Based on this representation of the group action of S_3 acting on $\mathbb{R}^2$, we direct our attention to the concept of S_3-invariance, S_3-equivariance and S_3-equivariant equivalence.

Definition 6.4. *A mapping $h : \mathbb{R}^2 \to \mathbb{R}$ is S_3-invariant if*

$$h(g\mathbf{u}) = h(\mathbf{u})$$

for all $g \in S_3$ *and* $\mathbf{u} \in \mathbb{R}^2$.

Definition 6.5. *A mapping* $f : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ *is* S_3*-equivariant if*

$$f(g\mathbf{u}, \lambda) = gf(\mathbf{u}, \lambda) \text{ for all } g \in S_3 \text{ and } \mathbf{u} \in \mathbb{R}^2.$$

Definition 6.6. *Two* S_3*-equivariant* C^∞*-mappings* $f : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ *and* $g : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ *are equivariantly equivalent, denoted by* $f \sim g$*, if there exist* $S : \mathbb{R}^2 \times \mathbb{R} \to L(\mathbb{R}^2, \mathbb{R}^2)$ *and* $U : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ *such that*

$$\begin{aligned}
&\det S(\mathbf{u}, \lambda) > 0, \\
&\quad U(0,0) = 0, \frac{\partial U}{\partial \mathbf{u}}(\mathbf{u}, \lambda) \text{ is positive definite} \\
&\quad S(g\mathbf{u}, \lambda) = gS(\mathbf{u}, \lambda)g^{-1}, U(g\mathbf{u}, \lambda) = gU(\mathbf{u}, \lambda) \text{ for all } g \in S_3, \mathbf{u} \in \mathbb{R}^2, \lambda \in \mathbb{R} \\
&\quad f(\mathbf{u}, \lambda) = S(\mathbf{u}, \lambda)g(U(\mathbf{u}, \lambda), \lambda).
\end{aligned}$$

The aim of Section 6.3.2 will be to show that the reduced bifurcation equation is in fact S_3-equivariant and equivariantly equivalent to its approximation up to fourth order. In order to verify the equivariant equivalence, we use the following concepts and results.

Theorem 6.7. [?, Theorem 1] *Any smooth* S_3*-invariant mapping* h *can be represented as*

$$h(\mathbf{u}) = \hat{h}(h_1(\mathbf{u}), h_2(\mathbf{u}))$$

where $h_1(\mathbf{u}) := u_1^2 + u_2^2$ *and* $h_2(\mathbf{u}) := u_1^3 - 3u_1u_2^2$.

Theorem 6.8. *Any S_3-equivariant mapping $f : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ can be represented by*

$$f(\mathbf{u}, \lambda) = a(h_1(\mathbf{u}), h_2(\mathbf{u}), \lambda) \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + b(h_1(\mathbf{u}), h_2(\mathbf{u}), \lambda) \begin{pmatrix} u_1^2 - u_2^2 \\ -2u_1u_2 \end{pmatrix}$$

with $h_1(\mathbf{u}) = u_1^2 + u_2^2$ and $h_2(\mathbf{u}) = u_1^3 - 3u_1u_2^2$.

Based on these results, we are now in the position to state the following proposition which yields the existence of a normal form under appropriate conditions.

Proposition 6.9. *Let $f : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ be of the form given in Theorem 6.8. Then*

$$f(\mathbf{u}, \lambda) \sim \epsilon\lambda \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} u_1^2 - u_2^2 \\ -2u_1u_2 \end{pmatrix}$$

for $\epsilon := \operatorname{sgn}\left(\frac{\partial a}{\partial \lambda}\right)$ if and only if

$$a(0,0,0) = 0, b(0,0,0) \neq 0 \text{ and } \frac{\partial a}{\partial \lambda}(0,0,0) \neq 0.$$

6.3.2 Existence of a transcritical bifurcation of the Onsager free-energy functional up to equivariance

The aim of this section is to find non-degeneracy conditions that allow us to reduce the problem of solving the bifurcation equation in (5.15) to an algebraic equation of a simple form and lower order. In particular, we show that $\hat{f}_{\mathrm{real}}$ is S_3-equivariantly equivalent to a mapping $G : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ by using the symmetry properties of f_{real}.

In order to prove that f_{real} is S_3-equivariant, it is sufficient to show that it is equivariant with respect to the generators g_2 and g_4 of the group action, see (6.13). This in turn is a consequence of Proposition 6.1. Notice that for two particular choices of Euler angles we have the following two Wigner matrices

$$R_1 = R\left(\tfrac{\pi}{2}, \pi, \pi\right) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

and

$$R_2 = R\left(\tfrac{\pi}{2}, \pi, -\tfrac{\pi}{2}\right) = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & -\frac{\sqrt{3}}{2} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 & -\frac{1}{2} \end{pmatrix}.$$

Both linear maps leave the subspace $\mathcal{S} = \{(0,0,x,0,y) | x, y \in \mathbb{R}\}$ invariant. Merely viewed on the space $\mathcal{S}$, they correspond to the two elements that generate S_3. Hence we conclude that f_{real} is S_3-equivariant and we know from Theorem 6.8 that it can therefore be written as

$$f_{\mathrm{real}}(\mathbf{u}, \lambda) = a(h_1(\mathbf{u}), h_2(\mathbf{u}), \lambda) \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + b(h_1(\mathbf{u}), h_2(\mathbf{u}), \lambda) \begin{pmatrix} u_1^2 - u_2^2 \\ -2u_1u_2 \end{pmatrix}.$$

Moreover, we can further deduce from Proposition 6.9 that it reduces to the normal form

$$\epsilon\lambda \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} u_1^2 - u_2^2 \\ -2u_1u_2 \end{pmatrix}$$

with $\epsilon := \operatorname{sgn}\left(\frac{\partial a}{\partial \lambda}\right)$ if and only if

$$a(0,0,0) = 0, b(0,0,0) \neq 0 \text{ and } \frac{\partial a}{\partial \lambda}(0,0,0) \neq 0.$$

Since it is not trivial to find the explicit form of the coefficients $a(\cdot,\cdot)$ and $b(\cdot,\cdot)$, it is not straightforward to verify that these conditions hold in case of the bifurcation equation in (5.15).

However, this is sufficient in the case of the reduced bifurcation equation $\hat{f}^{\mathcal{S}}_{\text{real}}$ in (6.12) because the first two derivatives of $f^{\mathcal{S}}_{\text{real}}$ and $\hat{f}^{\mathcal{S}}_{\text{real}}$ agree. In this case the coefficients are given by

$$\hat{a}(h_1(\mathbf{a}), h_2(\mathbf{a}), \lambda) = \lambda + \left(\frac{9}{3136(1+32\pi)} - \frac{5}{1792}\right)(a_0^2 + a_2^2)$$
$$\hat{b}(h_1(\mathbf{a}), h_2(\mathbf{a}), \lambda) = \frac{\sqrt{5\pi}}{448}.$$

Recall that Remark 5.8 shows that $\hat{f}_{\text{real}}$ is a fourth order approximation to f_{real}. In $\hat{f}^{\mathcal{S}}_{\text{real}}$ we have dropped the fourth order terms so that it agrees with $f_{\mathcal{S}}$ up to third order and therefore also verifies the non-degeneracy condition.

Thus, we see that all three non-degeneracy conditions in Proposition 6.9 hold and we can conclude that there exists a one-to-one correspondence between the set of solutions of $f^{\mathcal{S}}_{\text{real}}$ in (6.12) and

$$G(\mathbf{a}, \lambda) = \lambda \begin{pmatrix} a_0 \\ a_2 \end{pmatrix} + \begin{pmatrix} a_0^2 - a_2^2 \\ -2a_0 a_2 \end{pmatrix}.$$

The set of solutions of G can easily be computed. It is given by the trivial solution $\begin{pmatrix} a_0 \\ a_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and the three branches

$$\lambda \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \frac{\lambda}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \text{ and } \frac{\lambda}{2} \begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix}.$$

However, looking at the rotational symmetries of these three branches, we see that they in fact coincide after an application of a rotation. Thus, the solutions corresponding to all three branches are equivalent which proves the existence of a simple linear branch and thus the existence of a unique transcritical bifurcation up to rotations. This result has been summarised in Theorem 1.2.

Finally, let us mention that by using the same methods presented above and in Section 6.2, one is faced with a similar dimension reduction and a similar recognition problem which can be solved on a case to case basis.

Chapter 7

Other properties of the bifurcation diagram

We complete our bifurcation analysis of the Onsager model by proving other properties of the local and global bifurcation diagram. We mainly focus on general interaction kernels satisfying Assumption 1.3 or we work with the Onsager interaction potential in particular. First of all, we prove local uniaxiality of all solutions corresponding to the transcritical bifurcation from the isotropic state, see Section 7.1. Using the boundedness of all minimisers of the free-energy functional (see Lemma 3.3), we show that the free-energy functional is in fact strictly convex for high temperatures and that its trivial solution, $\rho_0 = \frac{1}{4\pi}$ is the unique global solution. In Section 7.2 we prove that the trivial solution is a local minimiser for high temperatures and that it is not a local minimiser for low temperatures. Finally, we focus again on the Onsager interaction potential and we show in Section 7.5 that any bifurcation branch either meets infinity or that it meets another bifurcation branch, thus, proving that all bifurcation branches are continuous and do not end suddenly.

7.1 Uniaxiality of solutions

Recall that the Euler-Lagrange operator corresponding to the Onsager free-energy functional is given by

$$E(\phi, \lambda) := \lambda\phi(p) - \frac{1}{Z(\phi)} \int_{\mathbb{S}^2} k(p \cdot q) \exp(-\phi(q))\, dq. \qquad \text{(see 4.2)}$$

Now, we restrict our attention to the uniaxial solutions of this problem which means that we assume that any solution $\rho_s : L^1(\mathbb{S}^2)$ is axially symmetric with respect to the z-axis. Thus, writing ρ in terms of spherical coordinates $\theta \in [0, \pi)$ and $\varphi \in [0, 2\pi)$ (see Section 4.2.1 for details), we assume that it only depends on θ and is independent of φ. In this case, where

$$\int_{\mathbb{S}^2} dp = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta \; d\theta,$$

the Onsager free-energy functional in (1.2) restricted to the set of axially symmetric probability densities can be rewritten as

$$\begin{aligned}\mathcal{F}_s(\rho_s) :=& \lambda \int_0^{\pi} \rho_s(\theta_p) \ln(\rho_s(\theta_p)) \sin\theta_p \; d\theta_p \\ &+ \frac{1}{2} \int_{A^2} K(\theta_p, \varphi_p, \theta_q, \varphi_q) \rho_s(\theta_q) \rho_s(\theta_p) \sin\theta_p \sin\theta_q \; d\theta_p d\theta_q d\varphi_p d\varphi_q\end{aligned}$$

for $A := [0, \pi] \times [0, 2\pi]$. The Euler-Lagrange equation corresponding to this restricted problem does not differ from the one of the full problem. The reason is that the Euler-Lagrange equation is derived by computing

$$\begin{aligned}
&\frac{d}{d\epsilon}\mathcal{F}_s(\rho_s+\epsilon z_s,\lambda)\Big|_{\epsilon=0}\\
&=\int_0^{\pi} z_s(\theta_p)\left[\lambda\ln\rho_s(\theta_p)+\int_A K(\theta_p,\varphi_p,\theta_q,\varphi_q)\rho_s(\theta_q)\sin\theta_q\,d\theta_q d\varphi_q\right]\sin\theta_p\,d\theta_p
\end{aligned}$$

where $z_s:[0,\pi)\to\mathbb{R}$ such that $\int_0^{\pi} z_s(\theta_p)\sin\theta_p\,d\theta_p=0$. In particular, the term within the square brackets does not depend on the variable φ_p.

Lemma 7.1. *The expression*

$$\int_{\theta_q=0}^{\pi}\int_{\varphi_q=0}^{2\pi} K(\theta_p,\varphi_p,\theta_q,\varphi_q)\rho(\theta_q)\sin\theta_q\;d\theta_q d\varphi_q$$

is independend of φ_p.

Proof. Let R_z be a rotation around the z-axis. Using the rotational invariance of the interaction kernel $k(p\cdot q)$, we see that

$$\begin{aligned}
\int_{\mathbb{S}^2} k(R_z p\cdot q)\exp(-\phi(q))\;dq &= \int_{\mathbb{S}^2} k(p\cdot R_z^t q)\exp(-\phi(q))\;dq\\
&= \int_{\mathbb{S}^2} k(p\cdot q)\exp(-\phi(R_z q))\;dq\\
&= \int_{\mathbb{S}^2} k(p\cdot q)\exp(-\phi(q))\;dq.
\end{aligned}$$

Thus, the expression is invariant with respect to rotations around the z-axis and therefore independent of the variable φ_p. $\square$

This allows us to apply the fundamental lemma of the calculus of variations with respect to the variable θ_p and this gives us the Euler-Lagrange equation

$$\lambda \ln \rho_s(\theta_p) + \int_A K(\theta_p, \varphi_p, \theta_q, \varphi_q)\rho_s(\theta_q) \sin\theta_q \; d\theta_q d\varphi_q = -\lambda \ln Z_s$$

where

$$Z_s = \int_A \exp\left(-\frac{1}{\lambda}\int_A^{2\pi} K(\theta_p, \varphi_p, \theta_q, \varphi_q)\rho_s(\theta_q) \sin\theta_q \; d\theta_q d\varphi_q\right) \sin\theta_p \; d\theta_p d\varphi_p$$

as before. Introducing the thermodynamic potential $\phi_s : \mathbb{S}^2 \to \mathbb{R}$ as

$$\phi_s(\theta_p) := \frac{1}{\lambda}\int_A K(\theta_p, \varphi_p, \theta_q, \varphi_q)\rho_s(\theta_q) \sin\theta_q \; d\theta_q d\varphi_q,$$

it follows that $\rho_s(\theta_p) = Z_s^{-1}\exp(-\phi_s(\theta_p))$ and we can rewrite the Euler-Lagrange equation as

$$\lambda\phi_s(\theta_p) - \frac{1}{Z_s}\int_{\mathbb{S}^2} K(\theta_p, \varphi_p, \theta_q, \varphi_q)\exp(-\phi_s(\theta_q)) \; d\theta_q \sin\theta_q d\varphi_q = 0.$$

Thus, we conclude that the Euler-Lagrange operator for uniaxial probability distributions is equivalently given by

$$E_s(\phi, \lambda) = \lambda\phi_s(\theta_p) - \frac{1}{Z}\int_{\mathbb{S}^2} K(\theta_p, \varphi_p, \theta_q, \varphi_q)\exp(-\phi_s(\theta_q)) \sin\theta_q d\theta_q d\varphi_q. \qquad (7.1)$$

A well-known concept that establishes a relationship between the symmetric solutions of a minimisation problem and the symmetrised problem is the principle of symmetric criticality [?]. It states that each critical point of the symmetric problem is a symmetric critical point of the general problem. In the above setting, this principle can be verified explicitly. Since the Euler-Lagrange operators E_s in (7.1) and E in (4.2) have exactly the same form, we can consider the corresponding Lyapunov-Schmidt decompositions for the general and the symmetric problem simultaneously. In particular, we split $\phi = u + v$ and $\phi_s = u_s + v_s$, respectively. The first step consists in solving

$$(1-P)E(u+v,\lambda) = 0 \text{ and}$$
$$(1-P)E_s(u_s+v_s,\lambda) = 0$$

for v in terms of u and v_s in terms of u_s, respectively. Taking the derivative with respect to v and v_s, respectively, we see that we can use the implicit function theorem in order to solve uniquely for v_s and v. Because $E(u_s+v_s,\lambda) = E_s(u_s+v_s,\lambda)$, it follows that

$$v(u_s) = v_s(u_s)$$

is axially symmetric. Therefore, solving the bifurcation equation of the full problem with $a_{-2} = a_{-1} = a_1 = a_2 = 0$ yields all uniaxial solutions. In particular, this equation is given by

$$\begin{aligned} f_s(a_0,\lambda) =& \frac{18\lambda a_0^3}{49\pi(1+32\pi)^2} + \lambda a_0 + \frac{\sqrt{\frac{5}{\pi}}(448\pi(13+2800\pi)+577)a_0^4}{5795328(1+32\pi)^2} \\ &+ \left(\frac{9}{3136(1+32\pi)} - \frac{5}{1792}\right)a_0^3 + \frac{1}{448}\sqrt{5\pi}a_0^2. \end{aligned}$$

This is now a bifurcation problem with a one-dimensional state variable and we say that it undergoes a transcritical bifurcation at $(0,0)$ if $(0,0)$ is a non-hyperbolic fixed point, that is

$$f(0,0) = 0 \text{ and } \frac{\partial f}{\partial a_0}(0,0) = 0,$$

and if the non-degeneracy conditions

$$\frac{\partial f}{\partial \lambda}(0,0) = 0, \quad \frac{\partial^2 f}{\partial a_0 \partial \lambda}(0,0) \neq 0 \quad \text{and} \quad \frac{\partial^2 f}{\partial a_0^2}(0,0) \neq 0$$

hold (these conditions can be found in [**?**, (3.1.65)-(3.1.68)]). It is easy to see that all of these conditions hold for $f_s(a_0, \lambda)$ and we may therefore deduce that a transcritical bifurcation occurs. Since we do have a unique transcritical solution in the case of the full problem and the symmetric problem, we conclude that these are the same. Therefore we proved the following statement.

Theorem 7.2. *All solutions of the Onsager free-energy functional are uniaxial in a neighbourhood of the trivial solution* $(\phi, \lambda) = (0, \lambda_2)$.

7.2 Local properties of the trivial solution $\rho_0 = \frac{1}{4\pi}$

We concentrate on proving conditions which ensure when the trivial solution is a local minimum and when it is not.

Proposition 7.3. *Let* U *be an interaction operator that diagonalises over the set* *of spherical harmonics, that is*

$$U(Y_l^m) = \mu_l Y_l^m.$$

Let $\mu_{\text{inf}} = \inf_l \mu_l$*, then for all* $\lambda > -\frac{\mu_{\text{inf}}}{4\pi}$ *the trivial solution* $\rho_0 = \frac{1}{4\pi}$ *is a local minimum. Moreover, for all* $0 < \lambda < -\frac{\mu_{\text{inf}}}{4\pi}$*, the trivial solution* $\rho_0 = \frac{1}{4\pi}$ *is not a local minimum.*

Proof. The second derivative of the Onsager free-energy functional in (1.2) at $\rho \in H^2(S^2)$ is given by

$$\begin{aligned} I(z,\lambda) = D_z^2\mathcal{F}(\rho) &= \frac{\partial^2}{\partial\epsilon^2}\mathcal{F}(\rho+\epsilon z)\bigg|_{\epsilon=0} \\ &= \lambda\int_{\mathbb{S}^2}\frac{z(p)^2}{\rho(p)}\,dp + \int_{\mathbb{S}^2\times\mathbb{S}^2} k(p\cdot q)z(p)z(q)\,dpdq \end{aligned} \tag{7.2}$$

with $z \in H^2(\mathbb{S}^2)$ such that $\int_{\mathbb{S}^2} z(p)\,dp = 0$. In particular, we may write

$$z(p) := \sum_{l=0}^{\infty}\sum_{m=-l}^{l} a_{lm}Y_l^m(p)$$

and taking into account that z integrates to zero, we may without loss of generality assume that $a_0 = 0$. On this basis, we can rewrite the second derivative at $\rho = \frac{1}{4\pi}$ as

$$I(z,\lambda) = 4\pi\lambda\int_{\mathbb{S}^2}\left(\sum_{l=1}^{\infty}\sum_{m=-l}^{l} a_{lm}Y_l^m(p)\right)^2 dp$$

$$
\begin{aligned}
&+\int_{\mathbb{S}^2}\left(\sum_{l=1}^{\infty}\sum_{m=-l}^{l} a_{lm}\int_{\mathbb{S}^2} k(p\cdot q)Y_l^m(p)\,dp\right)\sum_{l=1}^{\infty}\sum_{m=-l}^{l} a_{lm}Y_l^m(q)\,dq\\
=&4\pi\lambda\int_{\mathbb{S}^2}\left(\sum_{l=1}^{\infty}\sum_{m=-l}^{l} a_{lm}Y_l^m(p)\right)^2\,dp\\
&+\int_{\mathbb{S}^2}\sum_{l=1}^{\infty}\sum_{m=-l}^{l} a_{lm}\mu_l Y_l^m(q)\sum_{l=1}^{\infty}\sum_{m=-l}^{l} a_{lm}Y_l^m(q)\,dq.
\end{aligned}
$$

Viewing the spherical harmonics as an orthonormal basis in $L^2(\mathbb{S}^2)$, it follows that

$$
I(z,\lambda) = 4\pi\lambda\sum_{l=1}^{\infty}\sum_{m=-l}^{l}|a_{lm}|^2 + \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\mu_l|a_{lm}|^2. \tag{7.3}
$$

Hence the second derivative is positive, that is $I(z,\lambda) > 0$ for all $0 \neq z \in L^2(\mathbb{S}^2)$, if and only if $4\pi\lambda > -\mu_{\text{inf}}$. Thus, the trivial solution ρ_0 is a local minimiser of the bifurcation equation for all

$$
\lambda > -\frac{\mu_{\text{inf}}}{4\pi}.
$$

Moreover, we observe that the following holds

$$
\begin{aligned}
\mathcal{F}\left(\frac{1}{4\pi}+z(p)\right) &= \mathcal{F}\left(\frac{1}{4\pi}\right) + \mathcal{F}'\left(\frac{1}{4\pi}\right)z(p) + \frac{1}{2}\mathcal{F}''\left(\frac{1}{4\pi}\right)z(p) + \text{ h.o.t}\\
&= \mathcal{F}\left(\frac{1}{4\pi}\right) + \frac{1}{2}I(z(p),\lambda) + \text{ h.o.t}
\end{aligned}
$$

If we choose $z = sY_2^0$ with s close enough to zero, then $I(z(p),\lambda) < 0$. In fact, the higher order terms are negligible and we see that $\rho = \frac{1}{4\pi}$ is not a local minimiser for all $\lambda < -\frac{\mu_{\text{inf}}}{4\pi}$. □

Remark 7.4. *In the case of the Onsager interaction potential* $\mu_{\text{inf}} = \mu_2 = -\frac{\pi^2}{8}$

by Theorem 4.12.

7.3 Existence of a unique solution for large values of λ

We prove that the Onsager free-energy functional is strictly convex in ρ for all continuous interaction kernels and therefore that the isotropic state, represented by the uniform distribution $\rho_0 = \frac{1}{4\pi}$, is the unique solution if λ is big.

Theorem 7.5. *Let $k(\cdot)$ be a continuous interaction potential and let λ be given such that the following inequality holds*

$$8\pi M \exp(16M/\lambda) \leq \lambda$$

for $M := \max_{p,q\in\mathbb{S}^2} k(p\cdot q)$. Then the Onsager free-energy functional $\mathcal{F}$ is strictly convex on the set of all probability densities ρ bounded by $C^\star = \exp(16M/\lambda)$, see Lemma 3.3.

Proof. We know from Lemma 3.3 that it is enough to consider the minimisation problem among the set of probability densities $\rho \in L^1(\mathbb{S}^2)$ which are bounded by a constant $C^\star = \exp(16M/\lambda)$ where M denotes an upper bound on the kernel $k(p\cdot q)$. The idea of the proof is now to demonstrate that the second derivative of $\mathcal{F}$ is given by

$$\lambda \int_{\mathbb{S}^2} \frac{z^2(p)}{\rho(p)}\,dp + \int_{\mathbb{S}^2\times\mathbb{S}^2} k(p\cdot q)z(p)z(q)$$

see (7.2). Therefore an application of Jensen's inequality and imposing the condition that $8\pi M \leq \lambda/C^\star$ yield

$$
\begin{aligned}
\lambda \int_{\mathbb{S}^2} \frac{z^2(p)}{\rho(p)}\, dp + \int_{\mathbb{S}^2\times\mathbb{S}^2} & k(p\cdot q) z(p) z(q)\, dp\, dq \\
&\geq \lambda \int_{\mathbb{S}^2} \frac{z^2(p)}{\rho(p)}\, dp - M \left(4\pi \int_{\mathbb{S}^2} |z(p)|\, \frac{dp}{4\pi} \right)^2 \\
&\geq \lambda \int_{\mathbb{S}^2} \frac{z^2(p)}{\rho(p)}\, dp - M 4\pi \int_{\mathbb{S}^2} z(p)^2\, dp \\
&\geq \lambda \int_{\mathbb{S}^2} \frac{z^2(p)}{\rho(p)}\, dp - \frac{\lambda}{2C^\star} \int_{\mathbb{S}^2} z(p)^2 dp \\
&\geq \frac{\lambda}{2C^\star} \int_{\mathbb{S}^2} z^2(p)\, dp,
\end{aligned}
$$

proving that the Onsager functional is strictly convex. Rearranging this condition and plugging in the constant $C^\star = \exp(16M/\lambda)$ yields the above inequality $8\pi M \exp(16M/\lambda) \leq \lambda$. □

In fact Theorem 7.5 proves that the Onsager free-energy functional is a strongly convex functional for all probability densities $\rho \in \mathcal{S}$ as its second derivative is bounded away from zero by a factor which depends on the bifurcation parameter λ. Numerically, this value can be approximated by $\lambda^\star \approx 38.205$ when $M = 1$ (for example in the case of the Onsager interaction potential).

Corollary 7.6. *Let $k(\cdot)$ be a continuous interaction potential and let $\lambda^\star$ be chosen such that $8\pi M \exp(16M/\lambda) \leq \lambda$. Then the uniform density $\rho_0 = \frac{1}{4\pi}$ is the unique solution to the Onsager free-energy functional for all $\lambda \geq \lambda^\star$.*

Proof. The uniform density $\rho_0 = \frac{1}{4\pi}$ is indeed a solution to the Euler-Lagrange equation for all $\lambda \in \mathbb{R}$. By Corollary 3.4 and Theorem 7.5, the necessary optimality condition is also sufficient [?, Theorem 5.2.4]. $\square$

7.4 The Onsager free-energy functional is not convex in general

One condition proving that the functional $\mathcal{F}(\rho, \lambda)$ is convex is to show that its second derivative is positive definite for all $p \in \mathbb{S}^2$, see [?], that is

$$\frac{d^2\mathcal{F}(\rho + \epsilon z, \lambda)}{d^2\epsilon}\Big|_{\epsilon=0} \geq 0 \quad \forall z \text{ such that } \int_{\mathbb{S}^2} z(p)\, dp = 0.$$

In case of the Onsager free-energy functional, this condition reduces to

$$\lambda \int_{\mathbb{S}^2} \frac{z^2(p)}{\rho(p)}\, dp + \int_{\mathbb{S}^2 \times \mathbb{S}^2} k(p \cdot q) z(p) z(q)\, dp\, dq \geq 0 \tag{7.4}$$

for all $z \in L^1(\mathbb{S}^2)$ such that $\int_{\mathbb{S}^2} z(p)\, dp = 0$. Since it is well-known that the entropy term arising in the Onsager free-energy functional is convex, it would be sufficient to prove that the interaction term is convex as well. However. this is typically not the case.

We have seen in the previous section that the second derivative is not positive definite if $\lambda <= -\frac{\mu_{\inf}}{4\pi}$ following the arguments after Equation (7.3). In particular, for the Onsager kernel the energy functional is not convex for $\lambda <= \frac{\pi}{32}$.

7.5 Continuity of all bifurcation branches

We conclude this section by showing that every bifurcation branch of the Euler-Lagrange equation associated with the Onsager free-energy functional equipped with the Onsager kernel is either unbounded and meets infinity or that it meets another bifurcation branch.

The Euler-Lagrange equation in terms of the thermodynamic potential is given by

$$E(\phi, \lambda) = \lambda \phi(p) - \frac{1}{Z(\phi)} \int_{\mathbb{S}^2} k(p \cdot q) \exp(-\phi(q)) \, dq,$$

which is of the form $\lambda \mathrm{Id} - T$. It can be shown that T is in fact a compact operator.

Lemma 7.7.

$$T(\phi) = \frac{1}{Z(\phi)} \int_{\mathbb{S}^2} k(p \cdot q) \exp(-\phi(q)) dq$$

is a compact operator from $H^2(\mathbb{S}^2) \mapsto H^2(\mathbb{S}^2)$.

Proof. Similarly to the proofs of Lemma 4.2 and 4.3, we know that

$$\begin{aligned}
||T(\phi)||_{H^3(\mathbb{S}^2)} &\leq \frac{1}{4\pi} e^{||\phi||_\infty} ||U||_{L^2(\mathbb{S}^2) \to H^3(\mathbb{S}^2)} || \exp(-\phi)||_{L^2(\mathbb{S}^2)} \\
&\leq \frac{1}{4\pi} e^{||\phi||_\infty} ||U||_{L^2(\mathbb{S}^2) \to H^3(\mathbb{S}^2)} \exp(||\phi||_\infty) \\
&\leq \frac{1}{4\pi} e^{C_1 ||\phi||_{H^2(\mathbb{S}^2)}} ||U||_{L^2(\mathbb{S}^2) \to H^3(\mathbb{S}^2)} \exp(C_2 ||\phi||_{H^2(\mathbb{S}^2)}) \\
&\leq C_1 \exp(C_2 ||\phi||_{H^2(\mathbb{S}^2)}).
\end{aligned}$$

The statement follows because $H^3(\mathbb{S}^2)$ is compactly embedded in $H^2(\mathbb{S}^2)$. $\square$

It follows that the bifurcation problem can be rewritten as

$$\frac{1}{\lambda}T(\phi, \lambda) = \phi$$

and it is thus of the form of bifurcation problems considered by Rabinowitz [**?**].

Theorem 7.8. [**?**, Theorem 1.3] *Let $G : E \times \mathbb{R} \to E$ be a compact and continuous non-linear operator and consider the problem*

$$u = G(u, \lambda)$$

where $u \in E$ and $\lambda \in \mathbb{R}$. Moreover, let

$$G(u, \lambda) = \lambda Lu + H(u, \lambda)$$

where $H(u, \lambda)$ is $O(||u||)$ for u near the origin uniformly for bounded λ and let L be a compact and linear map on E. If λ is a real non-zero eigenvalue of L of odd multiplicity, then the solution set $\{(u, \lambda) \mid u = G(u, \lambda)\}$ possesses a maximal connected and closed subset C_u such that $(0, \lambda) \in C_u$ and C_u either

1. *meets infinity in E, or*
2. *meets $(0, \hat{\lambda})$ where $\lambda \neq \hat{\lambda}$ is a real non-zero eigenvalue of L.*

In particular, Rabinowitz shows that any eigenvalue of odd multiplicity is a bifurcation point and that any branch bifurcating from the trivial solution must either meet infinity or meet another bifurcation branch. In the case of the Onsager free-energy functional with Onsager potential, all eigenvalues have multiplicity $s = 2n + 1$ for $n \in \mathbb{N}$, thus we know that $(0, \lambda_s)$ is not an isolated solution but that it is instead a member of a non-trivial closed connected set described by Theorem 7.8.

Chapter 8

Conclusion

We presented a procedure to derive the eigenvalues of interaction operators of the form

$$U(\rho)(p) = \int_{\mathbb{S}^2 2} k(p \cdot q)\rho(q)\ dq$$

depending on kernels that are both continuous and rotationally symmetric. First of all we proved existence and boundedness from both below and above for all minimisers of this functional. Moreover, we derived an explicit expression for the eigenvalues of the Onsager free-energy functional involving the Onsager kernel. Based on this result, we know from [**?**] that all eigenvalues are bifurcation points and we proved that a transcritical bifurcation occurs at $\lambda_2 = \frac{\pi}{32}$ denoting the largest of these eigenvalues. Moreover, we proved that the corresponding solution is locally uniaxial. Globally, we showed that the trivial solution $\rho = \frac{1}{4\pi}$ is the unique solution for high values of λ. Finally, we verified that all bifurcation branches from the isotropic state of the Onsager free-energy functional equipped with the Onsager kernel either tend to infinity or meet another bifurcation branch.

In order to obtain a complete bifurcation diagram, it is left to show that no isolas occur, which means that we do not have any bifurcations that are isolated from all other solutions to our problem at hand. Our approach is not at all limited to the Onsager kernel and not even to quadratic forms given by interaction kernels.

Appendix A

The Sobolev space $H^2(\mathbb{S}^2)$ and its norms

Let us clarify the exact definitions and notation that we are using in Sections 4 and 5.

Definition A.1. *The Sobolev space $H^s(\mathbb{S}^2)$ is the completion of the smooth function space $C^\infty(\mathbb{S}^2)$ with respect to the norm*

$$||f||_{H^2(\mathbb{S}^2)} = \left(||f||^2_{L^2(\mathbb{S}^2)} + \langle f, -\Delta^\star f\rangle^2_{L^2(\mathbb{S}^2)} + ||\Delta^\star f||^2_{L^2(\mathbb{S}^2)} \right)^{1/2} \tag{A.1}$$

where $\Delta^\star$ denotes the Laplace-Beltrami operator on the sphere.

Lemma A.2. *The H^2-norm in (A.1) is equivalent to the norm*

$$||f||_{\hat{H}^2(\mathbb{S}^2)} = \left(\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(l + \frac{1}{2}\right)^4 |a_{lm}|^2 \right)^{1/2} \tag{A.2}$$

where a_{lm} denote the coefficients of the expansion of f in spherical harmonics, that is $f = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm} Y_l^m$.

Proof. It is well-known that spherical harmonics Y_l^m are the eigenfunctions of the

Laplace-Beltrami operator on the sphere. In particular,

$$-\Delta^\star Y_l^m = l(l+1)Y_l^m.$$

It follows that for $f = \sum_{l=0}^\infty \sum_{m=-l}^l a_{lm} Y_l^m$

$$\begin{aligned}
||f||^2_{L^2(\mathbb{S}^2)} &= \int_{\mathbb{S}^2} \left| \sum_{l=0}^\infty \sum_{m=-l}^l a_{lm} Y_l^m(p) \right|^2 dp \\
&= \sum_{l=0}^\infty \sum_{m=-l}^l \sum_{k=0}^\infty \sum_{n=-k}^k a_{lm} a_{kn} \int_{\mathbb{S}^2} Y_l^m(p) Y_k^n(p) dp \\
&= \sum_{l=0}^\infty \sum_{m=-l}^l \sum_{k=0}^\infty \sum_{n=-k}^k a_{lm} a_{kn} \delta_{kl} \delta_{nm} = \sum_{l=0}^\infty \sum_{m=-l}^l |a_{lm}|^2.
\end{aligned}$$

Similarly,

$$\begin{aligned}
\langle f, -\Delta^\star f\rangle^2_{L^2(\mathbb{S}^2)} &= -\int_{\mathbb{S}^2} \Delta^\star f(p) \cdot f(p) dp \\
&= \int_{\mathbb{S}^2} \left(\sum_{l=0}^\infty \sum_{m=-l}^l l(l+1) a_{lm} Y_l^m(p) \cdot \sum_{k=0}^\infty \sum_{n=-k}^k a_{kn} Y_k^n(p) \right) dp \\
&= \sum_{l=0}^\infty \sum_{m=-l}^l l(l+1)|a_{lm}|^2
\end{aligned}$$

and

$$||\Delta^\star f||^2_{L^2(\mathbb{S}^2)} = \int_{\mathbb{S}^2} |\Delta^\star f|^2 dp$$

$$
\begin{aligned}
&= \int_{\mathbb{S}^2} \Delta^\star(\Delta^\star f(p)) \cdot f(p) dp \\
&= \int_{\mathbb{S}^2} \left(\Delta^\star \left(\sum_{l=0}^{\infty} \sum_{m=-l}^{l} -l(l+1) a_{lm} Y_l^m(p) \right) \cdot \sum_{k=0}^{\infty} \sum_{n=-k}^{k} a_{kn} Y_k^n(p) \right) dp \\
&= \int_{\mathbb{S}^2} \left(\sum_{l=0}^{\infty} \sum_{m=-l}^{l} l^2(l+1)^2 a_{lm} Y_l^m(p) \cdot \sum_{k=0}^{\infty} \sum_{n=-k}^{k} a_{kn} Y_k^n(p) \right) dp \\
&= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} l^2(l+1)^2 |a_{lm}|^2.
\end{aligned}
$$

Hence

$$
\begin{aligned}
||f||^2_{\hat{H}^2(\mathbb{S}^2)} &= ||f||^2_{L^2(\mathbb{S}^2)} + \langle f, -\Delta^\star f \rangle^2_{L^2(\mathbb{S}^2)} + ||\Delta^\star f||^2_{L^2(\mathbb{S}^2)} \\
&= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(1 + l(l+1) + l^2(l+1)^2\right) |a_{lm}|^2.
\end{aligned}
$$

It is straightforward to see that

$$
\begin{aligned}
1 + l(l+1) + l^2(l+1)^2 &= 1 + l + 2l^2 + +2l^3 + l^4 \\
&\geq \frac{1}{16} + \frac{1}{2} l + \frac{3}{2} l^2 + 2l^3 + l^4 \\
&= \left(l + \frac{1}{2} \right)^4
\end{aligned}
$$

for all $l \geq 0$. Therefore $||f||_{H^2(\mathbb{S}^2)} \geq ||f||_{\hat{H}^2(\mathbb{S}^2)}$. To the contrary,

$$
\begin{aligned}
16 \left(l + \frac{1}{2} \right)^4 &= 1 + 8l + 12l^2 + 32l^3 + 16l^4 \geq 1 + l + 2l^2 + 2l^3 + l^4 \\
&= 1 + l(l+1) + l^2(l+1)^2
\end{aligned}
$$

and thus $||f||_{H^2(\mathbb{S}^2)} \leq 4||f||_{\hat{H}^2(\mathbb{S}^2)}$ which completes the proof. $\square$

Using very similar arguments, one can prove the following more general statement.

Corollary A.3. *The H^k-norm*

$$||\eta||_{H^k(\mathbb{S}^2)} = \left(\sum_{|\alpha| \leq k} \int_{\mathbb{S}^2} |D^\alpha \eta(p)|^2 \, dp \right)^{1/2}$$

is equivalent to the norm

$$||f||_{\hat{H}^k(\mathbb{S}^2)} = \left(\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(l + \frac{1}{2} \right)^{2k} |a_{lm}|^2 \right)^{1/2} \tag{A.3}$$

where a_{lm} denote the coefficients of the expansion of f in spherical harmonics, that is $f = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm} Y_l^m$. Notice that D^α acts in tangential direction to $\mathbb{S}^2$.

Appendix B

The exact form of the bifurcation equation in terms of real spherical harmonics up to fifth order

The bifurcation equation in terms of real spherical harmonics is given by

$$f_{\mathrm{real}}(u,\lambda)(p) = \sum_{m=-2}^{2} f_m(u,\lambda)Y_{2,m}(p). \tag{B.1}$$

with

$$\begin{aligned}
f_{-2} =& \lambda u_{-2} + \frac{1}{448}\sqrt{\frac{15\pi}{2}}u_{-1}^2 - \frac{1}{224}\sqrt{5\pi}u_{-2}u_0 - \frac{(-1+1120\pi)u_{-2}u_0^2}{12544(1+32\pi)} \\
&+ \frac{18\lambda u_{-2}u_0^2}{49\pi(1+32\pi)^2} + \frac{\sqrt{\frac{15}{2\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-1}^2u_0^2}{1931776(1+32\pi)^2} \\
&- \frac{\sqrt{\frac{5}{\pi}}\left(1-98\pi+4480\pi^2\right)u_{-2}u_0^3}{25872(1+32\pi)^2} + \frac{(-1+1120\pi)u_{-2}u_{-1}u_1}{6272(1+32\pi)} \\
&- \frac{36\lambda u_{-2}u_{-1}u_1}{49\pi(1+32\pi)^2} - \frac{\sqrt{\frac{15}{2\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-1}^3u_1}{965888(1+32\pi)^2} \\
&+ \frac{\sqrt{\frac{5}{\pi}}\left(23-9184\pi+250880\pi^2\right)u_{-2}u_{-1}u_0u_1}{965888(1+32\pi)^2}
\end{aligned}$$

$$
\begin{aligned}
&+\frac{5\sqrt{\frac{15}{2\pi}}\left(31+1120\pi+50176\pi^2\right)u_{-2}^2u_1^2}{965888(1+32\pi)^2}-\frac{(-1+1120\pi)u_{-2}^2u_2}{6272(1+32\pi)}\\
&+\frac{36\lambda u_{-2}^2u_2}{49\pi(1+32\pi)^2}+\frac{\sqrt{\frac{15}{2\pi}}\left(61+952\pi+125440\pi^2\right)u_{-2}u_{-1}^2u_2}{241472(1+32\pi)^2}\\
&-\frac{\sqrt{\frac{5}{\pi}}\left(61+952\pi+125440\pi^2\right)u_{-2}^2u_0u_2}{120736(1+32\pi)^2},\\
f_{-1}=&\lambda u_{-1}+\frac{1}{448}\sqrt{5\pi}u_{-1}u_0-\frac{(-1+1120\pi)u_{-1}u_0^2}{12544(1+32\pi)}+\frac{18\lambda u_{-1}u_0^2}{49\pi(1+32\pi)^2}\\
&+\frac{\sqrt{\frac{5}{\pi}}\left(577+5824\pi+1254400\pi^2\right)u_{-1}u_0^3}{5795328(1+32\pi)^2}-\frac{1}{224}\sqrt{\frac{15\pi}{2}}u_{-2}u_1\\
&+\frac{(-1+1120\pi)u_{-1}^2u_1}{6272(1+32\pi)}-\frac{36\lambda u_{-1}^2u_1}{49\pi(1+32\pi)^2}\\
&-\frac{\sqrt{\frac{5}{\pi}}\left(61+952\pi+125440\pi^2\right)u_{-1}^2u_0u_1}{241472(1+32\pi)^2}\\
&-\frac{\sqrt{\frac{15}{2\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-2}u_0^2u_1}{965888(1+32\pi)^2}\\
&+\frac{3\sqrt{\frac{15}{2\pi}}\left(111+672\pi+250880\pi^2\right)u_{-2}u_{-1}u_1^2}{965888(1+32\pi)^2}-\frac{(-1+1120\pi)u_{-2}u_{-1}u_2}{6272(1+32\pi)}\\
&+\frac{36\lambda u_{-2}u_{-1}u_2}{49\pi(1+32\pi)^2}+\frac{5\sqrt{\frac{15}{2\pi}}\left(31+1120\pi+50176\pi^2\right)u_{-1}^3u_2}{965888(1+32\pi)^2}\\
&-\frac{\sqrt{\frac{5}{\pi}}\left(221+12992\pi+250880\pi^2\right)u_{-2}u_{-1}u_0u_2}{965888(1+32\pi)^2}\\
&-\frac{\sqrt{\frac{15}{2\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-2}^2u_1u_2}{482944(1+32\pi)^2},\\
f_0=&\lambda u_0+\frac{1}{448}\sqrt{5\pi}u_0^2-\frac{(-1+1120\pi)u_0^3}{12544(1+32\pi)}+\frac{18\lambda u_0^3}{49\pi(1+32\pi)^2}
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{\sqrt{\frac{5}{\pi}}\left(577+5824\pi+1254400\pi^2\right)u_0^4}{5795328(1+32\pi)^2}-\frac{1}{448}\sqrt{5\pi}u_{-1}u_1\\
&+\frac{(-1+1120\pi)u_{-1}u_0u_1}{6272(1+32\pi)}-\frac{36\lambda u_{-1}u_0u_1}{49\pi(1+32\pi)^2}\\
&-\frac{\sqrt{\frac{5}{\pi}}\left(577+5824\pi+1254400\pi^2\right)u_{-1}u_0^2u_1}{1931776(1+32\pi)^2}\\
&+\frac{\sqrt{\frac{5}{\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-1}^2u_1^2}{965888(1+32\pi)^2}\\
&+\frac{5\sqrt{\frac{15}{2\pi}}\left(31+1120\pi+50176\pi^2\right)u_{-2}u_0u_1^2}{965888(1+32\pi)^2}-\frac{1}{224}\sqrt{5\pi}u_{-2}u_2\\
&-\frac{(-1+1120\pi)u_{-2}u_0u_2}{6272(1+32\pi)}+\frac{36\lambda u_{-2}u_0u_2}{49\pi(1+32\pi)^2}\\
&+\frac{5\sqrt{\frac{15}{2\pi}}\left(31+1120\pi+50176\pi^2\right)u_{-1}^2u_0u_2}{965888(1+32\pi)^2}\\
&-\frac{5\sqrt{\frac{5}{\pi}}\left(31+1120\pi+50176\pi^2\right)u_{-2}u_0^2u_2}{482944(1+32\pi)^2}\\
&+\frac{\sqrt{\frac{5}{\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-2}u_{-1}u_1u_2}{965888(1+32\pi)^2}\\
&-\frac{\left(-12365-2052416\pi-12020736\pi^2+1040449536\pi^3\right)u_{-2}u_{-1}u_0u_1u_2}{1997632\pi(1+32\pi)^3(5+512\pi)}\\
&-\frac{\sqrt{\frac{5}{\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-2}^2u_2^2}{482944(1+32\pi)^2},\\
f_1=&\lambda u_1+\frac{1}{448}\sqrt{5\pi}u_0u_1-\frac{(-1+1120\pi)u_0^2u_1}{12544(1+32\pi)}+\frac{18\lambda u_0^2u_1}{49\pi(1+32\pi)^2}\\
&+\frac{\sqrt{\frac{5}{\pi}}\left(577+5824\pi+1254400\pi^2\right)u_0^3u_1}{5795328(1+32\pi)^2}+\frac{(-1+1120\pi)u_{-1}u_1^2}{6272(1+32\pi)}
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{36\lambda u_{-1}u_1^2}{49\pi(1+32\pi)^2}-\frac{\sqrt{\frac{5}{\pi}}\left(61+952\pi+125440\pi^2\right)u_{-1}u_0u_1^2}{241472(1+32\pi)^2}\\
&+\frac{5\sqrt{\frac{15}{2\pi}}\left(31+1120\pi+50176\pi^2\right)u_{-2}u_1^3}{965888(1+32\pi)^2}-\frac{1}{224}\sqrt{\frac{15\pi}{2}}u_{-1}u_2\\
&-\frac{\sqrt{\frac{15}{2\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-1}u_0^2u_2}{965888(1+32\pi)^2}-\frac{(-1+1120\pi)u_{-2}u_1u_2}{6272(1+32\pi)}\\
&+\frac{36\lambda u_{-2}u_1u_2}{49\pi(1+32\pi)^2}+\frac{3\sqrt{\frac{15}{2\pi}}\left(111+672\pi+250880\pi^2\right)u_{-1}^2u_1u_2}{965888(1+32\pi)^2}\\
&-\frac{\sqrt{\frac{5}{\pi}}\left(221+12992\pi+250880\pi^2\right)u_{-2}u_0u_1u_2}{965888(1+32\pi)^2}\\
&-\frac{\sqrt{\frac{15}{2\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-2}u_{-1}u_2^2}{482944(1+32\pi)^2},
\end{aligned}
$$

and

$$
\begin{aligned}
f_2=&\lambda u_2+\frac{1}{448}\sqrt{\frac{15\pi}{2}}u_1^2\frac{\sqrt{\frac{15}{2\pi}}\left(89-1792\pi+250880\pi^2\right)u_0^2u_1^2}{1931776(1+32\pi)^2}\\
&-\frac{\sqrt{\frac{15}{2\pi}}\left(89-1792\pi+250880\pi^2\right)u_{-1}u_1^3}{965888(1+32\pi)^2}-\frac{1}{224}\sqrt{5\pi}u_0u_2\\
&-\frac{(-1+1120\pi)u_0^2u_2}{12544(1+32\pi)}+\frac{18\lambda u_0^2u_2}{49\pi(1+32\pi)^2}-\frac{\sqrt{\frac{5}{\pi}}\left(1-98\pi+4480\pi^2\right)u_0^3u_2}{25872(1+32\pi)^2}\\
&+\frac{(-1+1120\pi)u_{-1}u_1u_2}{6272(1+32\pi)}-\frac{36\lambda u_{-1}u_1u_2}{49\pi(1+32\pi)^2}\\
&+\frac{\sqrt{\frac{5}{\pi}}\left(23-9184\pi+250880\pi^2\right)u_{-1}u_0u_1u_2}{965888(1+32\pi)^2}\\
&+\frac{\sqrt{\frac{15}{2\pi}}\left(61+952\pi+125440\pi^2\right)u_{-2}u_1^2u_2}{241472(1+32\pi)^2}-\frac{(-1+1120\pi)u_{-2}u_2^2}{6272(1+32\pi)}
\end{aligned}
$$

$$+\frac{36\lambda u_{-2}u_2^2}{49\pi(1+32\pi)^2}+\frac{5\sqrt{\frac{15}{2\pi}}\left(31+1120\pi+50176\pi^2\right)u_{-1}^2u_2^2}{965888(1+32\pi)^2}$$
$$-\frac{\sqrt{\frac{5}{\pi}}\left(61+952\pi+125440\pi^2\right)u_{-2}u_0u_2^2}{120736(1+32\pi)^2}.$$

Appendix C

A local bifurcation analysis by Jakob Wachsmuth

The unpublished thesis of Jakob Wachsmuth [?] contains similar results about the local bifurcation structure of the Onsager free-energy functional with interaction potential satisfying Assumption 1.3. It was only drawn to the attention of the author after completion of our work on the bifurcation structure of the Onsager free-energy functional. The major differences between his and our work are as follows:

- Instead of working with the set of spherical harmonics, Wachsmuth uses an equivalent description of this set of functions, namely homogeneous polynomials restricted to the sphere. This allows him to perform an elegant dimension reduction to a state space of two dimensions.

- Wachsmuth does not derive an explicit expression for the set of eigenvalues of the interaction operator U. He shows that the Laplace-Beltrami operator and U commute which allows him to conclude that the spherical harmonics are indeed the eigenvectors of U as well. In contrast, we derive a procedure that allows us to compute the eigenvalues of U equipped with any kernel admitting an appropriate Taylor expansion, see Theorem 4.8.

- Wachsmuth imposes the assumption that the absolute values of the eigenvalues form a decreasing sequence. By proving that the interaction operator is compact in $H^2(\mathbb{S}^2)$ (see Lemma 7.7), we show that the sequence of eigenvalues corresponding to the interaction operator is always decreasing.

- Crucially, we prove local uniaxiality of the solutions occurring at the bifurcation point $\lambda^\star$ in Section 7.1, while Wachsmuth only shows that the solution is infinitesimally uniaxial.