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Magnetic confinement in stellarators: harmonic fields and shape differentiation

Robin Roussel

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Sorbonne Université

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Unité de recherche **Laboratoire Jacques-Louis Lions**

Thèse présentée par **Robin Roussel**

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Confinement magnétique dans les stellarators : champs harmoniques et différentiation de forme

Thèse dirigée par Ugo BOSCAIN
Mario SIGALOTTI

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Doctoral School **École Doctorale de Sciences Mathématiques de Paris Centre ED 386**

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Confinement magnétique dans les stellarators : champs harmoniques et différentiation de forme**Résumé**

Dans cette thèse, nous considérons des problèmes de différentiation de forme de champs harmoniques ayant pour applications l'étude de propriétés de confinement magnétique dans des stellarators.

Les stellarators sont des réacteurs à fusion ayant comme objectif de confiner un plasma dans une enceinte toroidale à l'aide de champs magnétiques. Contrairement aux tokamaks, les stellarators n'induisent pas directement de courant électrique dans le plasma, et les champs magnétiques utilisés peuvent donc être considérés comme des champs harmoniques en première approximation. Nous considérons ainsi dans cette thèse comment les variations de la forme géométrique du plasma modifient le champ harmonique associé ainsi que certaines de ses propriétés. Nous étudions ainsi dans un premier chapitre le problème général de différentiation de forme des champs harmoniques dans des domaines toroidaux. Dans un deuxième chapitre, nous définissons une fonction de forme correspondant à l'hélicité des champs harmoniques et étudions les problèmes de différentiation et d'optimisation de forme associés. Enfin, nous étudions dans un troisième chapitre la dynamique des applications de Poincaré associées aux champs harmoniques via une approche de différentiation de forme.

Mots clés : stellarators, champs harmoniques, différentiation de forme, hélicité, applications de Poincaré, théorie de Hodge, éléments finis extérieurs

Magnetic confinement in stellarators: harmonic fields and shape differentiation**Abstract**

In this thesis, we consider shape differentiation problems for harmonic fields with applications to the study of magnetic confinement in stellarators.

Stellarators are fusion reactors designed to confine a plasma in a toroidal chamber using magnetic fields. Unlike tokamaks, stellarators do not directly induce electric currents in the plasma so that the corresponding magnetic fields may be identified, as an initial approximation, with harmonic fields. In this thesis, we consider how variations in the geometric shape of the plasma modify the associated harmonic field and some of its properties. In the first chapter, we study the general problem of shape differentiation of harmonic fields in toroidal domains. In a second chapter, we define a shape function corresponding to the helicity of harmonic fields and study the associated shape differentiation and optimization problems. Finally, in a third chapter, we study the dynamics of Poincaré maps associated with harmonic fields via a shape differentiation approach.

Keywords: stellarators, harmonic fields, shape differentiation, helicity, Poincaré maps, Hodge theory, finite element exterior calculus

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1. beaucoup*

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2. Je crois me rappeler qu'il y avait un truc à Paris cet été, mais j'ai oublié quoi...

3. J'en oublie sans doute, il y en a eu beaucoup

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4. Challenge accepted : 23/07/23

5. Sauf : Spotify, Deezer, Amazon Music, Apple Music, YouTube Music, Qobuz, Tidal, Soundcloud, Instagram,

j'écris ces lignes, il est déjà 20h, je suis au labo depuis 8h30, et j'ai un jour de retard sur l'envoi de mon manuscrit pour l'impression. Et puis, j'ai pas envie de vous assommer encore plus qu'avec l'exposé auquel vous êtes en train d'assister⁶.

6. Ça se passe bien d'ailleurs, j'ai pas l'air trop stressé? Je suis tout pimpant avec mon costume, pas vrai?

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Chapter 1

Introduction

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1.1 General introduction

In this thesis, we are interested in some shape differentiation and optimization problems arising from the context of magnetic confinement in stellarator fusion reactors. Stellarators aim to confine a plasma in which fusion reactions take place by using an external magnetic field without inducing electric current inside the plasma. As such, we obtain from the Maxwell equations that the confining magnetic field may be well approximated by a curl free and divergence free vector field. We refer to such magnetic fields as *harmonic fields*.

The general approach of this manuscript is to consider how changing the shape of the plasma domain may affect the corresponding harmonic field as well as some of its properties which may be relevant in the context of magnetic confinement. In Chapter 2 we begin by considering the general problem of shape differentiation of harmonic fields, that is, how perturbing the shape of the plasma domain changes the corresponding harmonic field itself. In Chapter 3, we consider the helicity of harmonic fields, which is an important quantity in magnetohydrodynamics models. We proceed to study helicity of harmonic fields as a shape functional, compute the shape gradient of this quantity and propose a numerical scheme to evaluate helicity of harmonic fields and perform a numerical optimization of this functional. Finally, we consider in Chapter 4 the problem of shape differentiation for Poincaré maps of harmonic fields, that is, how perturbing the shape of the plasma domain affects the Poincaré map of the harmonic field of the underlying domain. In this context, we obtain a general shape differential formula and study two particular cases in which we are able to find explicit properties of the shape differential.

Before developing the contributions of this thesis, we begin by introducing the relevant scientific context in Chapter 1. This chapter is organized as follows. In Section 1.2, we introduce some relevant concepts for fusion reactors and, in particular, magnetic confinement of plasmas. We then give in Section 1.3 a first definition of harmonic fields in toroidal domains, which will be studied in the rest of the manuscript, and we expose some relevant mathematical objects and

problems in the context of magnetic confinement. Finally, we discuss the scientific contributions of this thesis and give a general overview of the rest of the manuscript in Section 1.4.

This thesis manuscript was prepared at the Laboratoire Jacques-Louis Lions under the supervision of Ugo Boscain¹ and Mario Sigalotti².

1.2 Physical context

In this section, we introduce some key concepts for magnetic confinement in fusion reactors. In Section 1.2.1, we give a general introduction to the basic principles of power production by nuclear fusion. In particular, we motivate the necessity of plasmas and the basic idea of magnetic confinement. Afterwards, we introduce in Section 1.2.2 three models to describe the dynamics of plasmas and discuss their physical and computational relevance. After that, we introduce in Section 1.2.3 a simpler Lagrangian model to describe the dynamics of charged particles in electromagnetic fields and discuss some of its implications. In particular, we use this to motivate the necessity of a poloidal component in magnetic fields used for confinement. Finally, we introduce two families of fusion reactors in Section 1.2.4, the tokamak and the stellarator. In this section, we explain that the key difference between the two approaches is the way in which a poloidal component is obtained for the magnetic field. For an introduction to the key concepts of magnetic confinement, in particular in the case of stellarators, we refer the interested reader to [IPW20].

1.2.1 Fusion reactors

Fusion type reactors aim to produce energy using nuclear fusion. It is known that while atoms with large atomic numbers tend to release energy by splitting, smaller atoms release energy by fusing. Indeed, the binding energy of atoms tends to increase with the number of atomic nuclei up to Iron-56 after which it slowly decreases (see Fig. 1.1). However, although small atoms release energy when fusing, igniting the fusion reactions necessitates high energies. Indeed, as positively charged particles repel each other, one needs to overcome the Coulomb barrier in order for the strong nuclear force to fuse nuclei together, that is, atoms need to have enough kinetic energy when colliding to overcome the large Coulomb potential energy when the distance between the atomic nuclei is of the order of the size of a proton³. As temperature is proportional to the average kinetic energy of the atoms, we find that fusion reactions necessitate high temperatures. In particular, the kinetic energy of the atoms needs to be much higher than their ionization energy, so that nuclear fusion takes place in a plasma, that is, a mixture of electrons and positively charged ions. Although one may think that using Hydrogen is the best option as it has no internal binding energy, it is known that hydrogen-hydrogen fusion has a small cross-section so that fusion reactions happen with low probability. In fact, it is known that the fusion reaction with the highest reactivity is given by deuterium and tritium, that is, isotopes of the Hydrogen with one and two neutrons respectively. This reaction is then optimal at a temperature of the order of 100MK, or about ten times the temperature of the sun.

Research for fusion power started as early as the 1940s as this option allows generating large amounts of energy with low quantities of reactants. Furthermore, deuterium can be easily extracted from water while tritium, which is a radioactive isotope of hydrogen, can be produced through a process called tritium breeding. Also, the byproducts of deuterium-tritium fusion

1. <https://www.ljll.fr/~boscain/>

2. <https://www.ljll.fr/~sigalotti/>

3. Statistically, the kinetic energy needed to achieve fusion is in fact smaller than the Coulomb barrier because of quantum tunneling.

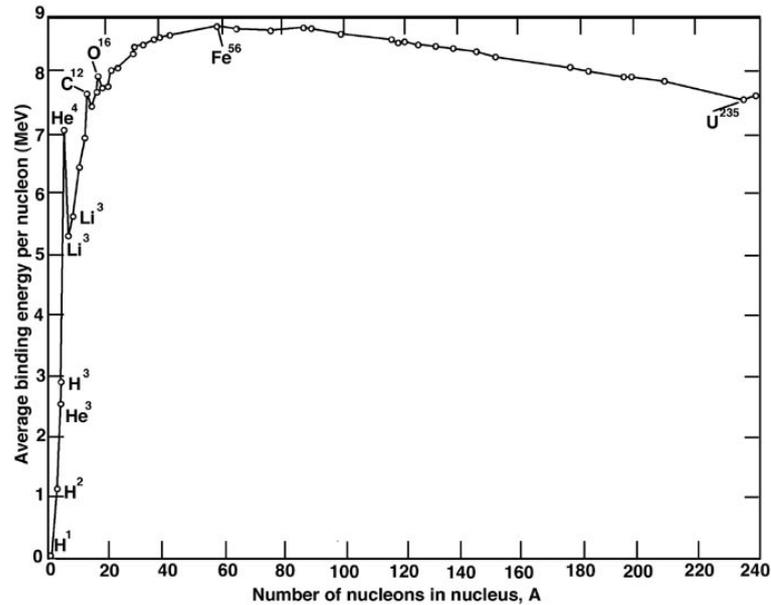


Figure 1.1 – Binding energy of atoms in function of the number of nucleons. Source: Nuclear binding energy Wikipedia page

reaction are simply helium atoms and neutrons, so that, in contrast to fission reactors, one does not have to handle radioactive waste. However, achieving stable fusion reactors for power production comes with many challenges so that, up to now, research on fusion power is purely experimental and not industrial.

As we just saw, fusion reactions occur at very high temperatures. In particular, the needed energies for fusion reactions are orders of magnitudes higher than ionization energies so that fusion occurs in plasmas. Moreover, the high temperatures of the plasma imply that it diffuses extremely quickly. For nuclear reactions occurring in stars, this diffusion is compensated by gravitational forces which cannot be used in man made fusion reactors. One of the most challenging aspects of fusion reactors is thus to confine the plasma in a small enough region to maintain high enough pressure and temperature for nuclear fusion. One approach, which will not be further discussed in this thesis, is inertial confinement, which uses lasers to confine the plasma in a small region. The other common approach is magnetic confinement, used for example in tokamaks and stellarators. Indeed, since the plasma is an ionized gas, the charge separation implies that it interacts with magnetic fields. The goal of magnetic confinement is thus to confine the plasma in a chamber, which is toroidally shaped for stellarators and tokamaks, through the use of an external magnetic field generated by electrical currents circulating in coils outside the fusion chamber. As will be discussed later in the introduction, the coupled dynamics of the plasma and the magnetic field are intricate so that finding magnetic fields which are well-suited for magnetic confinement is a challenging problem. Magnetic confinement devices also come with many physical and engineering challenges, such as the design and production of high temperature superconducting coils in order to generate the needed magnetic field.

1.2.2 Plasma models

As in the general context of particle dynamics, one can study plasmas at three different levels. First, the microscopic level aims to describe the motion of individual charged particles and their coupling with an external electromagnetic field. Second, the mesoscopic level gives a statistical description of the plasma, that is, we are only interested in the particle density in phase space rather than the description of each individual particle. Finally, the macroscopic scale gives a fluid description of the plasma, with objects such as the velocity, temperature and pressure fields of the plasma, and their coupling with the electromagnetic field.

Microscopic model

Suppose we are given a set of N particles, with position x_i , velocity v_i , charge q_i and mass m_i , as well as an external magnetic field given by E_{ext} and B_{ext} , two vector fields of \mathbb{R}^3 . For a given particle, its motion is described by the second Newton law

$$\begin{aligned}\dot{x}_i &= v_i, \\ m_i \dot{v}_i &= F_i(x_i, v_i),\end{aligned}$$

where F_i is the force applied to the i -th particle. If the particles only experiences electromagnetic forces, F_i is given by the Lorentz force

$$F_i(x, v) = q_i (E_i(x) + v \times B_i(x)).$$

E_i and B_i are the total electromagnetic fields experienced by the particle, which differ from E_{ext} and B_{ext} through the electromagnetic fields generated by the other $N - 1$ particles. These fields are given by

$$\begin{aligned}E_i(x) &= E_{\text{ext}}(x) + \sum_{j \neq i} \frac{q_j}{4\pi\epsilon_0} \frac{x - x_j}{|x - x_j|^3}, \\ B_i(x) &= B_{\text{ext}}(x) + \sum_{j \neq i} \frac{\mu_0 q_j}{4\pi} \frac{v_j \times (x - x_j)}{|x - x_j|^3}.\end{aligned}$$

Combining the expressions of the total electromagnetic fields and the Lorentz force into the equations of motion, we see that we obtain a $6N$ -dimensional system of coupled nonlinear ODEs. If one wants to simulate plasmas on the scales of reactors, the number of particles is impossible to track⁴. Even if one wants to simulate for example a few thousand or millions of atoms, computations become quickly very expensive as the number of interactions evolves as N^2 .

Vlasov–Maxwell equations

For practical purposes, it is often unnecessary to track individual particles. To this aim, the Vlasov–Maxwell equations give a mesoscopic description of charged particles given by a density function f on phase space, that is, a function of position and momentum. Intuitively, given a small volume element $dx dp$ centered on a point (x, p) in phase space, $f(x, p) dx dp$ gives the number of particles at position x and momentum p in this volume element.

More specifically, in the case of a monoatomic plasma, the mesoscopic description is given by two density functions; f_e for the electrons, and f_i for the positively charged ions. The evolution

4. For example, one gram of Deuterium corresponds to $N = 3,0 \times 10^{23}$ particles.

equations of these quantities is then the following.

$$\begin{aligned}\partial_t f_e + v_e \cdot \nabla_x f_e - e \left(E + \frac{v_e}{c} \times B \right) \cdot \nabla_p f_e &= 0, \\ \partial_t f_i + v_i \cdot \nabla_x f_i + Z_i e \left(E + \frac{v_i}{c} \times B \right) \cdot \nabla_p f_i &= 0,\end{aligned}\tag{1.1}$$

where the velocity v_α of the species α is related to its momentum p through the mass of an individual particle m_α by $v_\alpha = p/m_\alpha$ ⁵, c is the speed of light in a vacuum, e is the elementary charge of a proton and Z_i is the atomic number of the ions. Each equation can be seen as a transport equation in phase space, where the first transport term indicates that the position is transported by the velocity while the second term indicates that momentum is transported by the Lorentz force. The electromagnetic fields are then given by solutions to the Maxwell equations

$$\begin{aligned}\operatorname{curl} B &= \frac{4\pi j}{c} + \frac{1}{c} \partial_t E, \\ \operatorname{curl} E &= -\frac{1}{c} \partial_t B, \\ \operatorname{div} B &= 0, \\ \operatorname{div} E &= 4\pi \rho.\end{aligned}$$

Finally, the charge density ρ and current density j are given by the density functions by

$$\begin{aligned}\rho &= e \int_{\mathbb{R}^3} Z_i f_i - f_e dp, \\ j &= e \int_{\mathbb{R}^3} Z_i f_i v_i - f_e v_e dp.\end{aligned}$$

Combining the Maxwell equations with the evolution equations, we obtain a nonlinear nonlocal system of PDEs called the Vlasov–Maxwell system. One may also add a collision operator on the right hand side of Eq. (1.1) to obtain the Vlasov–Maxwell–Boltzmann system.

Magnetohydrodynamics

The last model we will discuss in this section to describe plasmas is a fluid model referred to as magnetohydrodynamics (MHD). For derivations of MHD equations from the Vlasov–Maxwell–Boltzmann system, we refer to [JM12; AS19; Zha21]. The MHD equations describe the evolution of macroscopic fluid quantities given by the velocity field u , the mass density n and pressure p . The mass density n satisfies the conservation law

$$\partial_t n + \operatorname{div}(nu) = 0,$$

while the velocity field satisfies the law of motion

$$n(\partial_t u + u \cdot \nabla u) - \nu \Delta u = j \times B - \nabla p,$$

where ν is the fluid viscosity and p is given by the equation of state

$$\frac{d}{dt} \left(\frac{p}{n^\gamma} \right) = 0.$$

5. This formula is valid when p is negligible in comparison to $m_\alpha c$. Otherwise, one needs to use the relativistic formula.

Moreover, combining Ohm's law

$$E + u \times B = \eta J,$$

where η is the magnetic resistivity, with Maxwell's equations, we obtain the following equation of motion for the magnetic field

$$\partial_t B = \text{curl}(u \times B) + \frac{\eta}{\mu_0} \Delta B.$$

The case where viscosity and magnetic resistivity are zero is referred to as ideal MHD. We also note that the last equation may be seen as a transport diffusion equation for the magnetic field when seen as a two-form (see Section 1.3.2 for the transport part).

The notion of MHD equilibrium is also important when designing magnetic fields for fusion reactors. In this case, the velocity field of the fluid is assumed to be zero, and the magnetic field to be time independent. In the ideal case, the MHD equations are thus reduced to the force balance equation

$$j \times B = \nabla p,$$

as well as the Gauss and Ampère laws for the magnetic field

$$\text{div } B = 0, \quad \text{curl } B = \mu_0 j.$$

As will be discussed in Section 1.3.3, solving for MHD equilibria is often used for preliminary designs of magnetic fields in stellarators. It is then common to study more subtle kinetic phenomena of plasma dynamics, such as neoclassical transport or bootstrap currents, starting from this MHD equilibrium (see for example [Bei+90] for the case of the W7X reactor). We also note that as the harmonic fields we will study in the main contributions verify $j = 0$, they correspond to MHD equilibria with constant pressure.

1.2.3 Trajectories of charged particles in magnetic fields

As the plasma models we discussed in Section 1.2.2 are complex to work with for explicit computations, we introduce a common simple model used to describe trajectories of charged particles in a plasma. In this model, we consider a single charged particle traveling in an electromagnetic field. Thus, we consider no influence of the particle on the electromagnetic field, and no particle to particle interaction as opposed to what was done in the complete microscopic model given in Section 1.2.2. We are thus led to consider the following ODE

$$\begin{aligned} \dot{x}(t) &= v(t), \\ m\dot{v}(t) &= q(E(x(t)) + v \times B(x(t))), \end{aligned}$$

where E and B are given electromagnetic fields.

Particles in a uniform magnetic field

We first consider the case of a particle in a uniform magnetic field. Let $(e_{\parallel}, e_{\perp}^1, e_{\perp}^2)$ be a positively oriented orthonormal basis of \mathbb{R}^3 , and consider the magnetic field

$$B = b e_{\parallel}.$$

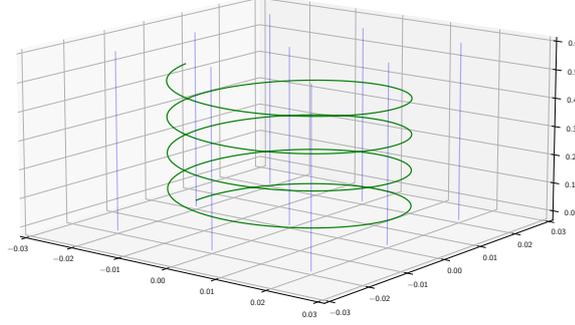


Figure 1.2 – Trajectory of a charged particle in a uniform magnetic field. Field lines are in blue and the trajectory is in green.

Using the orthogonal decomposition $v = v_{\perp} + v_{\parallel}e_{\parallel}$, the ODE satisfied by the velocity vector becomes

$$\begin{aligned}\dot{v}_{\parallel} &= 0, \\ \dot{v}_{\perp} &= \frac{qb}{m}v_{\perp} \times e_{\parallel}.\end{aligned}$$

Using the relations $e_{\perp}^1 \times e_{\parallel} = -e_{\perp}^2$ and $e_{\perp}^2 \times e_{\parallel} = e_{\perp}^1$, we obtain that v_{\perp} verifies the equations of a harmonic oscillator with angular frequency qb/m . As a result, we find that charged particles travel in the direction of the magnetic field with constant velocity while oscillating around field lines (see Fig. 1.2). Importantly, the orientation of the oscillation is determined by the sign of the charge and the amplitude of the oscillation in space, which is given by $m|v_{\perp}|/(qb)$, is inversely proportional to the strength of the magnetic field. The oscillation radius and angular frequencies are referred to as the gyroradius and gyrofrequency respectively. In the case of a Deuterium plasma heated at 100MK in a uniform field of 1T, average electrons will have a gyroradius of $1,9 \times 10^{-4}m$ and a gyrofrequency of $1,8 \times 10^{11}s^{-1}$, while deuterium ions will have an average gyroradius of $1,9 \times 10^{-2}m$ and a gyrofrequency of $4,8 \times 10^7s^{-1}$. Compared the typical time and space scales of a fusion reactor, we therefore see that the oscillations are narrow and fast so that one can make the approximation that charged particles follow the magnetic field lines.

Particles in non-uniform fields and the gyroaveraged Lagrangian

We now consider the motion of a charged particle in a general time independent electromagnetic field. To do so, we use the Lagrangian framework, and more specifically the gyroaveraged Lagrangian. Although our notations are slightly different, this section is largely inspired by and synthesizes [IPW20, Section 5.2].

First, we recall that the Lagrangian giving the motions of particles in a potential is given as a function of the position and velocity by the difference of the kinetic energy and the potential

energy. In the case of an electromagnetic field, if we have an electric potential $E = \nabla\Phi$ and a vector magnetic potential $B = \text{curl } A$, the Lagrangian is given by

$$L(x, \dot{x}) = \frac{1}{2}m|\dot{x}|^2 + q\dot{x} \cdot A(x) - q\Phi(x).$$

We now suppose that there exists a global positively oriented orthonormal frame (e_1, e_2, e_3) such that the magnetic field is given by $B(x) = b(x)e_1(x)$. In this case, the first key idea of the gyroaveraged Lagrangian is to decompose the position of the particle as a guiding center motion and a gyroradius r in the $(e_2(R), e_3(R))$ plane, that is, we define

$$x = R + r(R),$$

where R is in \mathbb{R}^3 and r is given by

$$r = \rho(-\cos\varphi e_2(R) + \sin\varphi e_3(R)).$$

The aim is to try to separate the fast oscillations around the field lines from the gradual drift of the particles away from the field lines coming from non-uniformities in the magnetic field. We thus describe points in \mathbb{R}^3 using three parameters for the guiding center and two parameters for the gyromotion.

After defining the general Lagrangian and the gyrocoordinates, the next step is to take the average of the Lagrangian in the new coordinates with respect to the variable φ . Intuitively, r should be a small correction, so that the angle variable φ does not play an important role in the description of the Lagrangian. After making an assumption on the smallness of some parameters related to the gyromotion, we obtain the following gyroaveraged Lagrangian

$$\mathcal{L}(R, \rho, \dot{R}, \dot{\varphi}) = \frac{1}{2}m\left((\dot{R} \cdot e_1(R))^2 + \rho^2\dot{\varphi}^2\right) + q\dot{R} \cdot A(R) - q\frac{\dot{\varphi}\rho^2}{2}b(R) - q\Phi(R).$$

We refer the interested reader to [IPW20, Section 5.2] for the details of the computations and the smallness assumptions.

From the Euler–Lagrange equations, one then obtains $\dot{\varphi} = \omega(R) := qb(R)/m$, which corresponds to a space-dependent version of the gyrofrequency introduced previously. From the independence of the gyroaveraged Lagrangian with respect to φ , we also obtain that the magnetic moment $\mu(r, R) = (r\omega(R))^2/(2b(R))$ is an invariant of the dynamics generated by the gyroaverage Lagrangian. We say that μ is an adiabatic invariant as variations in this quantity for the full dynamics happen on timescales much longer than that of the gyromotion. Once we have these quantities, we can discuss the evolution equations for the gyromotion using the gyroaveraged approximation. More specifically, we consider the normal part of the change in R , which is the orthogonal projection of \dot{R} onto the $(e_2(R), e_3(R))$ plane denoted \dot{R}_\perp . Indeed, this term gives us the drift of the gyromotion away from the magnetic field lines, and thus allows us to understand the qualitative difference between the motion of charged particles in non-uniform fields and in uniform fields. We obtain the following formula

$$\dot{R}_\perp = \frac{v_\parallel^2(\dot{R}, R)}{\omega(R)}e_1(R) \times \kappa(R) + \frac{\mu}{\omega(R)}e_1(R) \times \nabla b(R) + \frac{E(R) \times B(R)}{b(R)^2}. \quad (1.2)$$

The first term of the right-hand side is known as curvature drift. This term points in the direction perpendicular to the magnetic field and the curvature vector κ of the magnetic field lines, and its direction depends on the sign of the charge. The second term is referred to as grad-B drift, and

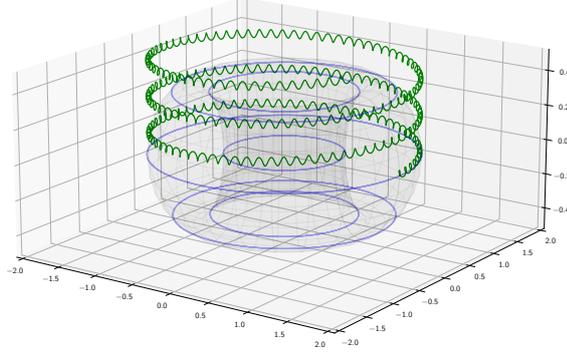


Figure 1.3 – Trajectory of a charged particle in a toroidal magnetic field. Field lines are in blue and the trajectory is in green. We see that the particle gradually drifts up and does not stay close to the invariant torus of the magnetic field.

points in the direction perpendicular to the magnetic field and the gradient of the magnetic field magnitude. The direction of this term is also dependent on the sign of the charge. Finally, the third term is in the direction perpendicular to the magnetic and electric field, and is independent of the sign of the charge. We also note that, as the first two terms depend on the sign of the charge, their contributions tend to generate charge separations in the plasma which leads to the creation of an additional electric field which aims to recover charge neutrality.

Although it seems like the first two terms of Eq. (1.2) inevitably leads to drifts away from the field lines in non-uniform fields, these drifts can be averaged out over time when we consider a magnetic field in a torus with a poloidal component, that is, a component in the short direction of the torus. Considering first the case of a purely toroidal magnetic field, we see that the first two contributions in Eq. (1.2) point in the e_z direction. As mentioned earlier, this will create a charge separation creating an electric field in the e_z direction (see Fig. 1.3), and thus, the last term of Eq. (1.2) will create a drift in the radial direction, independently of the charge of the particle. We thus see that a purely toroidal magnetic field cannot lead to good properties for magnetic confinement. However, in the case where the magnetic field has a poloidal component on invariant surfaces, the curvature and grad-B drifts will alternatively pull the guiding center away from and towards the invariant surface, so that the particle remains close to this surface over time (see Fig. 1.4). We thus understand that considering magnetic fields with invariant toroidal surfaces on which the field lines have a twist is a desirable property for magnetic confinement, as opposed to the purely toroidal case. For more precise computations justifying the necessity of a poloidal component in the axisymmetric case, we refer to [IPW20, Section 7.2].

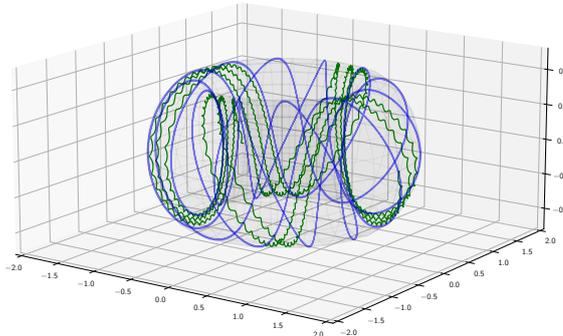


Figure 1.4 – Trajectory of a charged particle in a magnetic field with a poloidal component. Field lines are in blue and the trajectory is in green. We observe that the particle drifts away from the field lines but stays close to the invariant torus of the magnetic field.

1.2.4 Tokamaks and stellarators: two different approaches to generate twist

As we have seen in the previous section, the use of the gyroaveraged Lagrangian indicates that having a magnetic field with a poloidal component generating a twist on invariant tori is a desirable property for magnetic confinement. In this section, we introduce the tokamak and stellarator type reactors and explain how they correspond to two different approaches for introducing twist in the magnetic field.

Tokamaks

To simplify computations, one may wish to work with reactors where all relevant quantities are axisymmetric as this removes one degree of freedom. A standard fact is that, given a magnetic field B in an axisymmetric toroidal domain Ω of \mathbb{R}^3 which is tangent to $\partial\Omega$, B is either toroidal or has nonzero curl. For this fact, we refer to [IPW20, Section 7.6.1], but this can also be understood with basic properties of harmonic fields in toroidal domains which will be used throughout the thesis. Since the curl of the magnetic field is proportional to the electric current, we understand that the induction of current inside the plasma is necessary for magnetic confinement in axisymmetric toroidal domains.

Tokamak type reactors aim to preserve axisymmetry, and thus need to introduce an electrical current inside the plasma. The toroidal component of the magnetic field is generated by currents circulating in poloidal coils around the fusion chamber, while the electric current in the plasma necessary for the poloidal component is generated by an electric field induced by the presence of a transformer in the middle of the device (see Fig. 1.5). Since the induced electric field in the plasma depends on the time variation of the currents circulating in the transformer, tokamaks do not operate in steady-state but in short pulses. Furthermore, the introduction of induced currents can lead to instabilities of the plasma referred to as current driven instabilities [de 06].

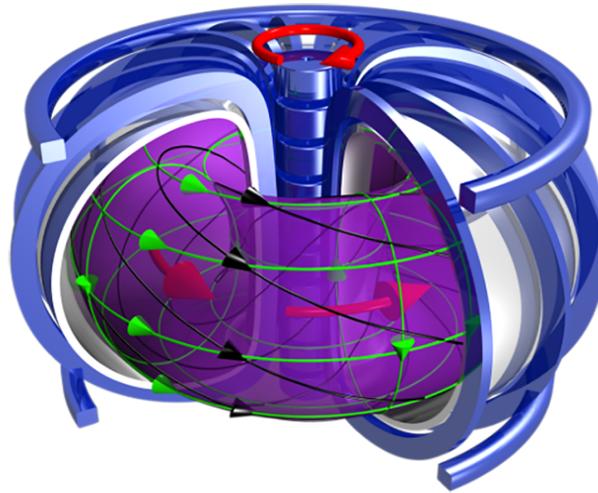


Figure 1.5 – The different components for the magnetic field of a tokamak. Source: International Atomic Energy Agency

Tokamaks reactors are therefore easier to design from a computational and engineering point of view, but their operation is a much more delicate task. The interested reader may find much more information on Tokamaks in [WW11].

Stellarators

As discussed in the previous paragraph, axisymmetric magnetic confinement necessitates the introduction of an electric current in the plasma in order to generate a poloidal twist. However, this current is generally induced by a transformer so that these devices cannot operate continuously. Furthermore, the induced currents lead to current driven instabilities.

The other main approach to generate a poloidal component on the magnetic field is to remove the assumption of axisymmetry. This leads to the notion of stellarator reactors (see Fig. 1.6). As a consequence, the necessary magnetic fields are much more complex to study theoretically. For example, as will be discussed in Section 1.3.3, while all axisymmetric magnetic fields in toroidal domains are foliated, constructing interesting magnetic fields such as MHD equilibria which are foliated without being axisymmetric is very challenging. For example, Grad conjectured in [Gra67] that there exists no smooth MHD equilibria with nonconstant pressure which are not axisymmetric. On the other hand, axisymmetric MHD equilibria can be reduced to the Grad–Shafranov equation, which is considerably easier to work with. Furthermore, from an engineering point of view, removing the axisymmetry assumption also leads to complications as, for example, one often needs to construct non-planar poloidal coils with different shapes in order to construct the desired non-axisymmetric magnetic fields. This modular coil approach was for example taken in the design of the W7X reactor [Bei+90]. However, these additional technicalities when designing stellarators come with the advantage that such reactors would greatly reduce current driven instabilities and allow for a steady state operation rather than the pulsed operation necessary for tokamaks.

Although, some experimental reactors have been built, such as the NCSX [Zar+01] or the W7X [Bei+90], no global collaboration project on the scale of ITER exists for stellarators. Indeed,

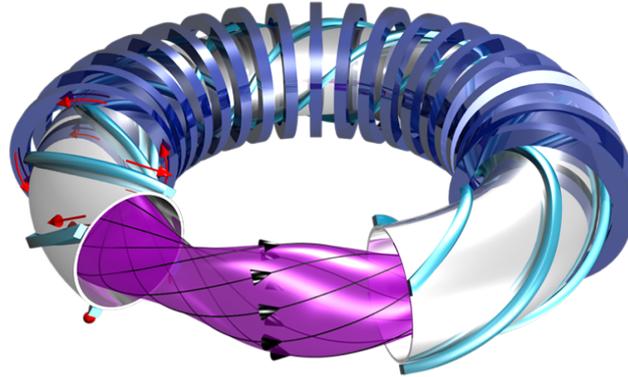


Figure 1.6 – The different components for the magnetic field of a stellarator. Source: International Atomic Energy Agency

even if the idea for stellarators predates the first tokamak⁶, it is only more recently that such reactors have started to gain traction again as the gradual increase of computational power now allows for more precise non-axisymmetric designs.

1.3 Underlying mathematical concepts

In this section, we introduce some mathematical concepts which will be used in the rest of the manuscript, or which are in general relevant in the context of magnetic confinement, and discuss some of the underlying theory and existing results. In Section 1.3.1, we give a definition of harmonic fields in regular toroidal domains, which is one of the key concepts of this manuscript. We in particular make the link with homology through the use of Hodge theory and the de Rham theorem to justify the normalization criterion which will be used for harmonic fields throughout the manuscript. The general definition for harmonic fields in less regular domains will be given in Section 2.2. In Section 1.3.2, we introduce the notion of helicity, which is a quadratic form on harmonic fields. We then discuss its physical and mathematical relevance in the context of MHD, introduce the topological interpretation of Arnold of this quantity, and discuss some ongoing literature for a related isoperimetric problem. Afterwards, we introduce the notion of foliations for magnetic fields in Section 1.3.3. Although these concepts will mostly be unused in the rest of the manuscript, we explain the key role that foliations play for the theoretical study of magnetic fields and the design of confining magnetic fields. In particular, we discuss Grad's conjecture in MHD, and discuss a similar issue for the existence of foliated harmonic fields. We then give the construction of a family of foliated harmonic fields which have trivial Poincaré maps but which are non-axisymmetric. Finally, we introduce a family of finite elements in Section 1.3.4 called finite element exterior calculus (FEEC) which is often used in the context of numerical electromagnetism. We begin by giving a general introduction to general finite elements before giving some of the constructions and main properties of FEEC.

⁶ The first concept for a stellarator was given in 1951 by Lyman Spitzer, while the first tokamak was built in 1954 in the Soviet Union. Tokamak designs then started giving more promising results by the end of the 1960s so that they gradually became the most studied type of fusion reactors.

1.3.1 Harmonic fields

As discussed earlier, stellarators aim to confine the plasma using magnetic fields without introducing any electrical current inside it. The aim of this section is to explain how this naturally leads to the notion of harmonic fields, and to introduce some underlying concepts in differential geometry and algebraic topology. More precisely, we will motivate the choice of normalization of harmonic fields using circulation along a toroidal loop. For convenience, we will only work with smooth manifolds with boundaries throughout this section. This means in particular that, when studying domains of \mathbb{R}^3 , we will assume that their boundaries are C^∞ , and not only Lipschitz for example. Therefore, not all the contents of this manuscript regarding harmonic fields will fall under this context. We still believe that the contents of this section may be useful for motivation purposes in more general contexts.

For useful elements of differential geometry, and more specifically Hodge theory, we refer for example to [AFW06; Sch95]. For an introduction to the aspects of homology and cohomology theory that will be used in this section, we refer to [Lee12, Chapters 17-18] and [Hat02].

Definition

Before introducing the notion of harmonic fields, we wish to motivate its definition from the context of stellarators.

First, since for time independent electromagnetic fields, the electrical current is proportional to the curl of the magnetic field, confining magnetic fields in stellarators should be curl free. Moreover, if we assume that the plasma is contained in a fixed domain Ω , the confining magnetic field should be tangent to $\partial\Omega$. Indeed, since charged particles locally wind around magnetic field lines as seen in Section 1.2.3, the magnetic field should be tangent to the plasma domain Ω if we do not want charged particles to escape from Ω . These two observations lead us to the following definition of harmonic fields of a domain Ω

$$\mathcal{K}(\Omega) = \{B \in L^2(\Omega)^3 \mid \operatorname{div} B = 0, \operatorname{curl} B = 0, B \cdot n = 0\},$$

where n is the unit outward pointing normal vector field on $\partial\Omega$, and the divergence and curl operators should be understood in the weak sense. Using the integration by parts formula

$$\int_{\Omega} (\operatorname{div} u)\varphi = - \int_{\Omega} u \cdot \nabla \varphi + \int_{\partial\Omega} (u \cdot n)\varphi,$$

it is also clear that a vector field is divergence free and tangent to the boundary if and only if it is L^2 orthogonal to $\nabla H^1(\Omega)$. Therefore, the set of harmonic vector fields may be written as

$$\mathcal{K}(\Omega) = H(\operatorname{curl}^0, \Omega) \cap \nabla H^1(\Omega)^\perp, \quad (1.3)$$

where $H(\operatorname{curl}^0, \Omega)$ is the set of curl free square integrable vector fields. In the rest of this section, we will investigate some links between this space and some geometrical objects arising from differential geometry, Hodge theory and algebraic topology. This will allow us to understand from a geometric perspective how fixing the toroidal circulation allows us to obtain a single harmonic field when Ω is bounded and has the topology of a full torus.

Vector fields and differential forms in three dimensions

Let M be an oriented n -dimensional Riemannian manifold with boundary and let us denote the space of smooth differential k -forms on M as $\Lambda^k(M)$. Since M is an oriented Riemannian

manifold, it is naturally equipped with a volume form $vol \in \Lambda^n(M)$. For q in M , we denote the set of k -forms on T_qM as $\text{Alt}^k(T_qM)$. The Riemannian structure on M induces a scalar product on $\text{Alt}(T_qM)$, which we denote \langle, \rangle . These structures allow to define the so-called Hodge star operator, which is an isomorphism from $\text{Alt}^k(T_qM)$ to $\text{Alt}^{n-k}(T_qM)$, and is characterized by

$$\alpha \wedge \beta = \langle * \alpha, \beta \rangle vol_q,$$

for all α in $\text{Alt}^k(T_qM)$ and β in $\text{Alt}^{n-k}(T_qM)$. Furthermore, the metric tensor g on M allows to define an isomorphism between T_qM and $(T_qM)' = \text{Alt}^1(T_qM)$ defined by

$$v^\flat = \iota_v g_q,$$

where v is in T_qM and ι_v is the interior product with v , and \flat and its inverse \sharp are the so-called musical isomorphisms of M .

Finally, for α, β in $\Lambda^k(M)$, we then have the inner product

$$\langle\langle \alpha, \beta \rangle\rangle_{L^2 \Lambda^k} = \int_M \langle \alpha, \beta \rangle vol.$$

This inner product allows to define the norm

$$\|\alpha\|_{H\Lambda^k}^2 = \langle\langle \alpha, \alpha \rangle\rangle_{L^2 \Lambda^k} + \langle\langle d\alpha, d\alpha \rangle\rangle_{L^2 \Lambda^k}.$$

$H\Lambda^k(M)$ is then defined as the completion of $\Lambda^k(M)$ using this norm. One can then define the set of closed and exact differential forms by

$$\mathcal{Z}^k(M) = \{\alpha \in H\Lambda^k(M) \mid d\alpha = 0\}, \quad \mathcal{B}^k(M) = dH\Lambda^{k-1}(M).$$

This allows us to define the space of harmonic forms as

$$\mathcal{H}^k(M) = \mathcal{Z}^k(M) \cap \mathcal{B}^k(M)^\perp, \quad (1.4)$$

where the orthogonal of $\mathcal{B}^k(M)$ is taken with respect to the L^2 inner product on $H\Lambda^k(M)$.

When M is three-dimensional, the Hodge star operator and musical isomorphisms allow us to obtain the following commutative diagram

$$\begin{array}{ccccccc} H\Lambda^0(M) & \xrightarrow{d} & H\Lambda^1(M) & \xrightarrow{d} & H\Lambda^2(M) & \xrightarrow{d} & H\Lambda^3(M) \\ \text{id} \downarrow & & \# \downarrow & & \#* \downarrow & & * \downarrow \\ H^1(M) & \xrightarrow{\nabla} & H(\text{curl}, M) & \xrightarrow{\text{curl}} & H(\text{div}, M) & \xrightarrow{\text{div}} & L^2(M) \end{array} \quad (1.5)$$

If $M = \bar{\Omega}$ is a manifold with boundary in \mathbb{R}^3 , this commutative diagram and Eqs. (1.3) and (1.4) allow us to obtain the following correspondence between the spaces of harmonic fields and harmonic 1-forms,

$$\mathcal{K}(\Omega) = \# \mathcal{H}^1(\bar{\Omega}),$$

which are therefore isomorphic.

Elements of Hodge theory

Let M be a smooth compact manifold with boundary. From $d \circ d = 0$, we obtain that the de Rham complex

$$0 \longrightarrow H\Lambda^0(M) \xrightarrow{d} H\Lambda^1(M) \xrightarrow{d} \cdots \xrightarrow{d} H\Lambda^{n-1}(M) \xrightarrow{d} H\Lambda^n(M) \longrightarrow 0 ,$$

is a cochain map. This therefore gives rise to a notion of cohomology called de Rham cohomology⁷. The de Rham cohomology spaces are thus defined as the quotient spaces

$$H_{\text{dR}}^k(M) = \mathcal{Z}^k(M)/\mathcal{B}^k(M).$$

It is then known that the space of harmonic forms $\mathcal{H}^k(M)$ is isomorphic to $H_{\text{dR}}^k(M)$. This follows from the fact that, when V is a closed subspace of a Hilbert space H , H/V is isomorphic to $H \cap V^\perp$. In other words, elements of H which are orthogonal to V give natural representatives in the quotient space H/V . The fact that $\mathcal{Z}^k(M)$ is L^2 closed is straightforward, while $\mathcal{B}^k(M)$ being L^2 closed follows from a Poincaré type inequality on differential forms (see [AFW06, Theorem 2.2 and 2.3]).

de Rham theorem and characterization of harmonic forms

We now aim to understand how the de Rham theorem allows us to characterize harmonic forms using integration along chains. To do so, we begin by shortly introducing singular homology to state the de Rham theorem. Let X be a topological space. A k -cell is a continuous map

$$c : \Delta^k \rightarrow X,$$

where Δ^k is the standard k -simplex. The space of k -chains $C_k(X)$ is then defined as the set of formal sums of k -cells, that is, the free abelian group generated by the set of k -cells. One can then define boundary maps $\partial : C_k(X) \rightarrow C_{k-1}(X)$ which verify $\partial_{k-1} \circ \partial_k = 0$. This therefore gives rise to a notion of homology, called singular homology, which is defined as

$$H_k(X) = \ker \partial_k / \text{im} \partial_{k+1}.$$

One should think of nonzero elements of $H_k(M)$ as equivalence classes of " k -dimensional submanifolds" with empty boundary, which are not the boundary of a " $(k+1)$ -dimensional submanifold". By dualizing the singular chain complex, we can then obtain a notion of singular cohomology. Let R be a ring, and consider the R -module of singular k -cochain to be defined as $C^k(X) = \text{Hom}(C_k(X), R)$, that is, the space of group homomorphisms from $C_k(X)$ to R . We then obtain a co-boundary map $d^k : C^k(X) \rightarrow C^{k+1}(X)$ defined by

$$d^k f(c) = f(\partial_{k+1} c).$$

We immediately obtain $d^{k+1} \circ d^k = 0$, so that we can define cohomology spaces $H^k(X, R)$ referred to as the singular cohomology groups of X .

7. Since we are working with Sobolev spaces instead of smooth forms, this is not technically the usual de Rham complex. However, in this context, the two cohomologies are isomorphic.

For a smooth manifold with boundary, we now define the map $I : \Lambda^k(M) \rightarrow C^k(M, \mathbb{R})$ by⁸

$$I(\alpha)(c) = \int_c \alpha.$$

Stoke's theorem then implies that this map is a cochain map, so that it induces a morphism between de Rham cohomology to singular cohomology over \mathbb{R} . Indeed, $I(d\alpha)(c) = I(\alpha)(\partial_{k+1}c) = d^k I(\alpha)(c)$. The de Rham theorem states that I induces an isomorphism between $H_{\text{dR}}^k(M)$ and $H^k(M, \mathbb{R})$.

In the case where $H_k(M)$ is finitely generated, we have an isomorphism from $\text{Hom}(H_k(M), \mathbb{R})$ to $H^k(M, \mathbb{R})$ ⁹. In this case, we have $H_k(M) = F_k \oplus T_k$, where $F_k \cong \mathbb{Z}^{\beta_k(M)}$ is the free part of $H_k(M)$, $\beta_k(M)$ being the k -th Betti number of M , and T_k is its torsion subgroup. Given c in T_k , there exists by definition an integer $i > 0$ such that $ic = 0$. Therefore, given f in $\text{Hom}(H_k(M), \mathbb{R})$, we have $f(c) = 0$ for all c in T_k . If we have $F_k = \bigoplus_{i=1}^{\beta_k(M)} \mathbb{Z}c_i$, we deduce that $f \in \text{Hom}(H_k(M), \mathbb{R})$ is uniquely determined by $f(c_i)$ for $1 \leq i \leq \beta_k(M)$.

To summarize what we have discussed so far, suppose that M is a smooth compact manifold with boundary. In this case, the spaces $\mathcal{H}^k(M)$ are finite dimensional, and the harmonic forms are smooth so that they may be integrated on k -chains [Sch95, Theorems 2.2.2 and 2.2.6]. We thus obtain the isomorphism $I : \mathcal{H}^k(M) \rightarrow \text{Hom}(H_k(M), \mathbb{R})$. We therefore find that, given $a_1, \dots, a_{\beta_k(M)}$ in \mathbb{R} , there exists a unique α in $\mathcal{H}^k(M)$ such that

$$\int_{c_i} \alpha = a_i,$$

for all $1 \leq i \leq \beta_k(M)$. In other words, given a set of generating cycles in the free part of $H_k(M)$, there exists a unique corresponding basis of $\mathcal{H}^k(M)$.

Harmonic fields in toroidal domains and toroidal circulation

We now wish to understand how one may apply the characterizations we discussed in the previous paragraphs for harmonic fields in toroidal domains.

Suppose $\Omega \subset \mathbb{R}^3$ is a toroidal domain, that is, $\bar{\Omega}$ is smoothly diffeomorphic to the full torus $S^1 \times D^2$. Since $S^1 \times D^2$ is homotopy equivalent to S^1 , we have $H_1(\bar{\Omega}) \cong H_1(S^1) \cong \mathbb{Z}$. Let γ' be a generator of $H_1(\bar{\Omega})$, with unit tangent vector field t' . We then have for α in $\Lambda^1(\bar{\Omega})$

$$\int_{\gamma'} \alpha = \int_{\gamma} \alpha^\# \cdot t'.$$

In view of the isomorphism $\mathcal{K}(\Omega) = \# \mathcal{H}^1(\bar{\Omega})$, we know that there exists a unique harmonic field $B(\Omega)$ in $\mathcal{K}(\Omega)$ such that

$$\int_{\gamma'} B(\Omega) \cdot t' = 1.$$

Therefore, given a toroidal domain Ω and γ' a generator of $H_1(\bar{\Omega})$, one can define the normalized harmonic field $B(\Omega)$. Strictly speaking, this field also depends on the choice of γ' . However, since

8. Strictly speaking, one should replace singular chains with smooth singular chains in order to define this integral properly. These two notions however define the same homology and cohomology [Lee12, Theorem 18.7].

9. This can be seen for example using the short exact sequence

$$0 \longrightarrow \text{Ext}(H_{k-1}(M), \mathbb{R}) \longrightarrow H^k(M, \mathbb{R}) \longrightarrow \text{Hom}(H_k(M), \mathbb{R}) \longrightarrow 0,$$

given by the universal coefficient theorem, and the fact that $\text{Ext}(H, \mathbb{R}) = 0$ for any finitely generated abelian group H . We refer to [Hat02, Section 3.1] for more details.

$H_1(\bar{\Omega}) \cong \mathbb{Z}$, the only generators of $H_1(\bar{\Omega})$ are $\pm\gamma'$, so that changing the generator changes $B(\Omega)$ only by a sign.

A large part of this manuscript aims at understanding how changing Ω affects $B(\Omega)$ and some of its properties. In particular, this will be done by giving variational formulations for $B(\Omega)$ in Chapter 2, which will also allow us to define the normalized harmonic field in toroidal domains with lower regularity.

1.3.2 Helicity

In this section, we introduce the notion of helicity of a magnetic field, and discuss some of its properties. First, we define the quantity, and make the connection between the Biot–Savart operator and vector potentials. Then, we discuss the physical relevance of helicity in MHD, both ideal and resistive. We then introduce a topological interpretation of the quantity due to Arnold, as a space average of the asymptotic linking number of the field lines. Finally, we discuss some open problems and results on helicity maximizers, and the related isoperimetric problem.

Definition

Let Ω be an open set of \mathbb{R}^3 . Given F in $L^2(\Omega)^3$, we define its helicity as

$$\mathbf{H}(F) = \frac{1}{4\pi} \int_{\Omega \times \Omega} F(y) \cdot \left(F(x) \times \frac{y-x}{|y-x|^3} \right) dx dy. \quad (1.6)$$

Introducing the Biot–Savart operator as

$$\text{BS}(F)(y) = \frac{1}{4\pi} \int_{\Omega} F(x) \times \frac{y-x}{|y-x|^3} dx, \quad (1.7)$$

we then obtain that BS is continuous from $L^2(\Omega)^3$ to itself [CDG01, Theorem D], and that $\mathbf{H}(F) = \int_{L^2} F \cdot \text{BS}(F)$. In physical contexts, $\mathbf{H}(F)$ is often referred to as the Biot–Savart or magnetic helicity of F .

For magnetic fields F of Ω , that is, divergence free vector fields which are tangent to $\partial\Omega$, it is known that $\text{BS}(F)$ is a vector potential of F , meaning that $\text{curl BS}(F) = F$ [CDG01]. When Ω is simply connected, it is known that all curl free vector fields are in $\nabla H^1(\Omega)$, so that any potential vector of a magnetic field F can be written as $A = \text{BS}(F) + \nabla\varphi$ for φ in $H^1(\Omega)$. Since being divergence free and tangent to the boundary is equivalent to being L^2 orthogonal to gradients, we obtain for any potential vector A of F

$$\int_{\Omega} F \cdot A = \mathbf{H}(F).$$

When Ω is not simply connected, not all curl free vector fields are gradients, so that this gauge invariance does not hold anymore for any magnetic field F . When Ω has the topology of a full torus, a gauge invariant formula can be recovered using the Bevir–Gray formula [BG80] which will be recalled in Section 3.2.1. We note that a similar formula can be obtained in more general cases for different topologies of Ω [MV19].

Relation with MHD and physical relevance

An important physical property of helicity is that it is conserved in ideal MHD assuming enough regularity on the solutions. In the case of a simply connected domain Ω , this can be

understood with the following geometric explanation, which is inspired from [Arn14]. We recall that the time evolution of B in ideal MHD reads as

$$\partial_t B = \text{curl}(u \times B),$$

v being the velocity field. We wish to prove that this corresponds to a transport equation when B is seen as a two-form. Therefore, we consider the two-form $\beta = \iota_B \text{vol}$ corresponding to B , where vol is the volume form on \mathbb{R}^3 . Since B is divergence free, β is closed, and we obtain using Cartan's formula

$$\mathcal{L}_u \beta = d\iota_u \beta,$$

where \mathcal{L}_v is the Lie derivative in the direction of u , and ι_u is the interior product with u . Using the usual identifications between vector fields and differential forms from Section 1.3.1, as well as the corresponding formulas for Lie derivatives (see Section 2.1.1), we see that the evolution equation of B is equivalent to

$$\partial_t \beta = \mathcal{L}_u \beta.$$

As a consequence, we have $\beta(t) = (\varphi^t)^* \beta(0)$, where φ^t is the flow of u at time t . This property is often referred to as the frozen-in flux theorem, or Alfvén's theorem. Physically, this result means that fluxes of B are conserved along surfaces which are transported by the flow of the velocity field. Furthermore, this also implies that the field lines of B are transported by φ^t , so that all their topological and dynamical properties are preserved. We suppose that Ω is a simply connected domain, and $\Omega_t = \varphi^t(\Omega)$. In this case, we know that if $B(t)$ is tangent to the boundary¹⁰, then for all vector potentials $A(t)$ of $B(t)$, we have

$$\text{H}(B(t)) = \int_{\Omega_t} B(t) \cdot A(t).$$

If $\alpha(0)$ is a one-form potential of $\beta(0)$, that is, $d\alpha(0) = \beta(0)$, the commutativity of the pullback and the exterior derivative implies $d((\varphi^t)^* \alpha(0)) = \beta(t)$, so that $\alpha(t) = (\varphi^t)^* \alpha(0)$ is a one-form potential of $\beta(t)$. The corresponding formula for helicity using differential forms is then given by

$$\begin{aligned} \text{H}(\beta(t)) &= \int_{\Omega_t} \beta(t) \wedge \alpha(t) \\ &= \int_{\Omega_t} (\varphi^t)^* (\beta(0) \wedge \alpha(0)). \end{aligned}$$

Finally, since pullbacks by orientation preserving diffeomorphisms preserve integrals, we deduce that

$$\begin{aligned} \text{H}(\beta(t)) &= \int_{\Omega} \beta(0) \wedge \alpha(0) \\ &= \text{H}(\beta(0)). \end{aligned}$$

A property that we also note is that, in the incompressible case, u being divergence free implies that φ^t is volume preserving. This implies that B being transported as a two form is equivalent to it being transported as a vector field. More precisely, we have $\beta = \iota_B \text{vol}$, so that for a volume

10. From the formula $\beta(t) = (\varphi^t)^* \beta(0)$, one can obtain that the tangency boundary condition is preserved over time.

preserving diffeomorphism φ , we compute

$$\begin{aligned}\varphi^*\beta(X, Y) &= \text{vol}(B, \varphi_*X, \varphi_*Y) \\ &= \text{vol}(\varphi_*((\varphi^{-1})_*B, \varphi_*X, \varphi_*Y)) \\ &= \varphi^*\text{vol}((\varphi^{-1})_*B, X, Y).\end{aligned}$$

φ being volume preserving, we deduce $\varphi^*\beta = \iota_{(\varphi^{-1})_*B}\text{vol}$. This gives us $B(t) = \left((\varphi^t)^{-1}\right)_*B(0)$. We also note that this argument for helicity conservation can be adapted in the case where Ω is not simply connected. One may do this by using the gauge invariant formulas from [MV19], or by proving that pullbacks of the Biot–Savart operator as one-forms behave well¹¹.

In the presence of small resistivity, Taylor conjectured that helicity is still approximately preserved [Tay74]. More specifically, Taylor discusses in this paper how, although the presence of arbitrarily small resistivity generally leads to magnetic reconnections, the global magnetic helicity of the system seems to be approximately preserved over time. This result was rigorously proven recently in [FL20] for simply connected domains and in [Far+22] in general. More specifically, it was proven that weak limits of Leray–Hopf solution preserve helicity in time as the viscosity and resistivity parameters tend to zero. However, it was also proven in [FLS24] that helicity preservation can sometimes fail in the ideal case when considering weak enough solutions.

Furthermore, the approximate conservation of helicity in presence of small resistivity leads to the Woltjer–Taylor relaxation theory. This theory conjectures that, in the presence of resistivity, magnetic energy decreases much faster than helicity. This then leads MHD solutions to relax towards minimizers of magnetic energy with fixed helicity. As shown by Woltjer [Wol58], such minimizers are force free (or Beltrami) fields, that is, magnetic fields verifying

$$\text{curl } B = \alpha B,$$

where α is a constant.

For more discussions on these concepts, as well as a review on the more recent mathematical results on the subject, we refer the reader to [FLS22].

Topological interpretation

We now wish to discuss a topological interpretation of the helicity defined by Eq. (1.6), which was first exhibited by Arnold.

Given two non-intersecting simple closed curves γ_1 and γ_2 of \mathbb{R}^3 , the Gauss linking number is denoted as $L(\gamma_1, \gamma_2)$. Intuitively, this quantity counts the number of times the two curves link with each other, where linkings with opposite orientations cancel out. When the curves $\gamma_i : S^1 \rightarrow \mathbb{R}^3$ are parametrized, Gauss found that this quantity can in fact be computed using the following integral formula

$$L(\gamma_1, \gamma_2) = \frac{1}{4\pi} \int_{S^1 \times S^1} \frac{\gamma_1(s) - \gamma_2(t)}{|\gamma_1(s) - \gamma_2(t)|^3} \cdot (\dot{\gamma}_1(s) \times \dot{\gamma}_2(t)) ds dt.$$

One can already notice a similarity between this formula for Linking number, and the helicity defined by Eq. (1.6). Indeed, it seems that the helicity of a magnetic field should correspond to the space average of the linking number of its field lines. This result was proven by Arnold in

¹¹. The Biot–Savart does not directly commute with this pullback, but we can prove that the commutator is always a gradient vector field, so that this does not affect the value of the helicity.

[Arn14]. Before stating the theorem, we give a few definitions which will allow us to understand some ideas of the proof.

Let F be a magnetic field of a bounded domain Ω , that is, F is divergence free and tangent to the boundary. For t in \mathbb{R} , we define φ^t as the flow of F at time t (which is a diffeomorphism of Ω as F is tangent to the boundary). One then wants to define an *asymptotic linking number* for the field lines of F . Indeed, we do not assume that the field lines are closed, so that the definition of Gauss is not applicable. This is done by choosing a way of closing the field lines. Given two points x and y in Ω , we define $\Delta(x_1, x_2)$ as a short path connecting x_1 and x_2 . Given x in Ω and $T > 0$, we define the closed curve $\Gamma_T(x)$ as the union of the curve $\{\varphi^t(x) \mid 0 \leq t \leq T\}$ and $\Delta(\varphi^T(x), x)$. Arnold then shows that, under some assumptions on the choices of small paths $\Delta(x, y)$, for almost all x_1, x_2, T_1, T_2 , the two curves $\Gamma_{T_1}(x_1)$ and $\Gamma_{T_2}(x_2)$ are non-intersecting, and that

$$\lambda(x_1, x_2) := \lim_{T_1, T_2 \rightarrow +\infty} \frac{L(\Gamma_{T_1}(x_1), \Gamma_{T_2}(x_2))}{T_1 T_2},$$

is equal to

$$\hat{\lambda}(x_1, x_2) := \lim_{T_1, T_2 \rightarrow +\infty} \frac{1}{T_1 T_2} \frac{1}{4\pi} \int_0^{T_1} \int_0^{T_2} \frac{\varphi^{t_1}(x_1) - \varphi^{t_2}(x_2)}{|\varphi^{t_1}(x_1) - \varphi^{t_2}(x_2)|^3} \cdot (\varphi^{t_1}(x_1) \times \varphi^{t_2}(x_2)),$$

for almost all x_1, x_2 . In particular, the asymptotic linking number λ does not depend on the choice of small paths to reconnect the field lines. Arnold then proves that

$$H(F) = \frac{1}{|\Omega \times \Omega|} \int_{\Omega \times \Omega} \lambda(x, y) dx dy.$$

Although the details of the proof are not discussed here, we note that Birkhoff's ergodic theorem is used so that F being divergence free is indeed crucial.

Helicity maximizers and isoperimetric problem

First, a natural problem one may ask is the existence of magnetic fields maximizing the absolute value of the helicity for a given domain Ω . More precisely, since helicity is a quadratic quantity, we search for maximizers in the unit L^2 sphere.

We introduce a modification of the Biot–Savart operator in order to obtain a simpler functional context. We define $H_0(\operatorname{div}^0, \Omega)$ as the space of square integrable divergence free vector fields of Ω which are tangent to $\partial\Omega$. Given a magnetic field F in $H_0(\operatorname{div}^0, \Omega)$, it is known that $\operatorname{BS}(F)$ is divergence free. However, it is not always tangent to the boundary. This inconvenient property can be corrected by introducing the modified Biot–Savart operator BS' , which is defined by

$$\operatorname{BS}'(F) = \operatorname{BS}(F) - \nabla\varphi_F,$$

where, for F in $H_0(\operatorname{div}^0, \Omega)$, φ_F is defined as the zero average solution to¹²

$$\begin{cases} \Delta\varphi_F = 0 & \text{in } \Omega, \\ \nabla\varphi_F \cdot n = \operatorname{BS}(F) \cdot n & \text{on } \partial\Omega. \end{cases}$$

¹² Since, for F in $H_0(\operatorname{div}^0, \Omega)$, $\operatorname{BS}(F)$ is divergence free, it is in $H(\operatorname{div}, \Omega)$. As a consequence, $\operatorname{BS}(F) \cdot n$ is in $H^{-1/2}(\partial\Omega)$, so that the PDE for φ_F is well posed. We refer to Section 2.2 for the relevant definitions and properties.

In other words, $\text{BS}'(F)$ is the L^2 projection of $\text{BS}(F)$ onto $H_0(\text{div}^0, \Omega)$. Importantly, $H_0(\text{div}^0, \Omega)$ being the space of vector fields which are L^2 orthogonal to $\nabla H^1(\Omega)$, we have

$$\int_{\Omega} \text{BS}'(F) \cdot F = \int_{\Omega} \text{BS}(F) \cdot F - \int_{\Omega} \nabla \varphi_F \cdot F \quad (1.8)$$

$$= \text{H}(F). \quad (1.9)$$

Therefore, this modification of the Biot–Savart operator does not change the value of the helicity. The operator $\text{BS}' : H_0(\text{div}^0, \Omega) \rightarrow H_0(\text{div}^0, \Omega)$ is known to be compact and self-adjoint [Can+00]. By the spectral theorem, $H_0(\text{div}^0, \Omega)$ admits a Hilbert basis composed of eigenfields of BS' with a corresponding sequence of eigenvalues which converges towards zero. Let λ be the largest eigenvalue in absolute value, and F a corresponding eigenfield. From the fact that BS , and thus BS' is a right inverse of the curl operator on $H_0(\text{div}^0, \Omega)$, it follows that

$$\text{curl } F = \frac{1}{\lambda} F.$$

In other words, F is also an eigenfield of the curl operator. Such vector fields are often referred to as Beltrami fields or force free fields¹³. We note however that eigenfields of the curl are in general not eigenfields of BS' .

Now, since $\text{H}(F) = \int_{\Omega} F \cdot \text{BS}'(F)$, we know that extremals of the helicity on the unit L^2 sphere are the eigenvectors of the modified Biot–Savart operator. Furthermore, $|\lambda|$ corresponds to the maximum of the absolute value of the helicity. Once we have this result, another natural question is to consider the corresponding isoperimetric problem. That is, for a fixed volume, can we find a domain which maximizes the largest eigenvalue of the modified Biot–Savart operator. This question was posed in [Can+99; Can+00], in which we can find computations suggesting that there may be no optimal shape. To the author’s knowledge, this problem was only revisited by Gerner in [Ger23a], who proved the existence of maximizers when imposing a uniform ball condition¹⁴ on the set of admissible shapes. There still seems to be no satisfactory result on the existence of optimal shapes without assumptions on the regularity of the domain. We still refer to the series of article by Enciso, Peralta-Salas and Gerner [EP23b; EGP24; Ger23b; EGP23; Ger23a] giving partial results of existence and non-existence for the related but different isoperimetric problem of the first curl eigenvalue.

1.3.3 Foliations

One important quantity for stellarator design is the rotational transform. Indeed, this quantity allows to quantify the presence of a poloidal component in the magnetic field, which, as was discussed in Section 1.2.3, is crucial for magnetic confinement of charged particles. However, in order to rigorously define this notion, one needs to assume that the plasma domain is foliated by invariant tori. Indeed, given an invariant torus of the magnetic field, often referred to as a flux surface, the rotational transform on it is defined as the average number of poloidal rotation per toroidal rotation of the field lines. This may be formalized mathematically as the rotation number of the Poincaré map of the magnetic field on a poloidal cut of the flux surface. One may

13. We note that force free fields also often refer to vector fields verifying $\text{curl } F = \alpha F$ where α may be non-constant in space. The name comes from the fact that such fields are the solutions to stationary MHD equations with constant pressure.

14. A set of shapes is said to verify a uniform ball condition if there exists $r > 0$ such that for all admissible shapes Ω and all $x \in \partial\Omega$, there exists a ball of radius r in the complement of Ω touching x , and a ball of radius r included in Ω touching x .

thus be able to associate the rotational transform with each invariant surface, so that a foliated magnetic field admits a rotational transform profile.

Magnetic coordinates, and MHD equilibria computations.

Suppose B is a magnetic field in a plasma domain Ω diffeomorphic to a full torus. We assume that S_ψ for $0 \leq \psi \leq 1$ is a foliation of $\bar{\Omega}$ into invariant manifolds, with S_0 diffeomorphic to a circle and S_ψ diffeomorphic to a torus for $0 < \psi \leq 1$. Furthermore, we assume that S_ψ is a foliation of the magnetic field, that is, B is tangent to S_ψ for all ψ . S_0 is referred to as the magnetic axis of B . We identify ψ with the function from $\bar{\Omega}$ to \mathbb{R} such that $\psi(x) = \psi$ if x is in S_ψ , which is assumed to be smooth. The tangency condition then becomes $B \cdot \nabla\psi = 0$. One can then define coordinates (ψ, θ, ϕ) in $\bar{\Omega} \setminus S_0$, such that, for fixed ψ , θ and ϕ are poloidal and toroidal coordinates respectively. Furthermore, one can construct these coordinates so that

$$\begin{aligned} B &= \nabla\psi \times \nabla\theta - \iota(\psi)\nabla\psi \times \nabla\phi \\ &= \sqrt{g}^{-1} (\partial_\phi + \iota(\psi)\partial_\theta), \end{aligned}$$

where $\iota(\psi)$ is the rotational transform of the invariant surface S_ψ . These types of coordinates are called magnetic coordinates [IPW20, Chapter 9]. Importantly, these coordinates linearize the magnetic field in the sense that they straighten the field lines on each invariant surface. Indeed, one can simply integrate the magnetic field so that the field lines take the form $\{(\psi_0, \theta_0 + \iota(\psi_0)s, \phi_0 + s) \mid s \in \mathbb{R}\}$ in these coordinates. One may find it surprising at first that assuming a toroidal foliation is enough to be able to construct such coordinates¹⁵. The existence of such coordinates in fact follows from the divergence free condition on the magnetic field, which allows to make a connection between the dynamics of the magnetic fields and Hamiltonian dynamics, where the toroidal angle should be understood as time [Mor00]. In this sense, one can understand the existence of magnetic coordinates as an Arnold–Liouville type theorem, giving action-angle coordinates trivializing the dynamics of the field.

When the magnetic field is also assumed to satisfy stationary ideal MHD equations, one can construct specific magnetic coordinates such as Boozer coordinates [IPW20, Section 9.3]. In this context, one can also mention the code VMEC [HvM86], which aims to find numerical ideal MHD equilibria given a set of prescribed flux surfaces and rotational transforms assuming the existence of a foliation. The code uses a Fourier parametrization for flux surfaces and components of the magnetic field, and performs a gradient descent type algorithm on a variational formulation for ideal MHD equilibria. VMEC has been widely used since its creation for preliminary designs of magnetic fields in experimental stellarators (see for example [Bei+90] for W7X).

Grad’s conjecture

An important topic in the context of foliations for stationary ideal MHD solutions is Grad’s conjecture. We recall that a magnetic field B is said to be an ideal MHD equilibrium if it verifies

$$\begin{aligned} B \times \text{curl } B &= \nabla p, \\ \text{div } B &= 0. \end{aligned}$$

From this equation, one obtains $B \cdot \nabla p = 0$, so that regular pressure level sets are invariant surfaces of the magnetic field. Grad conjectured in [Gra67] that all smooth MHD equilibria with

¹⁵ For example, the existence of such coordinates implies that, on each invariant torus, all field lines are either periodic or dense in the torus. We in particular cannot have hyperbolic periodic field lines on invariant tori.

nonconstant pressure should be axisymmetric. Indeed, in the case of axisymmetry, one can write B as

$$B = \nabla\psi \times \nabla\phi + g\nabla\phi,$$

where (R, ϕ, z) are the usual cylindrical coordinates, and g and ψ are scalar functions. In this case, the equations of ideal MHD equilibria reduce to the Grad–Shafranov equation

$$\partial_R^2\psi - \frac{1}{R}\partial_R\psi + \partial_z^2\psi = -R^2\frac{dp}{d\psi} - \frac{1}{2}\frac{dg^2}{d\psi}.$$

This scalar equation is better understood than the usual ideal MHD equilibrium equations (see for example [Ata+04] for explicit solutions and [BB80] for an existence result), and is often used for the construction of axisymmetric equilibria in tokamaks.

Some theoretical constructions

Although the existence of smooth non-axisymmetric ideal MHD equilibria with nonconstant pressure is still unknown, a recent family of solutions with stepped-pressure equilibria was recently constructed by Enciso, Luque and Peralta-Salas [ELP22]. We note that another similar result was found earlier by Bruno and Laurence for perturbations of axisymmetric domains [BL96] whereas the construction of Enciso et al. works with thin enlargements of generic closed curves of \mathbb{R}^3 . To discuss the construction of Enciso et al., we first give a few results for harmonic and Beltrami fields in thin tubes.

Let γ be a closed simple analytic curve of \mathbb{R}^3 . We denote by \hat{t} , \hat{n} and \hat{b} the tangent, normal and binormal vector fields on γ respectively, and κ and τ be the curvature and torsion. Given $\varepsilon > 0$ sufficiently small, we know that

$$\mathcal{T}_\varepsilon(\gamma) := \{x \in \mathbb{R}^3 \mid d(x, \gamma) < \varepsilon\}$$

is a toroidal domain of \mathbb{R}^3 with analytic boundary. Defining the coordinates

$$(x, y, z) = \gamma(\alpha) + \varepsilon r \cos\theta \hat{n}(\alpha) + \varepsilon r \sin\theta \hat{b}(\alpha),$$

Enciso et al. then prove in [EP15] that the harmonic field of $\mathcal{T}_\varepsilon(\gamma)$ can be approximated by

$$h = \chi(\partial_\alpha + \tau\partial_\theta),$$

where χ is a scalar function depending explicitly on the geometrical properties of the curve. The stepped pressure equilibria are then constructed in the following way. They start with a thin tube $\mathcal{T}_\varepsilon(\gamma)$, with γ and ε chosen such that there exists a Beltrami field B_1 with small eigenvalue which is conjugate to a diophantine vector field on $\partial\mathcal{T}_\varepsilon$. Using the approximate formula for harmonic fields in thin tubes discussed earlier, they prove that the set of curves verifying this condition is in fact generic. Once this field is obtained, they use a Cauchy–Kovalevskaya type theorem for the curl operator to extend the field to another Beltrami field B_2 with a different eigenvalue. To obtain that the constructed extension is an MHD equilibrium with a jump in pressure, one needs to verify that $|B_2|^2 - |B_1|^2$ is constant on $\partial\mathcal{T}_\varepsilon$. Using the Cauchy–Kovalevskaya type theorem, this is obtained through the existence of an analytic solution to a nonlinear Hamilton–Jacobi equation on \mathbb{T}^2 . The existence of such solutions is established with a quadratic Newton scheme, using the fact that B_1 is conjugate to a diophantine rotation on $\partial\mathcal{T}_\varepsilon(\gamma)$, similar to what is commonly done in KAM theory. Finally, using an additional twist assumption on $(B_2)_{\partial\mathcal{T}_\varepsilon}$, one shows that there is an accumulation of invariant tori for B_2 near $\partial\mathcal{T}_\varepsilon$, so that this construction may be repeated on

such invariant tori to construct an MHD equilibrium with an arbitrary number of pressure jumps.

Although this construction is a right step towards a resolution of Grad's conjecture, we believe that its complete resolution is still far from reach. Indeed, the pressure in such solutions is piecewise constant, so that it is not smooth. As a result, the constructed field does not a priori admit a tangent foliation, but a finite number of invariant tori. Even if this result is in itself an interesting construction, the author believes that the method could not easily be adapted to smooth solutions as it heavily uses Beltrami fields, which in themselves do not produce any change in pressure. We also note that the approximate formulas for harmonic fields in thin tubes were also used in [EP15; ELP20; EP23a] for constructions of knotted vortex tubes for the Euler equations, and the study of the dynamical properties of Beltrami fields.

Foliations for harmonic fields

To the author's knowledge, there are few explicit rigorous formulas for harmonic fields in toroidal domains, namely, the axisymmetric harmonic fields, and the approximate formula for thin tubes given in [EP15]. In particular, we believe that it is not known whether there exists foliated harmonic fields besides in the axisymmetric case, in which the field is purely toroidal. In this section, we construct other foliated fields with planar field lines by combining axisymmetric fields with different singular axes. We begin by constructing the usual axisymmetric solutions using a Hamiltonian formulation.

We equip $\mathbb{R}^3 \setminus \{x = y = 0\}$ with cylindrical coordinates (R, ϕ, z) and $\mathbb{R}^2 \setminus \{0\}$ with polar coordinates (R, ϕ) . We also define the projection $\pi : \mathbb{R}^3 \rightarrow \mathbb{R}^2$ by $\pi(x, y, z) = (x, y)$. Let H_0 be the Hamiltonian function defined in polar coordinates by

$$H_0(R) = \frac{1}{2\pi} \ln(R).$$

Then, one obtains that

$$\begin{aligned} b_0 &:= J\nabla H_0 \\ &= \frac{1}{2\pi} \nabla \phi, \end{aligned}$$

where, in Cartesian coordinates

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

is the canonical symplectic matrix in \mathbb{R}^2 . Since b_0 is a Hamiltonian vector field, it is divergence free, and since it is locally the gradient of a function, it is curl free. The field lines of b_0 are then positively oriented circles centered at the origin with period $1/R$. One then defines, for $\bar{x} = (x_1, \dots, x_N) \in (\mathbb{R}^2)^N$ and $\bar{\alpha} = (\alpha_1, \dots, \alpha_N) \in (R^+ \setminus \{0\})^N$

$$H_{\bar{x}, \bar{\alpha}} = \sum_{i=1}^N \alpha_i H_0(\cdot - x_i),$$

The set of points verifying $\nabla H_{\bar{x}, \bar{\alpha}} = 0$ is then a subset of the intersection of two polynomial curves without common factors, so that there is only a finite number of solutions. As a consequence, all but a finite number of level sets of $H_{\bar{x}, \bar{\alpha}}$ are regular. Furthermore, we have $\lim_{|x| \rightarrow \infty} H_{\bar{x}, \bar{\alpha}} = +\infty$ and $\lim_{x \rightarrow x_i} H_{\bar{x}, \bar{\alpha}} = -\infty$ so that all level sets of $H_{\bar{x}, \bar{\alpha}}$ are compact. Defining

$$b_{\bar{x}, \bar{\alpha}} = J\nabla H_{\bar{x}, \bar{\alpha}},$$

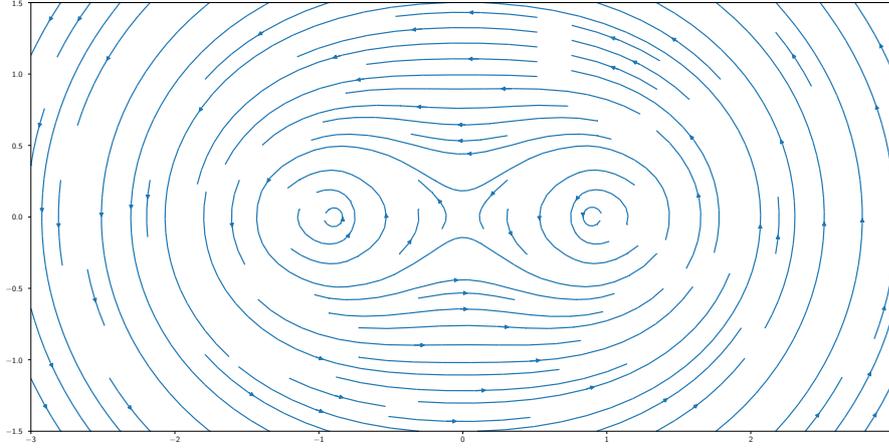


Figure 1.7 – Field lines of $b_{\bar{x}, \bar{\alpha}}$ for $\bar{x} = ((-1, 0), (1, 0))$ and $\bar{\alpha} = (1, 1)$. The field lines of $B_{\bar{x}, \bar{\alpha}}$ are the same on each horizontal plane of \mathbb{R}^3 .

we deduce that the trajectories generated by $b_{\bar{x}, \bar{\alpha}}$ starting on regular level sets are all periodic.

We now define $B_{\bar{x}, \bar{\alpha}}$ as the vector field of $\mathbb{R}^3 \setminus \cup_{i=1}^N \{\pi(x) = x_i\}$ obtained from $b_{\bar{x}, \bar{\alpha}}$ by lifting it on each horizontal plane. From the previous computations, it is clear that $B_{\bar{x}, \bar{\alpha}}$ is divergence and curl free, and that for all x such that $\pi(x)$ is a regular value of $H_{\bar{x}, \bar{\alpha}}$, the trajectory generated by $B_{\bar{x}, \bar{\alpha}}$ starting at x is planar and periodic. We refer to such trajectories as regular trajectories. We now choose a surface $S \subset \mathbb{R}^3$ diffeomorphic to an open disk, such that all the trajectories starting on S are regular. Moreover, we assume that if x and y are distinct points on S , then their trajectories are distinct. Defining Ω as the set of orbits starting on S , we obtain that Ω is a toroidal domain. Furthermore, $B_{\bar{x}, \bar{\alpha}}$ is by definition tangent to $\partial\Omega$, so that it is a harmonic field of $B_{\bar{x}, \bar{\alpha}}$.

The harmonic field we have constructed is foliated as all the field lines are closed, but if \bar{x} contains multiple points, it is not axisymmetric. We thus deduce that, contrary to the case of MHD equilibria where Grad conjectured that no smooth solutions exist with non-constant pressure without axisymmetry, one can easily construct non-axisymmetric harmonic fields which are foliated. However, the fields resulting from this construction have planar closed field lines, so that no twist is produced. The author believes that the question of existence of foliated harmonic fields in toroidal domains producing twist or non-trivial Poincaré maps is much more delicate.

1.3.4 Finite element method for electromagnetism

The most common way of writing Maxwell's equations is using the vectorial calculus language in three-dimensions, that is, using the gradient, curl and divergence operators. As a consequence, when setting variational formulations for these equations, one often encounters variational spaces involving only one of these operators such as $H^1(\Omega)$, $H(\text{curl}, \Omega)$ or $H(\text{div}, \Omega)$. When tackling the problem of finding numerical approximations using the finite element method, one therefore wishes to construct approximation spaces which are well-behaved with these differential operators. In the case of the gradient, the variational space is H^1 , so that the classical P_r elements may be

used. However, when dealing with the divergence or curl operators, which do not involve the whole Jacobian matrix, using P_r elements component-wise is not natural. Indeed, the obtained finite element spaces then discretize $H^1(\Omega)^3$, which is more restrictive than desired. For an example in which this discrepancy can cause issues, we refer to [AFW10, Section 2.3.2]. Indeed, it is shown that a vector Laplacian problem can be given by the minimization of a quadratic functional on $H(\text{curl}, \Omega) \cap H_0(\text{div}, \Omega)$. However, in the case of nonconvex polyhedra, this space is known to be a closed strict subspace of $H^1(\Omega)^3 \cap H_0(\text{div}, \Omega)$, so that using elements adapted to $H^1(\Omega)^3$ does not in general give us convergence of numerical solutions.

To remedy this problem, one needs to construct finite element spaces that are well adapted to the curl and divergence operators. This was first done in the late 1970s and early 1980s by Raviart, Thomas and Nedelec [RT77; Ned80]. Then, in the early 2000s, Arnold, Falk and Winther developed a more general theory referred to as finite element exterior calculus (FEEC) [AFW06; AFW10], which synthesizes and generalizes these finite elements to Hilbert complexes, and in particular, the de Rham complex. Although Arnold et al. gave a first comprehensive formulation of FEEC, one can note that similar constructions were made by Whitney in the 1950s when establishing a de Rham type theorem for simplicial cohomology [Whi57].

In the context of this manuscript, notions of FEEC will be used in Section 3.4 to obtain numerical approximations of harmonic fields in toroidal domains as well as vector potentials in order to construct a numerical method to compute the helicity of harmonic fields.

Finite element method

Before going into the specifics of FEEC, we give a small introduction to the general theory of finite elements. For general introductions to the finite element method, we refer the reader to the book of Ciarlet [Cia02] as well as the series of book of Ern and Guermond [EG21a; EG21b; EG21c]. We begin by giving a framework for variational problems.

For $\Omega \subset \mathbb{R}^n$ regular enough, typically Lipschitz, we consider a Hilbert space $V(\Omega)$. If Ω' is a subset of Ω , we have a bounded surjection $\pi : V(\Omega) \rightarrow V(\Omega')$. $V(\Omega)$ is typically a space of functions over Ω , and π a restriction operator. Given an invertible affine mapping F of \mathbb{R}^n , we also define an isomorphism $F^* : V(\Omega) \rightarrow V(F(\Omega))$. For example, if $V(\Omega)$ is a space of real valued functions over Ω , F^* may be the composition with F^{-1} . For Ω fixed, a a bilinear form on $V(\Omega)$ and l in $V(\Omega)'$, we now consider the following variational formulation. Find u in $V(\Omega)$ such that for all v in $V(\Omega)$,

$$a(u, v) = l(v).$$

We assume that this variational problem is well posed, that is, there exists a unique bounded resolvent R from $V(\Omega)'$ to $V(\Omega)$ verifying $a(R(l), v) = l(v)$ for all v .

Generally, the space $V(\Omega)$ has infinite dimension, so that explicitly solving this problem is impossible in practice. The aim of the finite element method is to consider finite dimensional subspaces $V_n(\Omega) \subset V(\Omega)$ on which solving the variational formulation becomes a classical linear inversion problem in finite dimensions. The hope is then that, by choosing n large enough, $V_n(\Omega)$ is a "good approximation" of $V(\Omega)$ so that the solution in $V_n(\Omega)$ is close to the one in $V(\Omega)$.

A more specific and standard definition for what are finite elements is the one of Ciarlet [Cia02]. A finite element is a triple $(K, \mathcal{V}, \mathcal{L})$ where

- $K \subset \mathbb{R}^n$ is a reference element, often a simplex or a hypercube, which is composed of subentities.
- \mathcal{V} is a finite dimensional space of polynomials on K ¹⁶.

16. More precisely, one may consider in general \mathcal{V} to be a subspace of $P \otimes E$, where P is a finite dimensional space of polynomials on K , and E a finite dimensional vector space. This allows for example to take into account vector valued functions by taking $E = \mathbb{R}^n$, or differential forms valued functions by taking $E = \text{Alt}^k(\mathbb{R}^n)$.

• $\mathcal{L} = \{l_1, \dots, l_k\}$ is a basis of \mathcal{V}' such that each l_i is associated to a subentity of K . Often, the functionals l_i are integral moments over subentities of K , such as point evaluation, or integration over edges. One may take the simple case of P_1 finite elements. In this case, K is the standard n dimensional simplex, \mathcal{V} is the space of polynomials of order at most 1 on K , and l_i is the evaluation on the i -th vertex of K .

Once a finite element is defined on a standard element K , one may define finite element spaces on meshes. Suppose Ω is a subset of \mathbb{R}^n equipped with a family of meshes $(\mathcal{T}_h)_{h>0}$ each composed of a finite set of affine invertible mappings $F_{i,h}$ in \mathbb{R}^n such that, Ω is the union over i of $\overline{F_{i,h}(K)}$, and for all i, j , the intersection of $\overline{F_{i,h}(K)}$ and $\overline{F_{j,h}(K)}$ is obtained by a sub-union of sets of the form $F_{i,h}(\sigma)$ or $F_{j,h}(\sigma)$ where the σ are taken over all the subentities of K . h is then defined to be the largest diameter of all the cells $F_{i,h}(K)$. One defines the finite element space $V_h(\Omega)$ as the set of v such that

- For all i , $F_{i,h}^*(v|_{F_{i,h}(K)})$ is in \mathcal{V} .
- Interelement continuity is satisfied, that is, corresponding linear functionals over a common subentity are equal when evaluated on v .

In the context of a global Hilbert space $V(\Omega)$ as in the beginning of this section, we say that $V_h(\Omega)$ is $V(\Omega)$ -conforming if the second point is equivalent to saying that v is in $V(\Omega)$.

Now that the finite element space $V_h(\Omega) \subset V(\Omega)$ is constructed, we return to the variational problem stated earlier. The discrete problem is the following. Find u_h in $V_h(\Omega)$ such that for all v_h in $V_h(\Omega)$

$$a(u_h, v_h) = l(v_h).$$

We also suppose that the discrete variational problem is well posed with resolvent $R_h : V(\Omega)' \rightarrow V_h(\Omega)$, which is for example a direct consequence of well-posedness in the continuous case when the Lax–Milgram theorem applies. When one wishes to prove convergence results of discrete solutions, the most common method comes in two steps.

First, we prove an approximation result which does not depend on the variational problem itself, but only on how well functions of $V_h(\Omega)$ can approximate functions of $V(\Omega)$. Often, such results are obtained either by assuming some regularity on the approximated function, or by measuring the error with respect to a weaker norm than the one of $V(\Omega)$. In the former case, assume that $\tilde{V}(\Omega)$ is a Hilbert space which injects continuously and densely in $V(\Omega)$. One then may wish to obtain estimates of the form

$$\inf_{v_h \in V_h(\Omega)} \|v - v_h\|_{V(\Omega)} \leq Ch^s \|v\|_{\tilde{V}(\Omega)},$$

for all v in $\tilde{V}(\Omega)$, where s is a positive constant. In other words, if one assumes some additional regularity on the target function, one may approximate it with functions in $V_h(\Omega)$. The order s is often bounded by two factors, the order of the polynomials in the finite element space and the difference of regularity between $\tilde{V}(\Omega)$ and $V(\Omega)$. To obtain such approximation results, it is also common to make some additional assumptions on the family of meshes, such as shape regularity or quasi-uniformity.

Once one has obtained approximation results for the finite element space, the second step is often to prove that the discrete solution is quasi-optimal. For example, when a verifies the hypotheses of Lax–Milgram, Céa’s lemma states that for all l in $V(\Omega)'$, we have

$$\|Rl - R_h l\|_{V(\Omega)} \leq C \inf_{v_h \in V_h(\Omega)} \|Rl - v_h\|.$$

In other words, $R_h l$ is, up to a constant independent of h , the optimal approximation of Rl in $V_h(\Omega)$. When combining this with the type of approximation results that was given earlier, we

obtain convergence in the case where the continuous solution Rl is in $\tilde{V}(\Omega)$. In the case of elliptic PDEs, such regularity assumptions are often obtained through elliptic regularity techniques. Otherwise, as was mentioned earlier, one can often obtain convergence in weaker norms without assuming any further regularity on the solution in the continuous case.

Finite element exterior calculus

As mentioned in the introduction of this section, one often needs to deal with finite element discretizations of variational spaces involving the curl and divergence operators when constructing numerical methods for electromagnetism. The first $H(\text{curl}, \Omega)$ and $H(\text{div}, \Omega)$ conforming finite elements were introduced by Raviart, Thomas and Nedelec in the late 70s and early 80s [RT77; Ned80]. However, we choose to introduce directly the framework of FEEC as given by Arnold et al. in [AFW06] in the context of differential forms. The link with the special cases of $H(\text{curl}, \Omega)$ and $H(\text{div}, \Omega)$ conforming spaces of Raviart, Thomas and Nedelec are then obtained as specific cases of FEEC when using the identifications between differential forms and vector fields in three dimensions (see Section 1.3.1). The precise construction and properties of FEEC spaces are technical, so we only choose to introduce some aspects of it. We refer the reader to [AFW06, Sections 2 to 6] for more details on the constructions and properties of these spaces.

Let $\mathcal{P}_r(\mathbb{R}^n)$ be the space of polynomials of degree at most r on \mathbb{R}^n . We then define the spaces of polynomial differential forms as

$$\mathcal{P}_r \Lambda^k(\mathbb{R}^n) = \mathcal{P}_r(\mathbb{R}^n) \otimes \text{Alt}^k(\mathbb{R}^n),$$

where $\text{Alt}^k(\mathbb{R}^n)$ is the space of k -multilinear antisymmetric forms on \mathbb{R}^n . We also introduce the space of reduced polynomial differential forms $\mathcal{P}_r^- \Lambda^k(\mathbb{R}^n)$, which is an intermediate space between $\mathcal{P}_{r-1} \Lambda^k(\mathbb{R}^n)$ and $\mathcal{P}_r \Lambda^k(\mathbb{R}^n)$, with $\mathcal{P}_r^- \Lambda^0(\mathbb{R}^n) = \mathcal{P}_r \Lambda^0(\mathbb{R}^n)$ and $\mathcal{P}_r^- \Lambda^n(\mathbb{R}^n) = \mathcal{P}_{r-1} \Lambda^n(\mathbb{R}^n)$. The definition and properties of these spaces involve the Koszul operator, which we choose to omit for conciseness.

Given an n -simplex T in \mathbb{R}^n , we now wish to define bases for $(\mathcal{P}_r \Lambda^k(T))'$ and $(\mathcal{P}_r^- \Lambda^k(T))'$. Since $\mathcal{P}_r \Lambda^k(T)$ is composed of k forms, a natural thing to consider is to integrate it against elements of $\Delta_k(T)$, the set of k -dimensional sub-simplices of T . Furthermore, one may integrate it on sub-simplices of dimension greater than k by taking the exterior product with polynomial differential forms. The general case for defining the degrees of freedom can be found in [AFW06], but we choose to introduce it only for the space $\mathcal{P}_1^- \Lambda^k(T)$, which corresponds to the Whitney forms [Whi57]. In this case, the degrees of freedom correspond to

$$l_f(\omega) = \int_f \omega$$

for all f in $\Delta_k(T)$.

When given a mesh \mathcal{T} of a domain Ω composed of n -simplices T_i , we define the spaces $\mathcal{P}_r \Lambda^k(\mathcal{T})$ as the set of differential forms ω in $L^2 \Lambda^k(\Omega)$ such that $\omega|_{T_i}$ is in $\mathcal{P}_r \Lambda^k(T_i)$ for all i , and which verifies interelement continuity. Defining $H \Lambda^k(\Omega)$ as the space of square integrable differential forms ω such that $d\omega$ is in $L^2 \Lambda^{k+1}(\Omega)$, we find that these spaces are $H \Lambda^k(\Omega)$ conforming, that is, interelement continuity is equivalent to requiring that ω is in $H \Lambda^k(\Omega)$. The spaces $\mathcal{P}_r^- \Lambda^k(\mathcal{T})$ are defined in the identical way and are also $H \Lambda^k(\Omega)$ -conforming.

One can then define projection operators from $L^2 \Lambda^k(\Omega)$ to $\mathcal{P}_r \Lambda^k(\mathcal{T})$ and $\mathcal{P}_r^- \Lambda^k(\mathcal{T})$ denoted Π . In this case, one cannot only use the canonical projections defined by identifying the degrees of freedom as the latter are not bounded in $L^2 \Lambda^k(\Omega)$. Therefore, these canonical projections are regularized using a smooth convolution kernel to obtain continuity. These smoothed projections

are constructed to obtain the following commutative diagrams

$$\begin{array}{ccc}
H\Lambda^k(\Omega) & \xrightarrow{d} & H\Lambda^{k+1}(\Omega) & & H\Lambda^k(\Omega) & \xrightarrow{d} & H\Lambda^{k+1}(\Omega) \\
\downarrow \Pi & & \downarrow \Pi & & \downarrow \Pi & & \downarrow \Pi \\
\mathcal{P}_r\Lambda^k(\mathcal{T}) & \xrightarrow{d} & \mathcal{P}_{r-1}\Lambda^{k+1}(\mathcal{T}) & & \mathcal{P}_r\Lambda^k(\mathcal{T}) & \xrightarrow{d} & \mathcal{P}_r^-\Lambda^{k+1}(\mathcal{T}) \\
\\
H\Lambda^k(\Omega) & \xrightarrow{d} & H\Lambda^{k+1}(\Omega) & & H\Lambda^k(\Omega) & \xrightarrow{d} & H\Lambda^{k+1}(\Omega) \\
\downarrow \Pi & & \downarrow \Pi & & \downarrow \Pi & & \downarrow \Pi \\
\mathcal{P}_r^-\Lambda^k(\mathcal{T}) & \xrightarrow{d} & \mathcal{P}_r^-\Lambda^{k+1}(\mathcal{T}) & & \mathcal{P}_r^-\Lambda^k(\mathcal{T}) & \xrightarrow{d} & \mathcal{P}_{r-1}\Lambda^{k+1}(\mathcal{T})
\end{array}$$

As a consequence, we can then combine any sequence of such diagrams to obtain a subcomplex of the de Rham sequence. In turn, the smoothed projections Π induce a linear map on cohomology spaces, which is in fact an isomorphism for the de Rham cohomology.

Although we choose to end this introduction to FEEC here, we note that many more constructions can be found in [AFW06; AFW10], such as approximation estimates, Hodge theory on the discrete de Rham complex and an application to the numerical resolution of the Hodge Laplacian. In the three dimensional vectorial setting, the spaces we will use in Section 3.4 are the spaces $\mathcal{P}_r^-\Lambda^k(\mathcal{T})$, which correspond to Lagrange, Nedelec first kind, Raviart-Thomas and discontinuous elements of degrees r , r , r and $r - 1$ respectively¹⁷.

1.4 Contributions of the thesis

In this manuscript, we are interested in studying magnetic confinement in stellarators using harmonic fields. As was discussed in Section 1.3.1, one may associate to each toroidal domain a normalized harmonic field. This allows to consider the problem through a shape optimization and shape differentiation approach. The scientific content of this thesis is mostly contained in the following published papers.

- R. Robin and R. Roussel. “Shape Optimization of Harmonic Helicity in Toroidal Domains”. In: *Journal of Optimization Theory and Applications* 204.1 (2024), p. 10. DOI: 10.1007/s10957-024-02588-y
- R. Roussel. “Shape Differentiation for Poincaré Maps of Harmonic Fields in Toroidal Domains”. In: *The Journal of Geometric Analysis* 35.1 (2024), p. 19. DOI: 10.1007/s12220-024-01849-6

1.4.1 Shape differentiation approach

As we saw in Section 1.3.1, one can associate with each toroidal domain Ω and a generator γ' of $H_1(\bar{\Omega})$ a unique harmonic field $B(\Omega)$ verifying

$$\int_{\gamma'} B(\Omega) \cdot t' = 1.$$

¹⁷. The fact that we obtain one lesser degree in the last case comes from the equality $\mathcal{P}_r^-\Lambda^n(\mathbb{R}^n) = \mathcal{P}_{r-1}\Lambda^n(\mathbb{R}^n)$.

One may then choose a cost function \mathcal{J} , which associates with each magnetic field a quantity describing an aspect of the quality of magnetic confinement. We may thus obtain a shape functional $\mathcal{J} \circ B$ which associates with each toroidal domain Ω the quantity $\mathcal{J}(B(\Omega))$. Strictly speaking, the harmonic field $B(\Omega)$ is only defined up to a sign, so that $\mathcal{J} \circ B$ may also depend on the choice of generator of $H_1(\bar{\Omega})$.

In practice however, it can be hard to obtain a simple functional \mathcal{J} which evaluates the quality of confinement directly from the magnetic field. In this manuscript, we therefore choose to use only two simple properties of magnetic fields, the magnetic helicity, and the Poincaré map on the boundary. We then study the shape derivatives of these shape functions, to obtain a numerical optimization scheme in the first case, and to obtain local properties on the Poincaré maps of harmonic fields under small perturbations of the domain in the second case.

One way to define shape differentials is the following. Consider a set of admissible shapes \mathcal{O} of \mathbb{R}^n , and a Banach space \mathcal{V} of vector fields of \mathbb{R}^n which leaves \mathcal{O} invariant. That is, if $\Omega \in \mathcal{O}$ is an admissible shape and $V \in \mathcal{V}$ is small enough, then $(I + V)(\Omega)$ is in \mathcal{O} . Considering a shape function $\mathcal{F} : \mathcal{O} \rightarrow \mathcal{W}$ where \mathcal{W} is a Banach space, we say that \mathcal{F} is shape differentiable at Ω with respect to deformations in \mathcal{V} if

$$\mathcal{F}((I + V)\Omega) = \mathcal{F}(\Omega) + \mathcal{F}'(\Omega; V) + o(\|V\|_{\mathcal{V}}),$$

where $\mathcal{F}'(\Omega) \in \mathcal{L}(\mathcal{V}, \mathcal{W})$ is a bounded linear map.

Finally, we note that although we choose to normalize the harmonic field using toroidal circulation, one could easily repeat this process for other normalizations. Suppose for example that we wish to normalize the harmonic field with respect to the L^2 norm. Considering a functional of the form $\mathcal{F} = \mathcal{J} \circ B$ as earlier, we may define

$$\tilde{\mathcal{F}}(\Omega) = \mathcal{J} \left(\frac{1}{\mathcal{N}(\Omega)} B(\Omega) \right),$$

where $\mathcal{N}(\Omega) = \|B(\Omega)\|_{L^2}$. Then, if \mathcal{F} is shape differentiable, we may obtain the shape derivative of $\tilde{\mathcal{F}}$ in practice using composition like formulas for differentials. In the simple case where $\mathcal{J} = H$ is the helicity (see Section 1.3.2), we obtain

$$\tilde{\mathcal{F}}(\Omega) = \frac{1}{\mathcal{N}(\Omega)^2} \mathcal{F}(\Omega),$$

so that

$$\tilde{\mathcal{F}}'(\Omega; V) = -\frac{(\mathcal{N}^2)'(\Omega; V)}{\mathcal{N}(\Omega)^4} \mathcal{F}(\Omega) + \frac{1}{\mathcal{N}(\Omega)^2} \mathcal{F}'(\Omega; V).$$

We therefore see that, when the normalization criterion may be differentiated, which is simple in the case of the square norm of the harmonic field using the techniques we will introduce in Section 3.3, one may obtain the shape derivative of the modified functional, although the formula may in general be more complex.

1.4.2 Shape differentiation of harmonic fields

In Chapter 2, we consider shape differentiation problems for normalized harmonic fields. Indeed, if one wishes to obtain derivatives of shape functionals defined using the normalized harmonic field, one needs to be able to differentiate it with respect to the shape.

Variational formulations for harmonic fields

In order to obtain the shape derivatives of the normalized harmonic field in a rigorous way, one needs to obtain a variational formulation for it. These formulations are given in Section 2.2. To obtain such a formulation, we consider a poloidal cutting surface Σ of a toroidal domain Ω , that is, a Lipschitz surface in Ω such that $\partial\Sigma \subset \partial\Omega$ is a poloidal loop¹⁸. $\Omega \setminus \Sigma$ is then a simply connected pseudo-Lipschitz domain, and the restriction of $B(\Omega)$ to it verifies $B(\Omega) = \nabla u$ where u is solution to

$$\begin{cases} \Delta u = 0 & \text{in } \Omega \setminus \Sigma, \\ \nabla u \cdot n = 0 & \text{on } \partial\Omega, \\ \llbracket u \rrbracket_{\Sigma} = 1, \end{cases}$$

where $\llbracket u \rrbracket_{\Sigma}$ denotes the jump of u across Σ (see for example [Amr+98]).

One can then obtain two variational formulations for this PDE. The first one is the following classical variational formulation for Poisson equations. Find u in $V_1(\Omega \setminus \Sigma)$ such that for all v in $H^1(\Omega)$

$$\int_{\Omega} \nabla u \cdot \nabla v = 0,$$

where $V_1(\Omega \setminus \Sigma)$ is the affine subspace of functions in $H^1(\Omega \setminus \Sigma)$ verifying $\llbracket u \rrbracket_{\Sigma} = 1$. The second one is given by the following mixed formulation. Find $(\sigma, u) \in H_0(\text{div}, \Omega) \times L_0^2(\Omega)$ such that, for all $(\tau, v) \in H_0(\text{div}, \Omega) \times L^2(\Omega)$ we have

$$\begin{aligned} \int_{\Omega} (\text{div } \sigma) v &= 0, \\ \int_{\Omega} \sigma \cdot \tau + \int_{\Omega} u (\text{div } \tau) &= \int_{\Sigma} \tau \cdot n_{\Sigma}, \end{aligned}$$

where $L_0^2(\Omega)$ is the set of zero average functions in $L^2(\Omega)$.

We observe that these two variational formulations give two different variational spaces for $B(\Omega)$, namely, $H(\text{curl}, \Omega)$ for the first one¹⁹ and $H_0(\text{div}, \Omega)$ for the second. In view of the vectorial de Rham complex

$$H^1(\Omega) \xrightarrow{\nabla} H(\text{curl}, \Omega) \xrightarrow{\text{curl}} H(\text{div}, \Omega) \xrightarrow{\text{div}} L^2(\Omega),$$

which is isomorphic to the de Rham complex on differential forms, we see that the first variational formulation gives a harmonic field which corresponds to a one-form while the second one gives a harmonic field which corresponds to a two-form²⁰.

Pullbacks of vector fields onto a fixed domain

We now consider the shape differentiability problem for harmonic fields. Let Ω be a Lipschitz toroidal domain and V a small enough Lipschitz vector field of \mathbb{R}^3 . Our aim is to express the harmonic field of the deformed domain $\Omega_V := (\mathbf{I} + V)(\Omega)$ as the sum of $B(\Omega)$, a term which is linear in V , and a higher order remainder. However, $B(\Omega_V)$ and $B(\Omega)$ do not live in the same

18. that is, a loop which is contractible in $\bar{\Omega}$ but which generates the first homology group of $\mathbb{R}^3 \setminus \Omega$.

19. Indeed, gradients of functions in $V_1(\Omega \setminus \Sigma)$ are in $H(\text{curl}, \Omega)$ [Amr+98, Lemma 3.11].

20. One can note that in the first case, $B(\Omega)$ corresponds to a harmonic one form, while in the second case, it corresponds to a harmonic two-form with essential boundary conditions. The equivalence between the two is given by Poincaré duality [AFW06].

space so that this naive approach does not work directly. To remedy this problem, we consider pullbacks of the harmonic fields in the deformed domain Ω_V back on to Ω .

As seen in the previous section, we have two variational formulations for $B(\Omega)$. The first one corresponds to seeing the harmonic field as a one-form, while the other one corresponds to seeing it as a two-form. One may thus consider two ways to pull $B(\Omega_V)$ onto Ω , by using a pullback as a one-form and by using a pullback as a two-form. Furthermore, each of these pullbacks denoted $\Phi_V^1 B(\Omega_V)$ and $\Phi_V^2 B(\Omega_V)$ preserve the variational spaces of the corresponding variational formulations. We then wish to obtain results of the form

$$\Phi_V^i B(\Omega_V) = B(\Omega) + B'_i(\Omega; V) + o(\|V\|).$$

The norms we will use for these differentiability results will differ in the two cases. We also note that one may pullback the harmonic field using the pushforward by $(I + V)^{-1}$. In this case, one preserves the field lines, but none of the variational spaces of the variational formulations are preserved by this transformation. These notions of pullbacks and all the relevant properties in the vectorial context will be given in Section 2.3.

Shape differentiability results

A general idea to prove shape differentiability of PDE solutions, as can be seen for example in [HP18], is to use an implicit function theorem on the variational formulation which is pulled back on the fixed domain Ω . As such, it is important to use definitions of pullbacks which preserve the variational spaces.

For the case of the mixed formulation of the normalized harmonic field, which is studied in Section 2.4, this procedure is obtained simply by using the pullback $\Phi_V^2 B(\Omega_V)$. Indeed, this transformation maps $H_0(\text{div}, \Omega_V)$ to $H_0(\text{div}, \Omega)$. One then obtains the differentiability of $V \mapsto \Phi_V^2 B(\Omega_V)$ from $W^{1,\infty}(\mathbb{R}^3)^3$ to $H_0(\text{div}, \Omega)$, which is given by Theorem 2.4.1. In the case of the classical formulation, which is studied in Section 2.5, there is the first difficulty that the variational space is an affine space. This can be remedied simply by choosing an arbitrary function in $V_1(\Omega \setminus \Sigma)$, and removing it from the solution to the pulled back variational formulation. Then, we prove that when Ω has smooth boundary, classical results from elliptic regularity allow us to use the implicit function theorem in more regular spaces. From this, we obtain the differentiability of the map $V \mapsto \Phi_V^1 B(\Omega_V)$ from $W^{k,\infty}(\mathbb{R}^3)^3$ to $H^{k+1}(\Omega)^3$, which is given by Theorem 2.5.1.

Expression of the shape derivatives

As we use two different pullbacks for the two variational formulations, it is clear that the resulting expressions for the shape derivative will differ. However, as we will see, the resulting shape derivative can be seen as the sum of two terms. First, a transport term given by the choice of the pullback, and then a Eulerian term independent of the choice of pullback.

To give an intuition for this expression of shape derivatives, we give the following argument. Let ω be a differential form on a manifold M and V a complete vector field on M . Then, one obtains

$$\frac{d}{dt}\Big|_{t=0} (e^{tV})^* \omega = \mathcal{L}_V \omega,$$

where e^{tV} is the flow of V at time t . If $t \mapsto \omega_t$ is now a differentiable path of differential forms, one obtains

$$\frac{d}{dt}\Big|_{t=0} (e^{tV})^* \omega_t = \mathcal{L}_V \omega_0 + \frac{d}{dt}\Big|_{t=0} \omega_t.$$

One sees that the total, or Lagrangian, derivative of $t \mapsto (e^{tV})^*$ decomposes as the sum of a Lie derivative $\mathcal{L}_V \omega_0$ and a Eulerian derivative. Furthermore, using Cartan's formula

$$\mathcal{L}_V \omega = d\iota_V \omega + \iota_V d\omega,$$

we define the equivalent Lie derivatives in the vectorial context

$$\begin{aligned}\mathcal{L}_V^1 u &= \nabla(u \cdot V) + \operatorname{curl} u \times V, \\ \mathcal{L}_V^2 u &= \operatorname{curl}(u \times V) + (\operatorname{div} u) V.\end{aligned}$$

In analogy with the previous computations, we define the Eulerian shape derivatives of the harmonic field as

$$B'_{i,\mathcal{E}}(\Omega; V) = B'_i(\Omega; V) - \mathcal{L}_V^i B(\Omega).$$

We then prove that for both cases of shape derivatives, we obtain $B'_{i,\mathcal{E}}(\Omega; V) = \nabla u_V$, where u_V solves

$$\begin{cases} \Delta u_V = 0 & \text{in } \Omega, \\ \nabla u_V \cdot n = \operatorname{div}_\Gamma(B(\Omega)(V \cdot n)) & \text{on } \partial\Omega, \end{cases} \quad (1.10)$$

where $\operatorname{div}_\Gamma$ is the tangential divergence on $\partial\Omega$.

1.4.3 Shape optimization of harmonic helicity

In Chapter 3, we consider the problem of shape optimization of harmonic helicity. Harmonic helicity is the shape functional defined as the helicity of the normalized harmonic field of a toroidal domain.

Bevir–Gray formula and potential vectors

We recall that the helicity of a magnetic field $F \in H_0(\operatorname{div}, \Omega)$ may be defined as

$$H(F) = \int_\Omega F \cdot \operatorname{BS}(F).$$

Also, the Biot–Savart operator BS is a convolution operator with a singular kernel. As a result, computing it numerically is not an easy task. However, we recall that the Biot–Savart operator gives a vector potential when evaluated on a magnetic field in $H_0(\operatorname{div}, \Omega)$, that is, $\operatorname{curl}(\operatorname{BS}(F)) = F$. Furthermore, when Ω is simply connected, the quantity $\int_\Omega F \cdot A$ is invariant on the choice of potential vector A of F . However, this gauge invariance no longer holds when Ω is not simply connected, and in particular when it is a toroidal domain. To remedy this problem, the Bevir–Gray formula [BG80] gives the following gauge invariant expression in the case of a toroidal domain

$$\int_\Omega F \cdot A - \left(\int_\gamma A \cdot t \right) \left(\int_{\gamma'} A \cdot t' \right), \quad (1.11)$$

where γ and γ' are poloidal and toroidal loops respectively. Furthermore, the toroidal circulation of $\operatorname{BS}(F)$ always vanishes [CDG01, Section III] so that this quantity is in fact equal to the helicity defined by the Biot–Savart operator. We also note that the Bevir–Gray formula was generalized in [MV19] for domains with more complex topology.

Given the Bevir–Gray formula, we now explain how one may choose specific vector potentials.

First, we use the Coulomb gauge, that is

$$\begin{cases} \operatorname{div} A = 0 & \text{in } \Omega, \\ A \cdot n = 0 & \text{on } \partial\Omega, \end{cases}$$

which is equivalent to saying that the chosen vector potential is L^2 orthogonal to gradient vector fields. However, since the space of harmonic fields is nonempty, this gauge is not sufficient to fix the vector potential. Indeed, adding a harmonic field to a Coulomb potential gives another Coulomb potential. One may choose two ways to fix the vector potentials. The first one is given by

$$\int_{\Omega} B(\Omega) \cdot A^1 = 0,$$

while the second one is given by

$$\int_{\gamma'} A^2 \cdot t' = 0.$$

When the chosen magnetic field is $B(\Omega)$, choosing the first vector potential A^1 makes the first term of Eq. (1.11) vanish, while the second choice A^2 makes the second term equal to zero.

Each vector potential comes with a variational formulation. The first one is the following mixed formulation for the vector Laplacian, adapted from [AFW06, Section 7] in the vectorial language. Find $(A^1(\Omega), u) \in H(\operatorname{curl}, \Omega) \times H(\operatorname{div}, \Omega)$ such that, for all $(\tau, v) \in H(\operatorname{curl}, \Omega) \times H(\operatorname{div}, \Omega)$

$$\begin{aligned} \int_{\Omega} A^1(\Omega) \cdot \tau &= \int_{\Omega} \operatorname{curl} \tau \cdot u, \\ \int_{\Omega} \operatorname{curl} A^1(\Omega) \cdot v + \int_{\Omega} (\operatorname{div} u)(\operatorname{div} v) &= \int_{\Omega} B(\Omega) \cdot v. \end{aligned}$$

The variational formulation for A^2 is the following, given in [Val19]. Find $(A^2(\Omega), u) \in \mathcal{Z}(\Omega) \times \nabla H^1(\Omega)$ such that for all $(\tau, v) \in \mathcal{Z}(\Omega) \times \nabla H^1(\Omega)$

$$\begin{aligned} \int_{\Omega} \operatorname{curl} A^2(\Omega) \cdot \operatorname{curl} \tau + \int_{\Omega} u \cdot \tau &= \int_{\Omega} B(\Omega) \cdot \operatorname{curl} \tau, \\ \int_{\Omega} A^2(\Omega) \cdot v &= 0, \end{aligned}$$

where

$$\mathcal{Z}(\Omega) = \left\{ u \in H(\operatorname{curl}, \Omega) \mid \operatorname{curl} u \cdot n = 0, \int_{\gamma'} u \cdot t' = 0 \right\}.$$

In fact, as is shown in [Val19], one finds that $A^2(\Omega)$ is equal to the modified Biot–Savart $BS'(B(\Omega))$ defined in Section 1.3.2.

Shape differentiation

We now define the harmonic helicity shape functional of a toroidal domain Ω as $\mathcal{H}(\Omega) = \mathbf{H}(B(\Omega))$. We begin Section 3.3 by proving some properties of this shape functional given in Proposition 3.3.2. Namely, we prove that given $\lambda > 0$, we have $\mathcal{H}(\lambda\Omega) = \lambda\mathcal{H}(\Omega)$, and that given a planar symmetry R , $\mathcal{H}(R\Omega) = -\mathcal{H}(\Omega)$. The first point indicates that a shape optimization problem for harmonic helicity should be considered at fixed volume, while the first point shows that domains with planar symmetries, in particular axisymmetric domains, have zero harmonic

helicity. The second property can also be understood using the characterization of helicity using the asymptotic linking numbers of the field lines given in Section 1.3.2. Indeed, applying a planar symmetry amounts to changing the orientation of the field lines, and thus, the sign of the linking numbers.

In Section 3.3, we then consider the shape differentiation problem of the harmonic helicity. We prove that it is differentiable for Lipschitz toroidal domains under Lipschitz deformations, and if Ω is s -regular²¹, then the shape derivative is given by the following formula

$$\mathcal{H}'(\Omega; V) = \int_{\partial\Omega} (B(\Omega) \cdot A^2(\Omega)) (V \cdot n).$$

This result is given in Theorem 3.3.4. In order to prove this theorem, we use the vector fields pullbacks introduced in Section 2.3. Moreover, we use the shape differentiability of the harmonic field when pulled back as a two-form given by Theorem 2.4.1, and we prove a similar result for the vector potential $V \mapsto A^2(\Omega_V)$ when pulling it back as a one-form. The rest of the proof then follows easily by pulling back the integral of $\mathcal{H}(\Omega_V)$ onto Ω , and using a variational formulation for the shape derivative of the harmonic field as a two-form.

Computing harmonic helicity using FEEC

In Section 3.4, we wish to obtain a numerical scheme to approximate the harmonic helicity of a domain and its shape gradient. Indeed, the PDEs for harmonic fields and their vector potentials use the classical vectorial calculus operators of electromagnetism, and it is thus natural to design numerical schemes to compute them using the FEEC framework introduced in Section 1.3.4.

Given a family of meshes $(\mathcal{T}_h)_{h>0}$ of a toroidal domain Ω , we consider the scalar and vectorial equivalents of the FEEC spaces $\mathcal{P}_r^- \Lambda^k(\mathcal{T}_h)$ introduced in Section 1.3.4. These correspond to the Lagrange, Raviart–Thomas, Nedelec first kind and discontinuous elements of degree r , r , r and $r - 1$ respectively for k going from 0 to 3. We then use these spaces to solve the different variational formulations for the harmonic field of Ω and its vector potentials in these finite element spaces. Furthermore, we prove the L^2 convergence of these numerical solutions to the continuous ones using classical estimates of FEEC that can be found in [AFW06]. As a consequence, the harmonic field being the L^2 product of $B(\Omega)$ with $A^2(\Omega)$, we find that the harmonic helicity of the discrete harmonic field converges to the harmonic helicity of Ω . These results are given by Propositions 3.4.7 and 3.4.9 and Theorem 3.4.12. Finally, we prove that the numerical shape gradient converges to the continuous one. This is done using trace inequalities in cells of the mesh from [EG21a].

Numerical results and shape optimization for stellarators

Finally, we give in Section 3.5 some numerical results for computation of harmonic fields, vector potentials and harmonic helicity using the scheme described in Section 3.4. The scheme is implemented in the python library FEniCSx [Scr+22b; Scr+22a; Aln+14], with meshes generated by Gmsh [GR09]. The boundary of the toroidal domains are parametrized in cylindrical coordinates by $\left(R(u, v), \frac{2\pi v}{N_p}, Z(u, v)\right)$, where N_p is an integer describing the discrete rotational symmetry of the domain and R and Z are given by a Fourier expansion. In practice, we fix a finite number of Fourier coefficients to perform numerical computations.

We then present some plots for harmonic fields and vector potentials in a section of the NCSX plasma domain, and perform a numerical convergence test. Finally, we perform numerical shape

21. We refer to Section 2.2.1 for the definition of s -regular domains.

optimizations by using the numerical shape gradient on the Fourier coefficients of the surface. To this end, we propose two optimization programs. In the first one, we aim to bound the perimeter and the curvature of the surface, while in the second, we aim to bound the volume and the curvature. In both cases, we impose a bound on the curvature to ensure that the surfaces are regular enough. Physically, this can be understood as producing surfaces with high curvature can be challenging from an engineering perspective. Moreover, imposing uniform ball conditions on the surface, which in particular imply bounds on the curvature, is a classical tool to ensure existence of optimal shapes [PRS24; Ger23a].

1.4.4 Shape differentiation for Poincaré maps of harmonic fields

In Chapter 4 of this manuscript, we consider the problem of shape differentiation for the Poincaré maps of harmonic fields in toroidal domains. As was mentioned in Section 1.3.3, magnetic fields used for plasma confinement in toroidal devices should have a poloidal component, which can be quantified using the rotational transform. However, defining this object necessitates the assumption of a toroidal foliation of the magnetic field, which as was discussed in Section 1.3.3, is far from trivial for harmonic fields. We therefore choose to only study the Poincaré map of the harmonic field on the boundary of the toroidal domain, as the boundary is by definition an invariant surface of the harmonic field. This allows us to obtain a Poincaré map as a diffeomorphism of the circle, to which we can associate a rotation number corresponding to the rotational transform on the boundary. We then study the Poincaré maps of harmonic fields using shape differentiation techniques. To the author's knowledge, this is a new approach to study the dynamics generated by solutions to vectorial PDEs.

Definition using admissible embeddings

In order to properly define the boundary Poincaré map as a diffeomorphism of the circle, one needs some additional data on the toroidal domain. First, we need to choose a poloidal Poincaré cut of the boundary. Then, in order to obtain a diffeomorphism of the circle, and not of the Poincaré cut itself, one needs to choose coordinates on this Poincaré cut.

This necessary data is obtained through the definition of admissible embeddings from the two-dimensional torus to \mathbb{R}^3 denoted $\text{Emb}_{\text{ad}}(\mathbb{T}^2; \mathbb{R}^3)$ given in Definition 4.2.1. Intuitively, an embedding is said to be admissible if its image is the boundary of a toroidal domain Ω , if the embedding define toroidal and poloidal coordinates, and if the poloidal cuts correspond to Poincaré cuts of $B(\Omega)$. This allows us to define a mapping

$$\Pi : \text{Emb}_{\text{ad}}(\mathbb{T}^2; \mathbb{R}^3) \rightarrow \text{Diff}(S^1),$$

which associates to each admissible embedding the Poincaré map of the underlying domain $B(\Omega)$ on the poloidal cut $\phi = 0$ with coordinates on this cut induced by the embedding. The precise definition of this map is given in Section 4.2.

Shape differentiation in the general case

In Section 4.3, we aim to study local properties of the mapping Π using a shape differentiation approach. We do note that Π is not technically a shape function as it also depends on the choice of embedding. However, the chosen approach is largely inspired by shape differentiation, and uses results from Chapter 2 for shape differentiability of harmonic fields.

The shape differentiation process is the following. Suppose \mathcal{E} is an admissible embedding, and $t \mapsto P_t$ is a smooth path of diffeomorphisms of \mathbb{R}^3 starting at the identity with $\frac{d}{dt}|_{t=0} P_t = V$.

Defining $\mathcal{E}_t = P_t \circ \mathcal{E}$, we wish to write

$$\Pi(\mathcal{E}_t) = \Pi(\mathcal{E}) + \Pi'(\mathcal{E}; V) + o(\|V\|).$$

In order to prove such a result, we adapt the shape differentiation result for harmonic field from Section 2.5 by replacing the pullback as one-forms by the pushforward by P_t^{-1} . Indeed, this pushforward maps field lines of $B(P_t(\Omega))$ to field lines of $(P_t^{-1})_* B(P_t(\Omega))$, and thus preserves the dynamics. The shape differentiability result then follows easily from the definition of the Poincaré map, and from the differentiation of a flow with respect to a parameter. The general shape differentiability of Π is given by Theorem 4.3.5.

Although we choose not to include the general formula in this section, we introduce the simpler formula in the case where $B(\Omega)$ is rectified on the boundary in the coordinates $(\phi, \theta) = \mathcal{E}^{-1}$ induced by \mathcal{E} . We suppose that $B(\Omega) = \chi(\partial_\phi + \omega\partial_\theta)$, where χ is a smooth function of $\partial\Omega$ and ω is a real number corresponding to the rotational transform of $B(\Omega)$ on $\partial\Omega$. In this case, we obtain

$$\Pi'(\mathcal{E}; V) = \int_{S^1} (X'_V)^\theta(\phi, \theta + \omega\phi) d\phi,$$

where

$$(X'_V)^\theta = f \frac{2\text{III}(B(\Omega), B(\Omega)^\perp)}{\sqrt{g}\chi^2} + \left\langle \vec{\omega}, \nabla_{\mathbb{T}^2} (\omega V_\Gamma^\phi - V_\Gamma^\theta) \right\rangle + \frac{1}{\sqrt{g}\chi^2} B(\Omega)^\perp \cdot \nabla_\Gamma u_V. \quad (1.12)$$

Here, f is the normal component of V and V_Γ its tangential component. The precise definition of all the terms will be introduced throughout Chapter 4, but we already give a short interpretation of all three terms. Intuitively, the first term corresponds to the fact that, through the normal component of V , we are changing the shape of the domain, and thus the surface on which we study the dynamics of the harmonic field. In this case, the term III is the second fundamental form of $\partial\Omega$. The second term indicates how changing the coordinates on $\partial\Omega$ affects the Poincaré map. In particular, this term does not affect the rotation number of the Poincaré map. Finally, the third term comes from the fact that changing the shape of the domain affects the harmonic field, and thus its dynamics.

Image of the differential in the axisymmetric case

In Section 4.4, we consider the case of the standard axisymmetric torus given by the following embedding

$$\mathcal{E}(\phi, \theta) = ((R_T + r_P \cos(2\pi\theta)) \cos(2\pi\phi), (R_T + r_P \cos(2\pi\theta)) \sin(2\pi\phi), r_P \sin(2\pi\theta)),$$

where R_T is the major radius, and $r_P < R_T$ is the minor radius. We then prove Theorem 4.4.1 which states that for all smooth vector fields V of \mathbb{R}^3 , we have

$$\Pi'(\mathcal{E}; V) = 0.$$

This means that one needs to go to second order in order to obtain information of the local behavior of Π around \mathcal{E} . To prove this result, we first show that the first term of Eq. (1.12) vanishes. To do this, we compute the second fundamental of $\partial\Omega$ and show that the harmonic field, which is explicit in this case, is everywhere aligned with the principal directions of curvature. Then, we obtain simply that the second term of Eq. (1.12) is of zero average along all toroidal curves, so that its contribution to $\Pi'(\mathcal{E}; V)$ also vanishes. Finally, we exhibit some symmetries of

the function u_V which solves Eq. (1.10) to prove that the last term of Eq. (1.12) always vanishes when integrated along toroidal curves.

We also note that, although we chose the standard torus for simplicity, the method applies to all smooth axisymmetric tori, so that Theorem 4.4.1 remains valid in general.

Image of the differential in the diophantine case

In Section 4.5, we study the case where $B(\Omega)$ is a diophantine vector field on $\partial\Omega$.

We recall that a real number ω is said to be diophantine if there exist positive constants C, τ such that, for all $p/q \in \mathbb{Q}$

$$|\omega - p/q| \geq C|q|^{-(\tau+1)}.$$

For all $\tau > 1$, we know that the set of diophantine numbers is of full measure in the reals. We now suppose that for the coordinates (ϕ, θ) associated to an admissible embedding, we have $B(\Omega) = \chi(\partial_\phi + \omega\partial_\theta)$ where ω is diophantine. We then prove that, under the additional assumption that $\mathbb{III}(B(\Omega), B(\Omega)^\perp)$ vanishes nowhere, the mapping

$$\begin{cases} \text{Vec}(\mathbb{R}^3) \rightarrow \mathcal{C}^\infty(S^1) \\ V \mapsto \Pi'(\mathcal{E}; V) \end{cases}$$

is surjective. This result is given by Theorem 4.5.1. In order to prove this theorem, we proceed in two steps. First, we consider only tangential vector fields so that only the second term of Eq. (1.12) is nonzero. We then prove that, by choosing the right tangential vector field, one may obtain any zero average smooth function of the circle as $\Pi'(\mathcal{E}; V_\Gamma)$. This is done by solving two cohomological equations. From this, we know that the image of $V \mapsto \Pi'(\mathcal{E}; V)$ is of codimension at most one. As a result, we only need to generate the extra dimension in order to prove surjectivity. This is done using the assumption on $\mathbb{III}(B(\Omega), B(\Omega)^\perp)$, and a specific normal deformation field so that the third term of Eq. (1.12) vanishes.

Chapter 2

Shape differentiation of harmonic fields

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2.1 Introduction

In the context of stellarator fusion reactors, one aims to confine a plasma inside a toroidal chamber without inducing additional electric currents into the plasma. As such, using Maxwell's equation, one obtains in first approximation that magnetic fields in stellarators should be divergence free and curl free. We thus define the set of harmonic fields of a domain Ω of \mathbb{R}^3 as

$$\mathcal{K}(\Omega) = \{u \in L^2(\Omega)^3 \mid \operatorname{div} u = 0, \operatorname{curl} u = 0, u \cdot n = 0\}.$$

As we discussed in Section 1.3.1 using elements of differential geometry and algebraic topology, if Ω is a Lipschitz toroidal domain, $\mathcal{K}(\Omega)$ is one-dimensional. Furthermore, given γ' a generator of $H_1(\bar{\Omega})$ with t' a unit tangent vector field of γ' , there exists a unique harmonic field $B(\Omega)$ satisfying

$$\int_{\gamma'} B(\Omega) \cdot t' = 1,$$

which is referred to as the harmonic field of Ω . This approach allows us to consider the design of magnetic fields in stellarators using a shape optimization approach. That is, considering a

cost function \mathcal{J} defined for magnetic fields, and a set of admissible toroidal domains \mathcal{O} , we can consider the minimization problem associated to the shape functional¹.

$$\mathcal{J} \circ B : \begin{cases} \mathcal{O} \rightarrow \mathbb{R} \\ \Omega \mapsto \mathcal{J}(B(\Omega)) \end{cases} .$$

One may also consider a shape function taking values in spaces other than \mathbb{R} to obtain more precise data on the harmonic fields, which will for example be the case in Chapter 4 when studying Poincaré maps. We note that, from a physical point of view, the choice of cost function is in general a complicated task as many aspects come into the design of magnetic fields in fusion reactors, and the associated costs are often hard to express directly from the magnetic field itself.

When dealing with shape functionals, it is often useful to obtain an expression for the shape derivative. First, this can be used numerically to perform gradient descents on the shape functional. Second, this can be used theoretically to study the local behavior of the shape functional, such as finding critical shapes, or in general, finding the image of the differential when the shape function takes values in spaces other than \mathbb{R} . Given a set of admissible domains \mathcal{O} of \mathbb{R}^n , and an open ball \mathcal{B} centered at zero in a Banach space \mathcal{V} of vector fields in \mathbb{R}^n , we say that a shape functional $\mathcal{F} : \mathcal{O} \rightarrow \mathbb{R}$ is Fréchet shape differentiable at Ω with respect to deformations in \mathcal{V} if:

- \mathcal{O} is \mathcal{B} invariant. That is, for all V in \mathcal{B} and Ω in \mathcal{O} , $\Omega_V := (\mathbf{I} + V)(\Omega)$ is in \mathcal{O} .
- There exists $\mathcal{F}'(\Omega; \cdot)$ in \mathcal{V}' such that

$$\mathcal{F}(\Omega_V) = \mathcal{F}(\Omega) + \mathcal{F}'(\Omega; V) + o(\|V\|_{\mathcal{V}}).$$

If we have as earlier a shape functional of the form $\mathcal{J} \circ B$, we see that, in order to obtain its shape derivative, we need first to differentiate $V \mapsto B(\Omega_V)$. Intuitively, we would obtain a formula of the form

$$(\mathcal{J} \circ B)'(\Omega; V) = \mathcal{J}'(B(\Omega); B'(\Omega; V)).$$

However, this formula only makes sense in a formal way. Indeed, since $B(\Omega)$ is a vector field in Ω , changing the domain changes the space in which the harmonic field is defined, and one cannot make sense of

$$B(\Omega_V) = B(\Omega) + B'(\Omega; V) + o(\|V\|_{\mathcal{V}}).$$

To remedy this problem, we define ways to pull vector fields back from Ω_V onto Ω . Given Φ_V which maps vector fields of Ω_V to vector fields of Ω , one may hope to obtain the differentiability of $V \mapsto \Phi_V B(\Omega_V)$ with respect to a certain norm for vector fields of Ω . Naively, one may define such a transformation by composing the vector field with $(\mathbf{I} + V)$ component-wise. However, this approach is not geometrically meaningful, and does not in general lead to simple expressions for shape derivatives. Given a vector field u of Ω_V , we identify three natural ways to pull it back onto Ω :

- By taking the pushforward of u by $(\mathbf{I} + V)^{-1}$, that is,

$$\Phi_V^{\text{vf}} u = (\mathbf{I} + V)_*^{-1} u.$$

- By taking the pullback of u by $\mathbf{I} + V$ when seen as a one-form, that is,

$$(\Phi_V^1 u)^{\flat} = (\mathbf{I} + V)^* (u^{\flat}).$$

1. To be rigorous, this function may also depend on the choice of generator γ' , and thus not exactly be a shape functional.

- By taking the pullback of u by $I + V$ when seen as a two-form, that is,

$$*(\Phi_V^2 u)^\flat = (I + V)^*(*u^\flat)$$

Here, \flat is the isometry taking vector fields to one-forms, and $*$ is the Hodge-star operator mapping one-forms to two-forms. We refer the reader to Section 1.3.1 for a short introduction to these concepts, and to [Lee18] for more precise definitions. We note however that all the computations of this chapter will be done using vector fields, so that these descriptions are only used to motivate the definitions of the transformations.

The goal of this chapter is thus to obtain shape differentiability results for mappings of the form $V \mapsto \Phi_V B(\Omega_V)$ and expressions for the corresponding shape derivatives. As we have seen, the way in which we choose to pull vector fields back onto a fixed domain may change the results of the shape derivative. Furthermore, as we will see in Section 2.5 requiring more regularity on the set of admissible shapes and deformations may lead to shape differentiability results with respect to stronger norms. Although we have mentioned the transformation Φ_V^{vf} , we will not be studying the shape differentiability of harmonic fields using it. This comes from the fact that, although this transformation may have desirable geometric properties (such as preserving the field lines), it is less convenient to work with when using the variational formulations of the harmonic fields we will introduce in Section 2.2.2. A shape differentiability result using this transformation will however be given in Chapter 4 when considering Poincaré maps of harmonic fields.

To obtain the shape differentiability of harmonic fields, we will be using a classical approach of shape differentiation for PDE solutions given for example in [HP18]. The idea is to consider pulled back versions of the variational formulations of $B(\Omega_V)$ onto the fixed domain Ω . Afterwards, if the chosen pullback Φ_V preserves the variational space, one can prove the differentiability of $V \mapsto \Phi_V B(\Omega_V)$ using an implicit function argument on the pulled back variational formulation. Therefore, to the author's knowledge, the novelty of our results does not lie on the general approach to prove shape differentiability of PDE solutions, but on the chosen pullbacks which commute with the vectorial de Rham complex and thus preserve the usual variational spaces of electromagnetism.

2.1.1 Lagrangian and Eulerian derivatives

As was mentioned earlier, we will be studying throughout this chapter the shape differentiability properties of harmonic fields using pullbacks onto a fixed reference domain, that is, differentiability of maps of the form $V \mapsto \Phi_V B(\Omega_V)$. Using a simplified framework, we will understand in this section how the choice of pullback affects the resulting notion of shape derivative.

Let M be a smooth manifold. Given a diffeomorphism Φ of M and T a (p, q) tensor field over M^2 , we define the pullback of T by Φ as

$$\Phi^* T(\omega_1, \dots, \omega_p, X_1, \dots, X_q) = T(\Phi^* \omega_1, \dots, \Phi^* \omega_p, (\Phi^{-1})_* X_1, \dots, (\Phi^{-1})_* X_q).$$

Given V a complete vector field of M and e^{tV} its flow at time t , we then define the Lie derivative of T in the direction V as

$$\mathcal{L}_V T = \frac{d}{dt} \Big|_{t=0} (e^{tV})^* T.$$

One verifies that we then recover usual formulas for Lie derivatives, that is, for vector fields

$$\mathcal{L}_V X = [V, X],$$

2. Vector fields correspond to $(p, q) = (1, 0)$ and k -forms to $(p, q) = (0, k)$

is the Lie bracket, and for k -forms

$$\mathcal{L}_V \omega = \iota_V d\omega + d\iota_V \omega, \quad (2.1)$$

is Cartan's formula. If $t \mapsto T_t$ is now a differentiable path of tensor fields, we obtain

$$\frac{d}{dt} \Big|_{t=0} (e^{tV})^* T_t = \mathcal{L}_V T_0 + \frac{d}{dt} \Big|_{t=0} T_t. \quad (2.2)$$

We refer to the derivative of $t \mapsto T_t$ as the *Eulerian* derivative, and the derivative of $t \mapsto (e^{tV})^* T_t$ as the *Lagrangian* derivative. We then observe that the Lagrangian derivative decomposes as the sum of a transport term, given by the Lie derivative, and of the Eulerian derivative.

Suppose now that \mathcal{O} is a collection of admissible open sets of M , and that to each Ω in \mathcal{O} , one may associate a (p, q) tensor field $T(\Omega)$ of Ω . Assuming that, given Ω in \mathcal{O} , the mapping $V \mapsto (I + V)^* T(\Omega_V)$ is differentiable with differential $T'(\Omega; V)$, we define in analogy with Eq. (2.2)

$$T'_{\mathcal{E}}(\Omega; V) := T'(\Omega; V) - \mathcal{L}_V T(\Omega),$$

as the Eulerian derivative of $\Omega \mapsto T(\Omega)$. That is, since we use a pullback to define the shape differential, we obtain a derivative analogous to the Lagrangian one. We therefore subtract the Lie derivative in order to obtain the Eulerian one.

As was explained earlier, we have three natural ways of viewing harmonic fields, which lead to three notions of pullbacks and shape derivatives. What we will observe in the main results of the chapter is that the Eulerian derivative of the harmonic fields does not depend on how we choose our pullbacks. Using the identifications in three-dimensional manifolds given in Section 1.3.1 as well as Cartan's formula, we have the following notions of Lie derivatives which correspond respectively to Φ_V^{vf} , Φ_V^1 and Φ_V^2

$$\begin{aligned} \mathcal{L}_V^{\text{vf}} u &= [V, u], \\ \mathcal{L}_V^1 u &= \nabla(u \cdot V) + \text{curl } u \times V, \\ \mathcal{L}_V^2 u &= \text{curl}(u \times V) + (\text{div } u) V. \end{aligned}$$

The Eulerian derivatives of the harmonic field are then given by

$$\begin{aligned} B'_{\mathcal{E}, \text{vf}}(\Omega; V) &= B'_{\text{vf}}(\Omega; V) - [V, u], \\ B'_{\mathcal{E}, 1}(\Omega; V) &= B'_1(\Omega; V) - \nabla(B(\Omega) \cdot V), \\ B'_{\mathcal{E}, 2}(\Omega; V) &= B'_2(\Omega; V) - \text{curl}(B(\Omega) \times V), \end{aligned}$$

where $B'_{\text{vf}}(\Omega; V)$, $B'_1(\Omega; V)$ and $B'_2(\Omega; V)$ correspond respectively to the differentials of $V \mapsto \Phi_V^{\text{vf}} B(\Omega_V)$, $V \mapsto \Phi_V^1 B(\Omega_V)$ and $V \mapsto \Phi_V^2 B(\Omega_V)$ at zero. In the latter two cases, we will see in this chapter that, when we have sufficient regularity to define these objects, the Eulerian derivatives is equal to ∇u_V where u_V solves

$$\begin{cases} \Delta u_V = 0 & \text{in } \Omega, \\ \nabla u_V \cdot n = \text{div}_{\Gamma}(B(\Omega)(V \cdot n)) & \text{on } \partial\Omega. \end{cases}$$

The author also notes that shape differentiation using a differential form language was also studied in [HL13], although the chosen approach and the problems considered differ from our context.

2.1.2 Contents of the chapter

This chapter is organized as follows.

- In Section 2.2.1, we introduce the necessary Sobolev spaces as well as some geometrical constructions in Lipschitz toroidal domains which will be used throughout the chapter. In Section 2.2.2, we introduce two variational formulations for the harmonic fields. The first one, which was already used for example in [Amr+98; Alo+18], corresponds to a slight adaptation of classical Poisson equations with Neumann boundary conditions. The second one is given by a mixed formulation of the Poisson equation. For the first (resp. second) formulation, the natural functional space is $H(\text{curl}, \Omega)$ (resp. $H_0(\text{div}, \Omega)$), which behaves well when identifying vector fields as one-forms (resp. two-forms).
- In Section 2.3, we define rigorously the transformations Φ_V^k for k in $\{0, 1, 2, 3\}$, and prove some useful properties. As mentioned earlier, these transformations correspond to usual pullbacks of differential forms. As such, the required properties, such as commutativity with differential operators, preservation of the circulations (resp. fluxes) by Φ_V^1 (resp. Φ_V^2) are not surprising. However, we prove these results assuming as little regularity as possible, so that these properties are not immediate.
- In Section 2.4, we prove that for Ω a Lipschitz toroidal domain, the mapping $V \mapsto \Phi_V^2 B(\Omega_V)$ is smooth at zero in $H_0(\text{div}, \Omega)$. We also provide a formula for its differential $B_2'(\Omega; V)$ assuming some further regularity on the domain Ω . The shape differentiability is obtained using a classical implicit function argument with a pulled back version of the mixed formulation for the harmonic field. The expression of the shape derivative then comes from differentiating this variational formulation and using formulas proved in Section 2.3.
- In Section 2.5, we prove that for Ω a smooth toroidal domain, the mapping $V \mapsto \Phi_V^1 B(\Omega_V)$ is smooth in Sobolev spaces with higher regularity. The proof strategy is essentially the same as in Section 2.5, except that the implicit function argument is adapted using classical results of elliptic regularity to work with stronger norms. In this context, seeing the harmonic field as a one-form is convenient, as this naturally leads to more classical variational formulations used in elliptic regularity theory.

2.2 Harmonic fields in toroidal domains

2.2.1 Toroidal domains

We recall the definitions of the following classical functional spaces:

$$\begin{aligned} H(\text{curl}, \Omega) &= \{u \in L^2(\Omega)^3 \mid \text{curl } u \in L^2(\Omega)^3\}, \\ H(\text{div}, \Omega) &= \{u \in L^2(\Omega)^3 \mid \text{div } u \in L^2(\Omega)\}. \end{aligned} \quad (2.3)$$

On $H(\text{curl}, \Omega)$ and $H(\text{div}, \Omega)$, the tangential and normal traces $u \times n : \partial\Omega \rightarrow \mathbb{R}^3$ and $u \cdot n : \partial\Omega \rightarrow \mathbb{R}$ are defined respectively by

$$\int_{\partial\Omega} (u \times n) \cdot \varphi = \int_{\Omega} u \cdot \text{curl } \varphi - \int_{\Omega} \text{curl } u \cdot \varphi, \quad (2.4)$$

for every φ in $H^1(\Omega)^3$, and

$$\int_{\partial\Omega} (u \cdot n) \varphi = \int_{\Omega} u \cdot \nabla \varphi + \int_{\Omega} (\text{div } u) \varphi, \quad (2.5)$$

for every φ in $H^1(\Omega)$. Since the traces of $H^1(\Omega)^3$ and $H^1(\Omega)$ are $H^{1/2}(\partial\Omega)^3$ and $H^{1/2}(\partial\Omega)$ respectively, $u \times n$ can be defined in $H^{-1/2}(\partial\Omega)^3$, and $u \cdot n$ in $H^{-1/2}(\partial\Omega)$. Then, we can define

$$\begin{aligned} H_0(\text{curl}, \Omega) &= \{u \in H(\text{curl}, \Omega) \mid u \times n = 0\}, \\ H_0(\text{div}, \Omega) &= \{u \in H(\text{div}, \Omega) \mid u \cdot n = 0\}. \end{aligned} \quad (2.6)$$

We also denote by $L_0^2(\Omega)$ the set of functions in $L^2(\Omega)$ which have zero average in Ω . Introducing the following spaces where the differential operator vanishes will also prove to be useful

$$\begin{aligned} H(\text{curl}^0, \Omega) &= \{u \in H(\text{curl}, \Omega) \mid \text{curl } u = 0\}, \\ H(\text{div}^0, \Omega) &= \{u \in H(\text{div}, \Omega) \mid \text{div } u = 0\}, \\ H_0(\text{curl}^0, \Omega) &= H(\text{curl}^0, \Omega) \cap H_0(\text{curl}, \Omega), \\ H_0(\text{div}^0, \Omega) &= H(\text{div}^0, \Omega) \cap H_0(\text{div}, \Omega). \end{aligned} \quad (2.7)$$

We introduce a poloidal cut Σ of Ω , that is, a Lipschitz surface included in Ω , with boundary γ contained in $\partial\Omega$ which generates the first homology group of $\Omega^c = \mathbb{R}^3 \setminus \Omega$. Similarly, we introduce Σ' a Lipschitz surface in Ω^c with boundary γ' that generates the first homology group of $\bar{\Omega}$. Fig. 2.1 illustrates these objects. We refer to γ as a poloidal loop of Ω , and to γ' as a toroidal loop.

We also define t (resp. t') as a unit tangent vector field on γ (resp. γ'), and n_Σ (resp. $n_{\Sigma'}$) as a unit normal vector field on Σ (resp. Σ'). These vector fields define orientations on Σ , Σ' , γ and γ' which are compatible with each other. We refer to [Alo+18, Section 1] and [Amr+98, Section 3.a] for the constructions and more precise definitions of these objects.

Since $\Omega \setminus \Sigma$ is a pseudo-Lipschitz domain (see e.g. [Amr+98, Definition 3.1]), we can define two traces on Σ of functions in $H^1(\Omega \setminus \Sigma)$. For u in $H^1(\Omega \setminus \Sigma)$, $u|_{\Sigma^-}$ is the trace of u when approaching Σ in the direction of n_Σ , and $u|_{\Sigma^+}$ when approaching Σ in the other direction. We then define $\llbracket u \rrbracket_\Sigma = u|_{\Sigma^+} - u|_{\Sigma^-}$, which is a function of $H^{1/2}(\Sigma)$ representing the jump of u across Σ , and for c in \mathbb{R}

$$V_c(\Omega \setminus \Sigma) = \{u \in H^1(\Omega \setminus \Sigma) \mid \llbracket u \rrbracket_\Sigma = c\}.$$

We then have the identification $H^1(\Omega) \cong V_0(\Omega \setminus \Sigma)$. For u in $H^1(\Omega \setminus \Sigma)$, we also denote $\tilde{\nabla} u$ as the L^2 extension of ∇u on Ω . It is then known that v is in $H(\text{curl}^0, \Omega)$ if and only if there exists c in \mathbb{R} and u in $V_c(\Omega \setminus \Sigma)$ such that $v = \tilde{\nabla} u$ [Amr+98][Lemma 3.11].

Finally, we recall some results on the notion of s -regularity (see for example [AFW06, Section 7.8]). We say that a domain Ω is s -regular if $H_0(\text{div}, \Omega) \cap H(\text{curl}, \Omega)$ continuously injects in $H^s(\Omega)$, when equipped with the norm

$$\|u\|^2 = \|u\|_{L^2}^2 + \|\text{div } u\|_{L^2}^2 + \|\text{curl } u\|_{L^2}^2.$$

It is then known that Lipschitz domains are 1/2-regular, that polyhedral domains are s -regular for $1/2 < s \leq 1$, and that $\mathcal{C}^{1,1}$ domains are 1-regular.

3. In fact, as was shown in [BCS02], the space of tangential traces of $H(\text{curl}, \Omega)$ is $H^{-1/2}(\text{div}_\Gamma, \partial\Omega)$, so that it is a proper subspace of $H^{-1/2}(\partial\Omega)^3$.

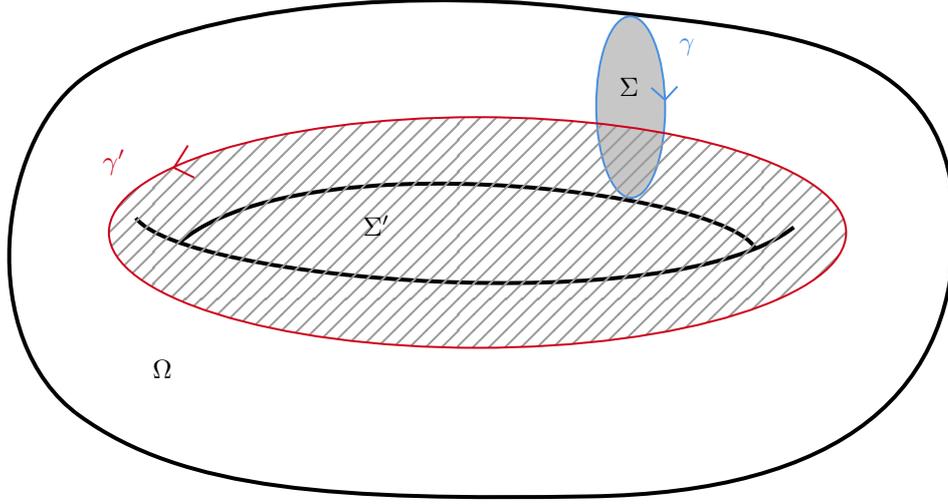


Figure 2.1 – Illustration of the curves γ and γ' , and the surfaces Σ and Σ'

2.2.2 Variational formulations for harmonic fields

The set of harmonic fields in Ω is defined in the following way

$$\begin{aligned} \mathcal{K}(\Omega) &= \{u \in L^2(\Omega)^3 \mid \operatorname{div} u = 0, \operatorname{curl} u = 0, u \cdot n = 0\} \\ &= H(\operatorname{curl}^0, \Omega) \cap H_0(\operatorname{div}^0, \Omega), \end{aligned} \quad (2.8)$$

As was explained in Section 1.3.1, this space is isomorphic to the first de Rham cohomology space of Ω , with each harmonic field giving a natural representative of the corresponding cohomology class. Another useful characterization is the following

$$\mathcal{K}(\Omega) = H(\operatorname{curl}^0, \Omega) \cap \nabla H^1(\Omega)^\perp.$$

Indeed, one can easily see using Eq. (2.5) that $H_0(\operatorname{div}^0, \Omega) = \nabla H^1(\Omega)^\perp$.

Hence, as shown in [Amr+98, Proposition 3.14], we can define the normalized harmonic field $B(\Omega)$ on Ω by $B(\Omega) = \tilde{\nabla} u$ with $u \in H^1(\Omega \setminus \Sigma)$ defined as follows. u is the unique solution of the variational problem. Find u in $V_1(\Omega \setminus \Sigma)$ such that, for all v in $H^1(\Omega)$

$$\int_{\Omega \setminus \Sigma} \nabla u \cdot \nabla v = 0, \quad (2.9)$$

for all $v \in H^1(\Omega)$.

Remark 2.2.1. *Although this characterization of the normalized harmonic field makes use of Σ , choosing another cutting surface may change B only up to a sign. Indeed, B is in $\mathcal{K}(\Omega)$ which is one-dimensional. Therefore, changing Σ may change B only by multiplying it by a constant. Furthermore, since B integrates to 1 along γ' , we see that this constant is equal to 1 if we preserve the orientation of Σ and γ' , and equal to -1 otherwise.*

Once we have the normalized harmonic field of Ω , we can define rigorously the circulation of vector fields in $H(\operatorname{curl}, \Omega)$ with curl tangent to the boundary. To do this, we define similarly

the harmonic field of $\Omega^{\text{ext}} = \mathcal{B} \cap \bar{\Omega}^c$, denoted B^{ext} , where \mathcal{B} is an open ball containing $\bar{\Omega}$. The normalized harmonic field of Ω^{ext} is the gradient of $u^{\text{ext}} \in V_1(\Omega^{\text{ext}} \setminus \Sigma')$, which verifies

$$\int_{\Omega^{\text{ext}} \setminus \Sigma'} \nabla u^{\text{ext}} \cdot \nabla v = 0, \quad (2.10)$$

for all v in $H^1(\Omega^{\text{ext}})$. Then, as in [Alo+18, Section 2], we are able to define the circulations of a vector field u in $H(\text{curl}, \Omega)$ with curl tangent to the boundary as

$$\int_{\gamma'} u \cdot t' = \int_{\Omega^{\text{ext}}} \text{curl } \tilde{u} \cdot B^{\text{ext}}, \quad (2.11)$$

$$\int_{\gamma} u \cdot t = \int_{\Omega} \text{curl } u \cdot B(\Omega), \quad (2.12)$$

where \tilde{u} is a continuous extension of u from $H(\text{curl}, \Omega)$ to $H(\text{curl}, \mathcal{B})$. Similarly, we can also write

$$\int_{\gamma'} u \cdot t' = - \int_{\partial\Omega} (u \times n) \cdot B^{\text{ext}}, \quad (2.13)$$

$$\int_{\gamma} u \cdot t = - \int_{\partial\Omega} (u \times n) \cdot B(\Omega). \quad (2.14)$$

Since these definitions of circulations correspond to the usual one for vector fields in $\mathcal{C}^\infty(\bar{\Omega} \setminus \bar{\Sigma})$, it is clear by density that for all u in $V_c(\Omega \setminus \Sigma)$, we have

$$\int_{\gamma'} \tilde{\nabla} u \cdot t' = c.$$

In particular, we recover that the toroidal circulation of $B(\Omega)$ is equal to one. Furthermore, since $H(\text{curl}^0, \Omega) = \cup_{c \in \mathbb{R}} \tilde{\nabla} V_c(\Omega \setminus \Sigma)$ (see [Amr+98, Lemma 3.11]), we obtain that a vector field of $H(\text{curl}^0, \Omega)$ is the gradient of a function in $H^1(\Omega)$ if and only if its circulation along γ' is zero.

Note that the definition of the normalized harmonic field in Eq. (2.9) is equivalent to the following mixed formulation. Since the variational space for the harmonic field in this formulation is $H_0(\text{div}, \Omega)$, it will prove to be useful when studying the shape derivative of the harmonic fields when pulled back as two-forms in Section 2.4.

Proposition 2.2.2. *There exists a unique solution to the following problem. Find $(B_{\text{div}}, u_{\text{div}}) \in H_0(\text{div}, \Omega) \times L_0^2(\Omega)$ such that, for all $(\tau, v) \in H_0(\text{div}, \Omega) \times L^2(\Omega)$ we have*

$$\begin{aligned} \int_{\Omega} (\text{div } B_{\text{div}}) v &= 0, \\ \int_{\Omega} B_{\text{div}} \cdot \tau + \int_{\Omega} u_{\text{div}} (\text{div } \tau) &= \int_{\Sigma} \tau \cdot n_{\Sigma}. \end{aligned} \quad (2.15)$$

Furthermore, we have $B_{\text{div}} = B(\Omega)$.

Proof. The left-hand side of Eq. (2.15) is the bilinear form for the mixed formulation of the Poisson equation with Neumann boundary conditions. As such, it is known to verify inf-sup conditions (see for example [EG21b, Section 51.1]), so that one only needs to prove the continuity of the linear form in the right-hand side to prove well-posedness. This can be obtained by

continuity of the normal trace from $H(\operatorname{div}, \Omega)$ to $H^{-1/2}(\Sigma)$. As a consequence, we get

$$\begin{aligned} \left| \int_{\Sigma} \tau \cdot n_{\Sigma} \right| &\leq \|1\|_{H^{1/2}(\Sigma)} \|\tau \cdot n_{\Sigma}\|_{H^{-1/2}(\Sigma)} \\ &\leq C \|\tau\|_{H(\operatorname{div}, \Omega)}. \end{aligned}$$

To prove that B_{div} and $B(\Omega)$ coincide, we show that B_{div} is a harmonic field, and that they are normalized in the same way. Equality then follows from the fact that the set of harmonic fields is one-dimensional. To find that B_{div} is a harmonic field, we prove it is orthogonal to $\nabla H^1(\Omega)$ and $\operatorname{curl} H_0(\operatorname{curl}, \Omega)$.

The first fact follows from the first equation of (2.15). Indeed, we find that $\operatorname{div} B_{\operatorname{div}} = 0$, so that $B_{\operatorname{div}} \in H_0(\operatorname{div}^0, \Omega) = \nabla H^1(\Omega)^{\perp}$.

Now, take $\tau = \operatorname{curl} \sigma$ in the second equation of (2.15), with $\sigma \in H_0(\operatorname{curl}, \Omega)$. As a consequence, we have $\operatorname{div} \tau = 0$, and

$$\int_{\Sigma} \tau \cdot n_{\Sigma} = \int_{\gamma} \sigma \cdot t = 0.$$

This gives us $\int_{\Omega} B_{\operatorname{div}} \cdot \tau = 0$ for all $\tau \in \operatorname{curl} H_0(\operatorname{curl}, \Omega)$. Since B_{div} is orthogonal to both $\nabla H^1(\Omega)$ and $\operatorname{curl} H_0(\operatorname{curl}, \Omega)$, we get that it is a harmonic field by Hodge decomposition (see Proposition A.1 of Appendix A).

Finally, we set $B_{\operatorname{div}} = \lambda B(\Omega)$, and want to prove that $\lambda = 1$. First, by plugging $\tau = B_{\operatorname{div}}$ in Eq. (2.15), we get

$$\|B_{\operatorname{div}}\|^2 = \int_{\Sigma} B_{\operatorname{div}} \cdot n_{\Sigma}.$$

Now, using the jump condition on u as defined in Eq. (2.9), and an integration by parts, we get

$$\begin{aligned} \|B(\Omega)\|^2 &= \int_{\Omega \setminus \Sigma} B(\Omega) \cdot \nabla u \\ &= \int_{\Sigma} B(\Omega) \cdot n_{\Sigma}. \end{aligned}$$

Now, on the one side we have

$$\int_{\Sigma} B_{\operatorname{div}} \cdot n_{\Sigma} = \lambda \int_{\Sigma} B(\Omega) \cdot n_{\Sigma},$$

and on the other side

$$\begin{aligned} \int_{\Sigma} B_{\operatorname{div}} \cdot n_{\Sigma} &= \|B_{\operatorname{div}}\|^2 \\ &= \lambda^2 \|B(\Omega)\|^2 \\ &= \lambda^2 \int_{\Sigma} B(\Omega) \cdot n_{\Sigma}. \end{aligned}$$

Since $B(\Omega)$ and B_{div} are both nonzero, we come to the conclusion that $\lambda = 1$. \square

2.3 Pullbacks on the de Rham complex

In this section, we define maps which allow us to transform elements of our functional spaces on a deformed domain Ω_V back to Ω . These transformations correspond to pullbacks in the language of differential forms, and their formulas are given by the Piola mappings, which are often encountered in finite element exterior calculus. This non-naive treatment is needed as composition by $I + V$ does not map $H(\text{curl}, \Omega_V)$ (resp. $H(\text{div}, \Omega_V)$) to $H(\text{curl}, \Omega)$ (resp. $H(\text{div}, \Omega)$).

For $k \geq 1$, we define

$$\mathcal{B}_k = \{V \in W^{k,\infty}(\mathbb{R}^3)^3 \mid \|DV\|_{L^\infty} < 1\},$$

where DV denotes the Jacobian matrix of V in Cartesian coordinates, and we use an operator norm on matrices. It is then clear that, for V in \mathcal{B}_k , $I + V$ is a $W^{k,\infty}$ diffeomorphism of \mathbb{R}^3 . Throughout this section, Ω is a Lipschitz toroidal domain as defined in Section 2.2.1. As a consequence, $\Omega_V = (I + V)(\Omega)$ is also a Lipschitz toroidal domain for V in \mathcal{B}_1 , and the curves γ_V , γ'_V and surfaces Σ_V , Σ'_V are given by the image by $I + V$ of the corresponding objects in Ω .

Definition 2.3.1. *Let u_0 and u_3 be in $L^p(\Omega_V)$, u_1 and u_2 be in $L^p(\Omega_V)^3$ for p in $[1, \infty]$, and V be in \mathcal{B}_1 . We define*

$$\begin{aligned}\Phi_V^0 u_0 &= u_0 \circ (I + V), \\ \Phi_V^1 u_1 &= (I + DV^T) u_1 \circ (I + V), \\ \Phi_V^2 u_2 &= J_V (I + DV)^{-1} u_2 \circ (I + V), \\ \Phi_V^3 u_3 &= J_V u_3 \circ (I + V).\end{aligned}$$

where $J_V := \det(I + DV)$.

Before giving the key properties of these transformations, we start by stating the following useful algebraic identities. These can be found by direct computations.

Lemma 2.3.2. *We have the following identities.*

$$\begin{aligned}(\Phi_V^0 u) (\Phi_V^3 v) &= \Phi_V^3 (uv) && \forall u, v \in L^2(\Omega_V), \\ (\Phi_V^1 u) \cdot (\Phi_V^2 v) &= \Phi_V^3 (u \cdot v) && \forall u, v \in L^2(\Omega_V)^3, \\ (\alpha(V) \Phi_V^1 u) \cdot (\Phi_V^1 v) &= \Phi_V^3 (u \cdot v) && \forall u, v \in L^2(\Omega_V)^3, \\ (\alpha(V)^{-1} \Phi_V^2 u) \cdot (\Phi_V^2 v) &= \Phi_V^3 (u \cdot v) && \forall u, v \in L^2(\Omega_V)^3,\end{aligned}$$

where $\alpha(V) = J_V (I + DV)^{-1} (I + DV^T)^{-1}$.

Proposition 2.3.3. *Let c be a real number. The diagram*

$$\begin{array}{ccccccc} V_c(\Omega_V \setminus \Sigma_V) & \xrightarrow{\tilde{\nabla}} & H(\text{curl}, \Omega_V) & \xrightarrow{\text{curl}} & H(\text{div}, \Omega_V) & \xrightarrow{\text{div}} & L^2(\Omega_V) \\ \Phi_V^0 \downarrow & & \Phi_V^1 \downarrow & & \Phi_V^2 \downarrow & & \Phi_V^3 \downarrow \\ V_c(\Omega \setminus \Sigma) & \xrightarrow{\tilde{\nabla}} & H(\text{curl}, \Omega) & \xrightarrow{\text{curl}} & H(\text{div}, \Omega) & \xrightarrow{\text{div}} & L^2(\Omega) \end{array}$$

is commutative. Furthermore, the same diagram can be made when $c = 0$ with the corresponding traceless spaces.

Proof. We begin by proving the commutativity of the first cell of the diagram. First, from [Amr+98][Lemma 3.11], we know that $\tilde{\nabla}$ maps $V_c(\Omega_V \setminus \Sigma_V)$ to $H(\text{curl}^0, \Omega_V)$. Then, if u is in

$H^1(\Omega_V \setminus \Sigma_V)$, $\Phi_V^0 u = u \circ (I+V)$ is in $H^1(\Omega \setminus \Sigma)$ as $I+V$ is a Lipschitz diffeomorphism. Furthermore, it is clear that $[[u]]_{\Sigma_V} \circ (I+V) = [[\Phi_V^0 u]]_{\Sigma}$, so that Φ_V^0 maps $V_c(\Omega_V \setminus \Sigma_V)$ to $V_c(\Omega \setminus \Sigma)$. We also have, using the composition formula for Jacobians, that

$$D(\Phi_V^0 u) = Du \circ (I+V)(I+DV),$$

so that, since $\nabla \Phi_V^0 u = D(\Phi_V^0 u)^T$, we obtain

$$\begin{aligned} \nabla \Phi_V^0 u &= (I+DV^T) \nabla u \circ (I+V) \\ &= \Phi_V^1 \nabla u. \end{aligned}$$

For the rest of the proof, we use smooth functions or vector fields u , and suppose that V is smooth for simplicity. The general statements can then be obtained by density, and continuity of the desired equalities with respect to the relevant norms.

We now prove that $\text{curl} \circ \Phi_V^1 = \Phi_V^2 \circ \text{curl}$ by taking u in $\mathcal{C}^\infty(\bar{\Omega}_V)^3$. We have

$$\begin{aligned} D(\Phi_V^1 u) &= D((I+DV^T)u \circ (I+V)) \\ &= D(DV^T)u \circ (I+V) + (I+DV^T)Du \circ (I+V)(I+DV), \end{aligned}$$

where $D(DV^T)u$ is a symmetric matrix given by

$$(D(DV^T)u)_{i,j} = \sum_{k=1}^3 \frac{\partial^2 V^k}{\partial x^i \partial x^j} u_k,$$

Therefore, we find

$$D(\Phi_V^1 u) - (D(\Phi_V^1 u))^T = (I+DV^T)(Du - Du^T) \circ (I+V)(I+DV).$$

Now, defining $\text{cr} : \mathfrak{so}(3) \rightarrow \mathbb{R}^3$, where $\mathfrak{so}(3)$ is the space of skew-symmetric matrices, by

$$\text{cr} \begin{pmatrix} 0 & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix},$$

we can prove that, for any invertible matrix B and skew-symmetric matrix A , $\text{cr}(B^T A B) = \det(B)B^{-1}\text{cr}(A)$. Since $\text{curl} u = \text{cr}(Du - Du^T)$, we find

$$\begin{aligned} \text{curl} \Phi_V^1 u &= J_V (I+DV)^{-1} \text{curl} u \circ (I+V) \\ &= \Phi_V^2 \text{curl} u. \end{aligned}$$

For the last commutativity relation $\text{div} \circ \Phi_V^2 = \Phi_V^3 \circ \text{div}$, we proceed by duality. Take u in $\mathcal{C}^\infty(\bar{\Omega}_V)^3$ and v in $\mathcal{C}_0^\infty(\Omega_V)$. First, we notice that the Φ_V^k are isomorphisms, as $(\Phi_V^k)^{-1} = \Phi_{(I+V)^{-1} \circ \Gamma}^k$. Therefore,

$$\begin{aligned} \int_{\Omega} (\text{div} \Phi_V^2 u) v &= - \int_{\Omega} (\Phi_V^2 u) \cdot \nabla v \\ &= - \int_{\Omega} (\Phi_V^2 u) \cdot \left[\Phi_V^1 \left(\nabla (\Phi_V^0)^{-1} v \right) \right], \end{aligned}$$

where we used $\Phi_V^1 \nabla v = \nabla \Phi_V^0 v$. Using Lemma 2.3.2, we then find

$$\begin{aligned} \int_{\Omega} (\operatorname{div} \Phi_V^2 u) v &= - \int_{\Omega} \Phi_V^3 \left(u \cdot \nabla (\Phi_V^0)^{-1} v \right) \\ &= - \int_{\Omega_V} u \cdot \nabla (\Phi_V^0)^{-1} v \\ &= \int_{\Omega_V} \operatorname{div} u \cdot (\Phi_V^0)^{-1} v \\ &= \int_{\Omega} (\Phi_V^3 \operatorname{div} u) v. \end{aligned}$$

Now, we prove that traceless functions or vector fields are preserved by the maps Φ_V^k . For $k = 0$, we simply take $u \in \mathcal{C}_0^\infty(\Omega)$, and verify that $u \circ (\mathbf{I} + V)$ is in $H_0^1(\Omega)$. We then find the desired result by density.

The proofs for $k = 1$ and $k = 2$ being similar, we only write the first one. Take u in $H_0(\operatorname{curl}, \Omega_V)$ and v in $H(\operatorname{curl}, \Omega)$. Then, we have

$$\begin{aligned} \int_{\partial\Omega} ((\Phi_V^1 u) \times n) \cdot v &= \int_{\Omega} \operatorname{curl} (\Phi_V^1 u) \cdot v - \int_{\Omega} (\Phi_V^1 u) \cdot \operatorname{curl} v \\ &= \int_{\Omega} \Phi_V^2 (\operatorname{curl} u) \cdot \Phi_V^1 \left((\Phi_V^1)^{-1} v \right) - \int_{\Omega} (\Phi_V^1 u) \cdot \Phi_V^2 \left(\operatorname{curl} (\Phi_V^1)^{-1} v \right) \\ &= \int_{\Omega_V} \operatorname{curl} u \cdot \left((\Phi_V^1)^{-1} v \right) - \int_{\Omega_V} u \cdot \left(\operatorname{curl} (\Phi_V^1)^{-1} v \right) \\ &= 0, \end{aligned}$$

so that $\Phi_V^1 u$ is in $H_0(\operatorname{curl}, \Omega)$ as claimed. \square

As the Φ_V^k transformations correspond to pullbacks of k -forms, it is not surprising that Φ_V^1 preserves circulations, and Φ_V^2 preserves fluxes. This result is given by the following lemma.

Lemma 2.3.4. *Let u be in $H(\operatorname{curl}, \Omega_V)$ with $\operatorname{curl} u \cdot n = 0$, and v be in $H_0(\operatorname{div}, \Omega_V)$. We then have the following identities*

$$\begin{aligned} \int_{\gamma'_V} u \cdot t'_V &= \int_{\gamma'} \Phi_V^1 u \cdot t', \\ \int_{\Sigma_V} v \cdot n_{\Sigma_V} &= \int_{\Sigma} \Phi_V^2 v \cdot n_{\Sigma}. \end{aligned}$$

Proof. For the first equality, we suppose that u is smooth so that we can study the circulation in the usual sense. The general case then follows from a density argument, and the continuity of the circulation as defined in [Alo+18, Section 2] with respect to the $H(\operatorname{curl}, \Omega)$ norm. We identify γ' with a Lipschitz embedding $\gamma' : S^1 \rightarrow \partial\Omega$, so that the derivative $\dot{\gamma}'(s)$ is defined for a.e. $s \in S^1$. γ'_V is then identified as the embedding $(\mathbf{I} + V) \circ \gamma'$, for which the derivative is given by

$$\dot{\gamma}'_V = ((\mathbf{I} + DV) \circ \gamma') \dot{\gamma}'.$$

The circulation of u along γ'_V is then given by

$$\int_{\gamma'_V} u \cdot t'_V = \int_{S^1} [u \circ \gamma'_V](s) \cdot \dot{\gamma}'_V(s) ds.$$

Using the formula for γ'_V and its derivative as an embedding, we get

$$\begin{aligned} \int_{\gamma'_V} u \cdot t'_V &= \int_{S^1} [u \circ (\mathbf{I} + V) \circ \gamma'] (s) \cdot [((\mathbf{I} + DV) \circ \gamma') \dot{\gamma}'] (s) ds \\ &= \int_{S^1} [(\mathbf{I} + DV^T) u \circ (\mathbf{I} + V)] \circ \gamma'(s) \cdot \dot{\gamma}'(s) ds \\ &= \int_{\gamma'} \Phi_V^1 u \cdot t'. \end{aligned}$$

For the second equality, we choose $v \in H_0(\operatorname{div}, \Omega_V)$ and use the following equality given in [Alo+18, Lemma 1] for $\psi \in H^1(\Omega_V \setminus \Sigma_V)$

$$\int_{\Sigma_V} v \cdot n_{\Sigma_V} [\psi]_{\Sigma_V} = \int_{\Omega_V \setminus \Sigma_V} v \cdot \nabla \psi + \int_{\Omega_V \setminus \Sigma_V} (\operatorname{div} v) \psi. \quad (2.16)$$

Taking $\psi = u(\Omega_V)$ in $V_1(\Omega_V \setminus \Sigma_V)$ to be the solution of Eq. (2.9) in Ω_V , we get

$$\begin{aligned} \int_{\Sigma_V} v \cdot n_{\Sigma_V} &= \int_{\Omega_V \setminus \Sigma_V} v \cdot \nabla u(\Omega_V) + \int_{\Omega_V \setminus \Sigma_V} (\operatorname{div} v) u(\Omega_V) \\ &= \int_{\Omega \setminus \Sigma} (\Phi_V^2 v) \cdot \nabla (\Phi_V^0 u(\Omega_V)) + \int_{\Omega \setminus \Sigma} (\operatorname{div} \Phi_V^2 v) (\Phi_V^0 u(\Omega_V)) \\ &= \int_{\Sigma} (\Phi_V^2 v) \cdot n_{\Sigma} [[\Phi_V^0 u(\Omega_V)]]_{\Sigma}. \end{aligned}$$

From Proposition 2.3.3, we have that $\Phi_V^0 u(\Omega_V)$ is in $V_1(\Omega \setminus \Sigma)$ so that $[[\Phi_V^0 u(\Omega_V)]]_{\Sigma} = 1$, which proves the desired equality. \square

We know from Lemma 2.3.2 that when we pullback products in $H(\operatorname{curl}, \Omega)$ or $H(\operatorname{div}, \Omega)$, there is a non-homogeneous term $\alpha(V)$ which appears. We will have to consider such products in the next sections to differentiate the variational formulations of the harmonic fields. The next lemma shows how $V \mapsto \alpha(V)$ behaves under differentiation when integrated against products of vector fields.

Lemma 2.3.5. *Let k be a non-negative integer. Then, the mapping $V \mapsto \alpha(V)$ from \mathcal{B}_{k+1} to $W^{k, \infty}(\mathbb{R}^3; \mathcal{M}_3(\mathbb{R}))$ defined in Lemma 2.3.2 is smooth. Furthermore, denoting its differential at zero by $\alpha'(0; V)$, we have:*

- If u and v are in $H_0(\operatorname{div}, \Omega) \cap H(\operatorname{curl}, \Omega)$ and Ω is 1-regular

$$\begin{aligned} \int_{\Omega} (\alpha'(0; V)u) \cdot v &= \int_{\Omega} (\operatorname{div} u)V \cdot v + \int_{\Omega} \operatorname{curl}(u \times V) \cdot v - \int_{\Omega} (\operatorname{curl} u) \times V \cdot v \\ &\quad + \int_{\Omega} (\operatorname{div} v)u \cdot V. \end{aligned} \quad (2.17)$$

- If u is in $H_0(\operatorname{div}, \Omega) \cap H(\operatorname{curl}, \Omega)$, v is in $H(\operatorname{curl}, \Omega)$ and Ω is 1-regular

$$\begin{aligned} \int_{\Omega} (\alpha'(0; V)u) \cdot v &= \int_{\Omega} (\operatorname{div} u)V \cdot v + \int_{\Omega} (u \times V) \cdot \operatorname{curl} v - \int_{\partial\Omega} (u \times V) \times n \cdot v \\ &\quad - \int_{\Omega} (\operatorname{curl} u) \times V \cdot v - \int_{\Omega} \nabla(u \cdot V) \cdot v. \end{aligned} \quad (2.18)$$

- If u and v are in $H_0(\operatorname{div}, \Omega) \cap H(\operatorname{curl}, \Omega)$ and Ω is s -regular with $s > 1/2$

$$\begin{aligned} \int_{\Omega} (\alpha'(0; V)u) \cdot v &= \int_{\Omega} (\operatorname{div} u)V \cdot v + \int_{\Omega} (u \times V) \cdot \operatorname{curl} v + \int_{\partial\Omega} (u \cdot v)(V \cdot n) \\ &\quad - \int_{\Omega} (\operatorname{curl} u) \times V \cdot v + \int_{\Omega} (\operatorname{div} v)u \cdot V. \end{aligned} \quad (2.19)$$

Proof. We recall that $\alpha(V) = J_V(\mathbf{I} + DV)^{-1}(\mathbf{I} + DV^T)^{-1}$. To find that α is smooth, we simply notice that the maps defined on the unit ball of $\mathcal{M}_3(\mathbb{R})$ given by $A \mapsto (\mathbf{I} + A)^{-1}$, $A \mapsto (\mathbf{I} + A^T)^{-1}$ and $A \mapsto \det(\mathbf{I} + A)$ are smooth. We also have that $V \mapsto DV$ is linear and bounded from $W^{k+1, \infty}(\mathbb{R}^3)^3$ to $W^{k, \infty}(\mathbb{R}^3; \mathcal{M}_3(\mathbb{R}))$. We conclude by composition that α is smooth.

Using that the differential of the determinant and the inverse at the identity are, respectively, the trace and minus the identity, we find

$$\alpha'(0; V) = (\operatorname{div} V)\mathbf{I} - DV - DV^T.$$

To prove the different formulas, we begin by choosing u and v in $H^1(\Omega)^3$. Then, $u \cdot V$ and $u \times V$ are in H^1 , and we have

$$\begin{aligned} \nabla(u \cdot V) &= Du^T V + DV^T u, \\ \operatorname{curl}(u \times V) &= DuV - DVu - (\operatorname{div} u)V + (\operatorname{div} V)u. \end{aligned}$$

Combining these formulas, we find

$$\begin{aligned} \nabla(u \cdot V) - \operatorname{curl}(u \times V) &= -DuV + DVu + (\operatorname{div} u)V - (\operatorname{div} V)u + Du^T V + DV^T u \\ &= -\alpha'(0; V)u - (Du - Du^T)V + (\operatorname{div} u)V \\ &= -\alpha'(0; V)u - \operatorname{curl} u \times V + (\operatorname{div} u)V, \end{aligned}$$

so that

$$\alpha'(0; V)u = (\operatorname{div} u)V + \operatorname{curl}(u \times V) - \operatorname{curl} u \times V - \nabla(u \cdot V).$$

We therefore have

$$\int_{\Omega} (\alpha'(0; V)u) \cdot v = \int_{\Omega} (\operatorname{div} u)V \cdot v + \int_{\Omega} \operatorname{curl}(u \times V) \cdot v - \int_{\Omega} (\operatorname{curl} u) \times V \cdot v - \int_{\Omega} \nabla(u \cdot V) \cdot v.$$

For Eq. (2.17), Ω is assumed to be 1-regular so that $H_0(\operatorname{div}, \Omega) \cap H(\operatorname{curl}, \Omega)$ coincides with $H^1(\Omega)^3$. We find the relation using

$$\int_{\Omega} \nabla(u \times V) \cdot v = - \int_{\Omega} (\operatorname{div} v)(u \cdot V) + \int_{\partial\Omega} (v \cdot n)(u \cdot V).$$

For Eq. (2.18), we use

$$\int_{\Omega} \operatorname{curl}(u \times V) \cdot v = \int_{\Omega} (u \times V) \cdot \operatorname{curl} v - \int_{\partial\Omega} (u \times V) \times n \cdot v.$$

We then use that $u \times V$ is in $H^1(\Omega)^3$ so that its tangential trace is in $H^{1/2}(\Omega)^3$, and conclude by using the density of $H^1(\Omega)^3$ in $H(\operatorname{curl}, \Omega)$ and that the tangential trace is continuous from $H(\operatorname{curl}, \Omega)$ to $H^{-1/2}(\partial\Omega)^3$.

Finally, for Eq. (2.19), we use the two previous integration by parts formula, together with

$(u \times V) \times n = (u \cdot n)V - (V \cdot n)u$. We then conclude by density of $H^1(\Omega)^3$ in $H_0(\operatorname{div}, \Omega) \cap H(\operatorname{curl}, \Omega)$, and s -regularity with $s > 1/2$ to obtain convergence of the boundary integrals. \square

2.4 Shape differentiation as two-forms in the Lipschitz category

In this section we prove the differentiability of $V \mapsto \Phi_V^2 B_V$. As is classical in shape variation of PDEs (see for example [HP18, Chapter 5]), this is done using an implicit function argument on a pulled back version of the variational formulations. Since we are interested in the harmonic fields as two forms, we will be using the mixed formulation given by Eq. (2.15). Furthermore, we will obtain an expression for the shape derivative of $V \mapsto \Phi_V^2 B(\Omega_V)$. As expected, this is given by the sum of the Lie derivative of $B(\Omega)$ when seen as a two-form and of a "Eulerian" derivative which only depends on the normal trace of V .

Theorem 2.4.1. *The mapping*

$$\begin{cases} \mathcal{B}_1 \rightarrow H_0(\operatorname{div}, \Omega) \\ V \mapsto \Phi_V^2 B(\Omega_V) \end{cases},$$

is smooth at zero. Furthermore, if Ω is 1-regular (see Section 2.2.1), the differential of this mapping $B'_2(\Omega; V)$ is given by

$$B'_2(\Omega; V) = \operatorname{curl}(B(\Omega) \times V) + \nabla u_V,$$

where u_V verifies

$$\begin{cases} \Delta u_V = 0 & \text{in } \Omega, \\ \nabla u_V \cdot n = \operatorname{div}_\Gamma(B(\Omega)(V \cdot n)) & \text{on } \partial\Omega. \end{cases}$$

Proof. We denote by $(B(\Omega_V), u(\Omega_V))$ the solutions to Eq. (2.15) in Ω_V , that is

$$\int_{\Omega_V} B(\Omega_V) \cdot \tau + \int_{\Omega_V} u(\Omega_V) \operatorname{div} \tau = \int_{\Sigma_V} \tau \cdot n_{\Sigma_V}, \quad (2.20)$$

$$\int_{\Omega_V} \operatorname{div} B(\Omega_V) v = 0, \quad (2.21)$$

for all (τ, v) in $H_0(\operatorname{div}, \Omega_V) \times L^2(\Omega_V)$. The proof of Theorem 2.4.1 comes in two steps. First, we prove that $V \mapsto \Phi_V^2 B(\Omega_V)$ is smooth. Then, we find an expression for the differential of this mapping at zero.

Shape differentiability Pulling back Eq. (2.20) onto Ω , and using Lemmas 2.3.2, 2.3.4 and 2.3.5, we get

$$\begin{aligned} \int_{\Omega} \Phi_V^3(B(\Omega_V) \cdot \tau) + \int_{\Omega} \Phi_V^3(u(\Omega_V) \operatorname{div} \tau) &= \int_{\Sigma} (\Phi_V^2 \tau) \cdot n_{\Sigma}, \\ \int_{\Omega} (\alpha(V)^{-1} \Phi_V^2 B(\Omega_V)) \cdot (\Phi_V^2 \tau) + \int_{\Omega} (\Phi_V^0 u(\Omega_V)) (\operatorname{div} \Phi_V^2 \tau) &= \int_{\Sigma} (\Phi_V^2 \tau) \cdot n_{\Sigma}. \end{aligned} \quad (2.22)$$

Similarly, pulling back Eq. (2.21) onto Ω , we get

$$\int_{\Omega} (\operatorname{div} \Phi_V^2 B(\Omega_V)) (\Phi_V^0 v) = 0. \quad (2.23)$$

Of course, since the Φ_V^k define isomorphisms, we can take test functions (τ, v) in $H_0(\operatorname{div}, \Omega) \times L^2(\Omega)$. We now define

$$F : W^{1,\infty}(\mathbb{R}^3)^3 \times (H_0(\operatorname{div}, \Omega) \times L_0^2(\Omega)) \rightarrow (H_0(\operatorname{div}, \Omega) \times L^2(\Omega))'$$

by

$$F(V; \sigma, u)(\tau, v) = \int_{\Omega} (\alpha(V)^{-1}\sigma) \cdot \tau + \int_{\Omega} u \operatorname{div} \tau + \int_{\Omega} (\operatorname{div} \sigma) v - \int_{\Sigma} \tau \cdot n_{\Sigma},$$

so that $F(V; \Phi_V^2 B(\Omega_V), \Phi_V^0 u(\Omega_V)) = 0$.

Now, we know from Lemma 2.3.5 that $V \mapsto \alpha(V)^{-1}$ is smooth. Since $(\sigma, u) \mapsto F(V; \sigma, u)$ is linear and bounded, we deduce that F is smooth as well. Furthermore, denoting by $D_{\sigma, u} F$ the differential of F with respect to the (σ, u) variables, we have

$$D_{\sigma, u} F(0; B_0, u_0)(\sigma', u')(\tau, v) = \int_{\Omega} \sigma' \cdot \tau + \int_{\Omega} u' \operatorname{div} \tau + \int_{\Omega} (\operatorname{div} \sigma') v.$$

We therefore find that $D_{\sigma, u} F(0; B_0, u_0)$ is an isomorphism from $H_0(\operatorname{div}, \Omega) \times L_0^2(\Omega)$ to the dual space $(H_0(\operatorname{div}, \Omega) \times L^2(\Omega))'$ by the same inf-sup inequalities used to prove the well-posedness of Proposition 2.2.2. Using the implicit function theorem, we deduce that for small enough V , there is a unique smooth mapping $V \mapsto (\sigma(V), u(V))$ such that $F(V; \sigma(V), u(V)) = 0$. From uniqueness, we find that $(\sigma(V), u(V)) = (\Phi_V^2 B(\Omega_V), \Phi_V^0 u(\Omega_V))$.

Expression of the shape derivative We now wish to obtain the expression of the shape derivative of $\Phi_V^2 B(\Omega_V)$. We write the differential of $V \mapsto (\Phi_V^2 B(\Omega_V), \Phi_V^0 u(\Omega_V))$ at zero as $(B'_2(\Omega; V), u'_0(\Omega; V))$ and decompose it as

$$\begin{aligned} B'_2(\Omega; V) &= \operatorname{curl}(B(\Omega) \times V) + B'_{\mathcal{E}, 2}(\Omega; V), \\ u'_0(\Omega; V) &= B(\Omega) \cdot V + u'_{\mathcal{E}, 0}(\Omega; V). \end{aligned}$$

Assuming that Ω is 1-regular, we know that $B(\Omega)$ is in $H^1(\Omega)^3$, so that $B(\Omega) \times V$ is in $H^1(\Omega)^3$ and $B(\Omega) \cdot V$ is in $H^1(\Omega)$. Then, differentiating Eqs. (2.22) and (2.23) with respect to V and using Lemma 2.3.4 for the flux term, we obtain

$$\begin{aligned} \int_{\Omega} B'_2(\Omega; V) \cdot \tau + \int_{\Omega} u'_0(\Omega; V) \operatorname{div} \tau &= \int_{\Omega} (\alpha'(0; V) B(\Omega)) \cdot \tau, \\ \int_{\Omega} (\operatorname{div} B'_2(\Omega; V)) v &= 0, \end{aligned}$$

for all (τ, v) in $H_0(\operatorname{div}, \Omega) \times L^2(\Omega)$. Now, using Eq. (2.17) of Lemma 2.3.5, we have

$$\int_{\Omega} (\alpha'(0; V) B(\Omega)) \cdot \tau = \int_{\Omega} \operatorname{curl}(B(\Omega) \times V) \cdot \tau + \int_{\Omega} (\operatorname{div} \tau)(B(\Omega) \cdot V),$$

so that

$$\int_{\Omega} B'_{\mathcal{E}, 2}(\Omega; V) \cdot \tau + \int_{\Omega} u'_{\mathcal{E}, 0}(\Omega; V) \operatorname{div} \tau = 0, \quad (2.24)$$

$$\int_{\Omega} (\operatorname{div} B'_{\mathcal{E}, 2}(\Omega; V)) v = 0, \quad (2.25)$$

To prove that $B'_{\mathcal{E},2}(\Omega; V)$ is a gradient, we apply the Hodge decomposition Eq. (A.2) to Eq. (2.24). Taking $\tau = B(\Omega)$, we obtain $\int_{\Omega} B'_{\mathcal{E},2}(\Omega; V) \cdot B(\Omega) = 0$, so that $B'_{\mathcal{E},2}(\Omega; V)$ is orthogonal to $\mathcal{K}(\Omega)$. Taking τ in $\text{curl } H_0(\text{curl}, \Omega)$, we obtain $\int_{\Omega} B'_{\mathcal{E},2}(\Omega; V) \cdot \tau = 0$. We conclude that there exists a unique zero average function u_V in $H^1(\Omega)$ such that $B'_{\mathcal{E},2}(\Omega; V) = \nabla u_V$. Eq. (2.25) then implies $\Delta u_V = 0$. For the boundary condition, we know that $B'_2(\Omega; V) \cdot n = 0$, so that

$$\nabla u_V \cdot n = \text{curl}(V \times B(\Omega)) \cdot n.$$

From [BCS02, Section 4], we then know that $(V \times B(\Omega)) \times n$ is in $H^{-1/2}(\text{div}_{\Gamma}, \partial\Omega)$, and that

$$\text{curl}(V \times B(\Omega)) \cdot n = \text{div}_{\Gamma}((V \times B(\Omega)) \times n).$$

Finally, we use the formula $(a \times b) \times c = (a \cdot c)b - (b \cdot c)a$ to obtain the desired boundary condition for u_V . \square

2.5 Shape differentiation as one-forms in the smooth category

The aim of this section is to prove a shape differentiability result for the harmonic fields when pulled back as one-forms in the smooth category. We will thus be using the variational formulation given by Eq. (2.9), and will be able to use classical elliptic regularity results to deal with shape differentiability with higher regularity. Indeed, since Eq. (2.9) is essentially a classical variational formulation for the Poisson equation (instead of the mixed formulation used in Section 2.4), the corresponding pulled back variational formulation on the fixed domain Ω is a "div-A-grad" equation, for which the elliptic regularity theory is well known.

Throughout this section, we suppose that there exists a smooth diffeomorphism $\mathcal{F} : S^1 \times D^2 \rightarrow \bar{\Omega}$, so that, in particular, Ω is a toroidal domain with smooth boundary. This also implies from [Sch95][Theorem 2.2.7] that $B(\Omega)$ is in fact smooth up to the boundary. We denote the first component of \mathcal{F}^{-1} as ϕ , which is a smooth function from $\bar{\Omega}$ to S^1 . We also assume that the cutting surface $\bar{\Sigma}$ is given by $\mathcal{F}(\{0\} \times D^2)$. Therefore, \mathcal{F} defines a smooth diffeomorphism from $(0, 1) \times D^2$ to $\bar{\Omega} \setminus \bar{\Sigma}$. We denote the first component of its inverse by $\tilde{\phi}$, which is a smooth function from $\bar{\Omega} \setminus \bar{\Sigma}$ to \mathbb{R} .

The main theorem of this section is the following.

Theorem 2.5.1. *Let k be a positive integer. The mapping*

$$\begin{cases} \mathcal{B}_k \rightarrow H^{k+1}(\Omega)^3 \\ V \mapsto \Phi_V^1 B(\Omega_V) \end{cases},$$

is smooth at zero, and its differential verifies

$$B'_1(\Omega; V) = \nabla(V \cdot B(\Omega)) + \nabla u_V,$$

where u_V solves

$$\begin{cases} \Delta u_V = 0 & \text{in } \Omega, \\ \nabla u_V \cdot n = \text{div}_{\Gamma}(B(\Omega)(V \cdot n)) & \text{on } \partial\Omega. \end{cases}$$

Before proving Theorem 2.5.1, we prove the following technical Lemma.

Lemma 2.5.2. *$\tilde{\phi}$ is in $V_1(\Omega \setminus \Sigma)$, and its partial derivatives are in $\mathcal{C}^{\infty}(\bar{\Omega})$.*

In order to prove Lemma 2.5.2, we proceed with a differential geometry argument. To do so, we begin by recalling some elementary constructions from differential geometry.

Let M and N be smooth manifolds, with or without boundaries. We recall that, given a smooth function $F \in \mathcal{C}^\infty(M; N)$, we can associate its pushforward $F_* \in \mathcal{C}^\infty(TM; TN)$. Moreover, given a smooth vector field X of M , F_*X defines a vector field along F , that is, F_*X is a smooth map from M to TN verifying that $(F_*X)(x)$ is in $T_{F(x)}N$ for x in T_xM .

Denoting π as the quotient projection from \mathbb{R} to $S^1 = \mathbb{R}/\mathbb{Z}$ and $\hat{e}_{\mathbb{R}}$ as the canonical unit vector field on \mathbb{R} , we obtain in this particular case that $\pi_*\hat{e}_{\mathbb{R}}$ may be associated with a vector field of S^1 . We denote this vector field as \hat{e}_{S^1} . This comes from the fact that, for all x, x' such that $\pi(x) = \pi(x')$, we have $(\pi_*\hat{e}_{\mathbb{R}})(x) = (\pi_*\hat{e}_{\mathbb{R}})(x')$.

Proof of Lemma 2.5.2. For the first statement, it is clear from the definition of $\tilde{\phi}$ that its traces on Σ are equal to 1 and 0, so that the jump across Σ is equal to 1. As a consequence, we find that $\tilde{\phi}$ is indeed in $V_1(\Omega \setminus \Sigma)$.

For the second statement, we begin by noticing that, using the notations from the introduction of this section, we have $\pi \circ \tilde{\phi} = \phi|_{S^1 \setminus \{0\}}$. As a consequence, we obtain directly that $\pi \circ \tilde{\phi}$ extends to a smooth function from $\bar{\Omega}$ to S^1 . The idea is now to prove that the partial derivatives of $\tilde{\phi}$ may be obtained in a simple way from the pushforward of the canonical vector fields of $\bar{\Omega}$ by $\pi \circ \tilde{\phi}$. Let x^i be one of the canonical Cartesian coordinates of \mathbb{R}^3 .

On one side, since $\pi \circ \tilde{\phi}$ is a smooth function from $\bar{\Omega}$ to S^1 , we know that $(\pi \circ \tilde{\phi})_* \partial_{x^i}$ is a smooth vector field along $\pi \circ \tilde{\phi}$. As a consequence, there exists f_i in $\mathcal{C}^\infty(\bar{\Omega})$ such that, for all x in $\bar{\Omega}$.

$$((\pi \circ \tilde{\phi})_* \partial_{x^i})(x) = f_i(x) \hat{e}_{S^1}(\pi \circ \tilde{\phi}(x)).$$

On the other side, we know that for all x in $\Omega \setminus \Sigma$, we have

$$\begin{aligned} ((\pi \circ \tilde{\phi})_* \partial_{x^i})(x) &= \pi_* [\tilde{\phi}_* \partial_{x^i}(x)] \\ &= \pi_* [\partial_{x^i} \tilde{\phi}(x) \hat{e}_{\mathbb{R}}(\tilde{\phi}(x))] \\ &= \partial_{x^i} \tilde{\phi}(x) \pi_* [\hat{e}_{\mathbb{R}}(\tilde{\phi}(x))] \\ &= \partial_{x^i} \tilde{\phi}(x) \hat{e}_{S^1}(\pi \circ \tilde{\phi}(x)). \end{aligned}$$

From this, we find that $\partial_{x^i} \tilde{\phi}$ is equal to f_i on $\Omega \setminus \Sigma$. As a consequence, we obtain that $\partial_{x^i} \tilde{\phi}$ extends to a smooth function of $\bar{\Omega}$. \square

Proof of Theorem 2.5.1. The proof comes in two steps. First, we prove that $V \mapsto \Phi_V^1 B(\Omega_V)$ is indeed differentiable in the desired norms. This is given by an implicit function argument together with elliptic regularity results, which is similar to the proof of [HP18][Theorem 5.5.1]. Then, we obtain an expression for the shape derivative of $\Phi_V^1 B(\Omega_V)$. This is done by differentiating the pulled-back variational formulation given in Eq. (2.9) with respect to V , and using Lemma 2.3.5. As expected, we obtain the sum of the Lie derivative of $B(\Omega)$ as a one-form and of the "Eulerian" derivative which we also obtained in Theorem 2.4.1.

Shape differentiability We recall that $B(\Omega_V) = \tilde{\nabla} u(\Omega_V)$, where $u(\Omega_V)$ is the solution to the following variational problem. Find $u(\Omega_V)$ in $V_1(\Omega_V \setminus \Sigma_V)$ such that, for all v in $H^1(\Omega_V)$, we have

$$\int_{\Omega_V} \nabla u(\Omega_V) \cdot \nabla v = 0.$$

In order to work in $H^1(\Omega)$, we define $\tilde{u}(\Omega_V)$ by

$$\Phi_V^0 \tilde{u}(\Omega_V) = \Phi_V^0 u(\Omega_V) - \tilde{\phi}.$$

We then have, using Proposition 2.3.3

$$\int_{\Omega} (\alpha(V) \nabla (\Phi_V^0 \tilde{u}(\Omega_V))) \cdot (\nabla \Phi_V^0 v) = \int_{\Omega} \nabla \tilde{\phi} \cdot (\nabla \Phi_V^0 v)$$

for all v in $H^1(\Omega_V)$. Since Φ_V^0 is an isomorphism from $H^1(\Omega_V)$ to $H^1(\Omega)$, we obtain that

$$\int_{\Omega} (\alpha(V) \nabla (\Phi_V^0 \tilde{u}(\Omega_V))) \cdot \nabla v = \int_{\Omega} \nabla \tilde{\phi} \cdot \nabla v$$

for all v in $H^1(\Omega)$, which is the variational formulation of

$$\begin{cases} \operatorname{div} (\alpha(V) \nabla u) = \Delta \tilde{\phi}, & \text{in } \Omega, \\ (\alpha(V) \nabla u) \cdot n = 0, & \text{on } \partial\Omega. \end{cases}$$

We now proceed with an inverse function theorem argument. Since, using Lemma 2.5.2, we know that $\Delta \phi$ is in $\mathcal{C}^\infty(\bar{\Omega})$, we may define

$$F_k : \begin{cases} \mathcal{B}_{k+2} \times H^{k+2}(\Omega) \rightarrow H^k(\Omega) \times H^{k+1/2}(\partial\Omega) \\ (V, u) \mapsto (\operatorname{div} (\alpha(V) \nabla u) - \Delta \tilde{\phi}, (\alpha(V) \nabla u) \cdot n) \end{cases}.$$

From Lemma 2.3.5, we know that $V \mapsto \alpha(V)$ is smooth from \mathcal{B}_{k+2} to $W^{k+1, \infty}(\mathbb{R}^3; \mathcal{M}_3(\mathbb{R}))$ so that, since F_k is linear and bounded with respect to u , F_k is smooth as well. Furthermore, we have $F_k(0, \tilde{u}(\Omega)) = 0$ and

$$D_u F_k(0, \tilde{u}(\Omega))(v) = (\Delta v, \nabla v \cdot n).$$

From [Gri11][Section 2.5.1], we then know that $D_u F_k(0, \tilde{u}(\Omega))$ is an isomorphism from $H^{k+2}(\Omega)$ to $H^k(\Omega) \times H^{k+1/2}(\partial\Omega)$. Using the implicit function theorem, we know that, for $\|V\|_{W^{k+2, \infty}}$ small enough, there is a unique smooth mapping $V \mapsto u(V)$ such that $F_k(u(V), V) = 0$. From uniqueness, we deduce that $u(V) = \Phi_V^0 \tilde{u}(\Omega_V)$.

Finally, we are now able to conclude that $V \mapsto \Phi_V^1 B(\Omega_V)$ is smooth at zero. Indeed, we have by definition

$$\Phi_V^0 u(\Omega_V) = \tilde{u}(\Omega_V) + \tilde{\phi},$$

so that

$$\Phi_V^1 B(\Omega_V) = \nabla (\Phi_V^0 \tilde{u}(\Omega_V)) + \nabla \tilde{\phi}.$$

Since $\nabla \tilde{\phi}$ is in $H^{k+1}(\Omega)^3$, and $\mathcal{B}_{k+2} \ni V \mapsto \Phi_V^0 \tilde{u}(\Omega_V) \in H^{k+2}(\Omega)$ is smooth at zero, we deduce that $V \mapsto \Phi_V^1 B(\Omega_V) \in H^{k+1}(\Omega)^3$ is also smooth at zero.

Expression of the shape derivative We now wish to find an expression for the differential of $V \mapsto \Phi_V^1 B(\Omega_V)$, which we denote $B'_1(\Omega; V)$. We begin by writing

$$B'_1(\Omega; V) = \nabla(B(\Omega) \cdot V) + B'_{\mathcal{E},1}(\Omega; V).$$

Using Proposition 2.3.3, we know that $\operatorname{curl}(\Phi_V^1 B(\Omega_V)) = 0$, so that $B_1'(\Omega; V)$ is curl free. Similarly, using Lemma 2.3.4, we have

$$\int_{\gamma'} (\Phi_V^1 B(\Omega_V)) \cdot t' = 1,$$

so that

$$\int_{\gamma'} B_1'(\Omega; V) \cdot t' = 0.$$

Since $B_1'(\Omega; V)$ and $B_{\mathcal{E},1}'(\Omega; V)$ differ from each other by a gradient, we know that $B_{\mathcal{E},1}'(\Omega; V)$ is also curl free and circulation free. We then know that there exists a unique zero average function u_V in $H^1(\Omega)$ such that $B_{\mathcal{E},1}'(\Omega; V) = \nabla u_V$ (see Section 2.2.2). To obtain the variational formulation for u_V , we now write

$$\int_{\Omega} (\alpha(V) \Phi_V^1 B(\Omega_V)) \cdot \nabla v = 0,$$

for all v in $H^1(\Omega)$. Differentiating with respect to V , we obtain

$$\int_{\Omega} (\alpha'(0; V) B(\Omega)) \cdot \nabla v + \int_{\Omega} (\nabla(V \cdot B(\Omega)) + \nabla u_V) \cdot \nabla v = 0.$$

Using Eq. (2.18) of Lemma 2.3.5 for v in $\mathcal{C}^\infty(\bar{\Omega})$, as well as $(B(\Omega) \times V) \times n = -B(\Omega)(V \cdot n)$, we then obtain

$$\int_{\partial\Omega} (B(\Omega) \cdot \nabla v)(V \cdot n) - \int_{\Omega} \nabla(B(\Omega) \cdot V) \cdot \nabla v + \int_{\Omega} (\nabla(B(\Omega) \cdot V) + \nabla u_V) \cdot \nabla v = 0,$$

so that, integrating by part on the boundary term, we obtain

$$\int_{\Omega} \nabla u_V \cdot \nabla v = \int_{\partial\Omega} \operatorname{div}_{\Gamma}(B(\Omega)(V \cdot n)) v.$$

We are then able to conclude from density of $\mathcal{C}^\infty(\bar{\Omega})$ in $H^1(\Omega)$. □

2.6 Conclusion and perspectives

Conclusion In this chapter, we have studied the shape differentiability properties of normalized harmonic fields in toroidal domains. To this end, we have introduced in Section 2.2 two equivalent variational formulations for the normalized harmonic field, a first one where $H(\operatorname{curl}, \Omega)$ is the variational space, and second one where it is $H_0(\operatorname{div}, \Omega)$. We then defined in Section 2.3 ways to pull vector fields back from a deformed domain Ω_V onto a fixed one Ω . These transformations, which correspond to usual pullbacks in the differential forms setting, allow us to preserve the variational spaces of the variational formulations. Using these transformations, we then obtained a shape differentiability result for each variational formulation of the normalized harmonic fields. For the case of $H_0(\operatorname{div}, \Omega)$, we proved in Section 2.4 the smoothness of $V \mapsto \Phi_V^2 B(\Omega_V)$ and provided a formula for the differential under the assumption that Ω is 1-regular. For the case of $H(\operatorname{curl}, \Omega)$, we proved in Section 2.5 the smoothness of $V \mapsto \Phi_V^1 B(\Omega_V)$ from \mathcal{B}_k to $H^{k+1}(\Omega)^3$ under the additional assumption that Ω is smooth and gave a formula for the differential. In both cases, we found that the formula for the shape derivative is given by the sum of a Lie

derivative, corresponding to the choice of pullback, and a Eulerian part, independent of the choice of pullback.

Perspectives First, we saw in the introduction of this chapter that one may also pull the normalized harmonic fields back using the pushforward by $(I+V)^{-1}$. Although this transformation does not preserve the divergence or the curl, it is natural to use it when considering dynamical properties of the harmonic field. We will consider this way of transforming the normalized harmonic field in Chapter 4. In this case, we will adapt Theorem 2.5.1 to fit this case and find that the differential of $V \mapsto (I+V)_*^{-1}B(\Omega_V)$ at zero is unsurprisingly given by $B'_{\text{vf}}(\Omega; V) = [V, B_0] + \nabla u_V$.

On another note, we have proven that $V \mapsto \Phi_V^k B(\Omega_V)$ is not only differentiable at zero, but smooth. One may then wonder what the higher order shape derivatives of the harmonic fields may be, and under what regularity assumptions we may obtain geometrically meaningful formulas for these derivatives. Intuitively, one may expect that higher order derivative should be given by the sum of a composition of Lie derivatives by the deformation vector fields and of a Eulerian part independent on the choice of pullback. Having rigorous derivations for these formulas would necessitate adapting Lemma 2.3.5 to higher order derivatives of $V \mapsto \alpha(V)$, for which the computations may be more involved if one wishes to obtain geometrically meaningful terms.

Shape optimization of harmonic helicity

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3.1 Introduction

For a given vector field F on a three-dimensional domain Ω , we recall from Section 1.3.2 that its helicity (also known as magnetic or Biot–Savart helicity) is defined by the formula

$$\mathbf{H}(F) = \frac{1}{4\pi} \int_{\Omega \times \Omega} F(y) \cdot \left(F(x) \times \frac{y-x}{|y-x|^3} \right) dx dy. \quad (3.1)$$

This quantity plays an important role in plasma physics, fluid dynamics and magnetohydrodynamics (see e.g. [Arn66; AK21; FLS24]). In the context of electromagnetism, helicity of a magnetic field (called magnetic helicity) can be seen as a scalar quantifying the linkage of the magnetic field [Mof69; Arn14]. As was seen in Section 1.3.2, Eq. (3.1) can be interpreted as the average linking number of the field lines of F when it is a magnetic field, that is, divergence free and tangent to the boundary.

When working with magnetic fields of Ω , a natural connection with vector potentials appears. First note that if one introduces the Biot–Savart operator of F

$$\text{BS}(F)(y) = \frac{1}{4\pi} \int_{\Omega} \frac{F(x) \times (y-x)}{|y-x|^3} dx, \quad (3.2)$$

one obtains that the helicity of F is the L^2 inner product of F with $\text{BS}(F)$. For simply connected domains, the latter remains true if we replace $\text{BS}(F)$ by any vector potential of F (we recall that $\text{curl BS}(F) = F$). For three-dimensional domains that are not simply connected, the connection between helicity and vector potentials is slightly more involved and have been established by Bevir and Gray in [BG80] for toroidal domains¹ and [MV19] for more general ones. We recall the definition and main properties of the magnetic helicity in Section 3.2.1.

A classical mathematical problem related to helicity studied in e.g. [Can+00; Can+99; Val19; Mon23] is the maximization of the helicity on $H_0(\text{div}^0, \Omega)^2$ with fixed L^2 norm. The critical vector field of this optimization problem are in fact eigenfields of the curl operator which can be seen thanks to a modified Biot–Savart operator denoted here BS' [Can+00].

Elements of shape optimization were also discussed in [Can+00] and [Can+99] to characterize the domain with the highest eigenvalue of BS' for a given volume. Some properties of the maximizing fields on such a domain were given, but it is also unclear whether the optimal shape exists, as some computations suggest that it would have to be a singular sphere, with North and South Pole collapsed to a single point. Recent works on the existence of an optimal shape and its characterization for the related problem of the first curl eigenvalue can be found in [EP23b; Ger23b; Ger23a].

In this chapter, we are interested in a slightly different problem. Given a toroidal domain Ω , we consider the set of harmonic fields, that is the set of vector fields that are divergence free, curl free and tangent to the boundary. By classical results of Hodge theory, this set is a one-dimensional vector space. We are then interested in the helicity of the normalized harmonic field $B(\Omega)$ introduced in Chapter 2, where physically, the normalization is related to total flux of currents through the central hole of the torus. Thus, for any regular enough toroidal domain, we define a scalar quantity that we call the **harmonic helicity** of the domain Ω .

Designing a numerical scheme to compute this shape functional is not obvious. A close problem is the spectral approximation of the curl operator in multiply connected domains; this has been tackled in [LRV15; Alo+18] using the finite element method. For efficiency considerations, it is important to avoid the computation of the double integral in Eq. (3.1) and use another vector potential than the Biot–Savart. Using classical results on vector potentials characterizations [Amr+98] and tools from finite element exterior calculus [AFW06; AFW10], we provide efficient numerical approximation schemes and implementation for the harmonic helicity.

Physical motivations for considering harmonic helicity arise from the design of stellarators, advanced nuclear fusion devices that rely on the confinement of intensely hot plasma through a sophisticated magnetic field. A significant challenge arises due to the inherent impossibility of creating a non-zero magnetic field with constant magnitude on a toroidal domain. Additionally, variations in the magnetic field amplitude, typically inversely proportional to the major radius, result in a vertical drift, which can be mitigated through the implementation of a twisted magnetic field. Optimization of the shape of the coils is a very active field [Pau+18; PRS22]. A measure of the twisted nature of the magnetic field is expressed by the magnetic helicity. We refer to [IPW20] for a very nice introduction to the topic.

In contrast to Tokamaks, which are axisymmetric devices inducing a current inside the plasma

1. That is bounded open subsets of \mathbb{R}^3 homeomorphic to a full torus.
 2. we refer to Section 2.2.1 for the definition of this Hilbert space.

to generate a twisting magnetic field, stellarators aim for stability without requiring a current within the plasma. Consequently, the magnetic field employed to stabilize the plasma in a stellarator can be reasonably approximated as a harmonic field within the domain representing the plasma. Hence, we believe that the optimization of the shape of the plasma to increase the harmonic helicity could give rise to interesting new forms of plasma.

This chapter is organized as follows:

- In Section 3.2, we introduce the necessary functional framework for the rest of the chapter. We begin by recalling some aspects of the constructions given in Section 2.2 for toroidal domains and for the variational formulations of the normalized harmonic fields. Next, we give two PDE formulations to characterize vector potentials. Finally, we make the connection between vector potentials and the helicity through the Bevir–Gray formula.
- In Section 3.3, we begin by introducing the precise definition of the harmonic helicity of a toroidal domain. We then give a few basic properties of this shape functional, that is, its dependence on scaling and planar reflections of the domain. The rest of the section is dedicated to the computation of the shape derivative of the harmonic helicity. This is done using shape differentiation of several PDE problems and a subtle use of the transformations introduced in Section 2.3. To the best of the authors' knowledge, the employed methodology is original and may hold applicability in addressing new shape differentiation problems involving other Hilbert complexes.
- In Section 3.4, we recall the framework of finite element exterior calculus. We then use classical results on approximations of Hodge Laplacian problems. The adaptations of these tools to our problem is not straightforward and provides a method to compute both the helicity and the shape gradient.
- In Section 3.5, we provide numerical results of the proposed numerical methods on specific shapes motivated by the study of stellarator plasmas. Then we present two numerical experiments to improve the harmonic helicity of a standard plasma shape.

3.2 Prerequisites

We begin by recalling some elements of Section 2.2 for the functional framework and the variational formulations of the harmonic fields.

Let Ω be a Lipschitz toroidal domain, that is, a Lipschitz open set Ω such that $\bar{\Omega}$ is homeomorphic to the full torus $S^1 \times D^2$. As in Section 2.2.1, we introduce a toroidal and a poloidal loop on $\partial\Omega$ denoted as γ' and γ with unit tangent vector fields t' and t respectively. We are then able to define notions of circulations along γ' and γ as in Section 2.2.2 for vector fields with curl tangent to the boundary.

We also recall that $H(\text{curl}, \Omega)$ (resp. $H(\text{div}, \Omega)$) is the space of square integrable vector fields with curl in $L^2(\Omega)^3$ (resp. divergence in $L^2(\Omega)$). Furthermore, elements of $H(\text{curl}, \Omega)$ (resp. $H(\text{div}, \Omega)$) have tangential (resp. normal) traces in $H^{-1/2}$ with

$$\int_{\partial\Omega} (u \times n) \cdot \varphi = \int_{\Omega} u \cdot \text{curl} \varphi - \int_{\Omega} \text{curl} u \cdot \varphi, \quad (3.3)$$

for every φ in $H^1(\Omega)^3$, and

$$\int_{\partial\Omega} (u \cdot n) \varphi = \int_{\Omega} u \cdot \nabla \varphi + \int_{\Omega} (\text{div} u) \varphi, \quad (3.4)$$

for every φ in $H^1(\Omega)$. We also denote as $H(\text{curl}^0, \Omega)$ (resp. $H(\text{div}^0, \Omega)$) the space of square

integrable vector fields of Ω with vanishing curl (resp. divergence) and define $L_0^2(\Omega)$ as the space of square integrable functions of Ω with zero average. We finally recall that $H_0(\text{curl}, \Omega)$ (resp. $H_0(\text{div}, \Omega)$) is the space of vector fields in $H(\text{curl}, \Omega)$ (resp. $H(\text{div}, \Omega)$) with vanishing trace, and

$$\begin{aligned} H_0(\text{curl}^0, \Omega) &= H_0(\text{curl}, \Omega) \cap H(\text{curl}^0, \Omega) \\ H_0(\text{div}^0, \Omega) &= H_0(\text{div}, \Omega) \cap H(\text{div}^0, \Omega). \end{aligned}$$

The set of harmonic fields of Ω is then defined as

$$\begin{aligned} \mathcal{K}(\Omega) &= \{u \in L^2(\Omega)^3 \mid \text{div } u = 0, \text{ curl } u = 0, u \cdot n = 0\}, \\ &= H(\text{curl}^0, \Omega) \cap H_0(\text{div}^0, \Omega). \end{aligned}$$

This space has dimension equal to the first Betti number of Ω , so that it is one-dimensional for toroidal domains. We thus only need to prescribe a degree of freedom to single out an element of $\mathcal{K}(\Omega)$, which in our case is the circulation along the toroidal loop γ' .

We now recall how one may find variational formulations for the normalized harmonic field. We introduce as in Section 2.2.1 a Lipschitz cutting surface $\Sigma \subset \Omega$ with unit normal vector field n_Σ . $\Omega \setminus \Sigma$ is then a pseudo-Lipschitz domain, and we may define $\llbracket u \rrbracket_\Sigma$ as the jump of u along Σ in the direction of n_Σ for u in $H^1(\Omega \setminus \Sigma)$. To define the normalized harmonic field of Ω , we recall that there exists a unique function $u \in H^1(\Omega \setminus \Sigma)$ such that $\llbracket u \rrbracket_\Sigma = 1$ and for all v in $H^1(\Omega)$

$$\int_{\Omega \setminus \Sigma} \nabla u \cdot \nabla v = 0. \quad (3.5)$$

The normalized harmonic field $B(\Omega)$ is then defined as the L^2 extension of ∇u to Ω . Finally, we recall that Proposition 2.2.2 states that the following variational problem is well posed. Find $(B_{\text{div}}, u_{\text{div}}) \in H_0(\text{div}, \Omega) \times L_0^2(\Omega)$ such that, for all $(\tau, v) \in H_0(\text{div}, \Omega) \times L^2(\Omega)$ we have

$$\begin{aligned} \int_{\Omega} (\text{div } B_{\text{div}}) v &= 0, \\ \int_{\Omega} B_{\text{div}} \cdot \tau + \int_{\Omega} u_{\text{div}} (\text{div } \tau) &= \int_{\Sigma} \tau \cdot n_\Sigma. \end{aligned} \quad (3.6)$$

Furthermore, we have $B_{\text{div}} = B(\Omega)$.

3.2.1 Vector potentials and Bevir–Gray formula

As was mentioned earlier, the numerical computation of the Biot–Savart operator can be very costly. As a consequence, we chose to compute the helicity of the normalized harmonic field by substituting $\text{BS}(B(\Omega))$ by an appropriate vector potential of $B(\Omega)$. Indeed, since $\text{curl } \text{BS}(B(\Omega)) = B(\Omega)$, we know that any vector potential $A(\Omega)$ of $B(\Omega)$ can only differ from $\text{BS}(B)$ by the sum of a gradient and a harmonic field (see Eqs. (A.2) and (A.7) in Appendix A). Since vector fields of $H_0(\text{div}^0, \Omega)$ are orthogonal to gradient vector fields, we know that $\int_{\Omega} B(\Omega) \cdot A(\Omega)$ can differ from $\text{H}(B(\Omega))$ only through the harmonic part of the difference between $A(\Omega)$ and $\text{BS}(B(\Omega))$. However, this difference can be accounted for by modifying the formula of the magnetic helicity, giving a quantity which is invariant under a change of the vector potential. This is given by the well known Bevir–Gray formula [BG80] in toroidal domains, which was later generalized to a large class of non-simply connected domains in [MV19]. In our case, for a vector field F in

$H_0(\operatorname{div}^0, \Omega)$ and A any of its vector potentials, this invariant quantity is given by

$$\mathbb{H}(F) = \int_{\Omega} F \cdot A - \left(\int_{\gamma} A \cdot t \right) \left(\int_{\gamma'} A \cdot t' \right). \quad (3.7)$$

Note that $\operatorname{BS}(V)$ has zero circulation along γ' [CDG01, Section III.A], so that this invariant quantity does correspond to the usual Biot–Savart helicity.

From this formulation, a natural problem is to find good vector potentials, which are simple to study, both theoretically and numerically. Getting back to the helicity of the normalized harmonic field, we will study two natural vector potential candidates. First, a vector potential given by a classical vector Laplacian problem, which is orthogonal to $B(\Omega)$, therefore canceling the first term of Eq. (3.7). Second, a vector potential given in [Val19], which is of zero circulation along the toroidal loop γ' , therefore canceling the second term. As we will see in Section 3.5, using these two vector potentials also allows us to stay in a finite element exterior calculus setting throughout the numerical computation of the harmonic helicity, and its shape gradient.

The first vector potential, which we denote by $A^1(\Omega)$, is given by the following proposition.

Proposition 3.2.1. *There exists a unique $(A^1(\Omega), u) \in H(\operatorname{curl}, \Omega) \times H(\operatorname{div}, \Omega)$ such that, for all $(\tau, v) \in H(\operatorname{curl}, \Omega) \times H(\operatorname{div}, \Omega)$*

$$\int_{\Omega} A^1(\Omega) \cdot \tau = \int_{\Omega} \operatorname{curl} \tau \cdot u, \quad (3.8)$$

$$\int_{\Omega} \operatorname{curl} A^1(\Omega) \cdot v + \int_{\Omega} (\operatorname{div} u)(\operatorname{div} v) = \int_{\Omega} B(\Omega) \cdot v. \quad (3.9)$$

Furthermore, $A^1(\Omega)$ verifies

1. $A^1(\Omega)$ is in $H_0(\operatorname{div}^0, \Omega)$,
2. $\operatorname{curl} A^1(\Omega) = B(\Omega)$,
3. $\int_{\Omega} A^1(\Omega) \cdot B(\Omega) = 0$.

Proof. Since the second de Rham cohomology space of Ω is trivial, the space of harmonic 2-forms of Ω vanishes, and this variational problem is equivalent to [AFW06, Equation (7.1)] for the case $k = 2$. Existence and uniqueness is then given by [AFW06, Theorem 7.2].

To prove Item 1, we simply take τ in $\nabla H^1(\Omega)$ in Eq. (3.8). This gives us $\int_{\Omega} A^1(\Omega) \cdot \tau = 0$, so that $A^1(\Omega)$ is orthogonal to $\nabla H^1(\Omega)$, and therefore is in $H_0(\operatorname{div}^0, \Omega)$ by Eq. (A.4) in Appendix A. To find Item 2, we proceed with the same splitting analysis used in [AFW06]. We define using the Hodge decomposition Eq. (A.3), $u = u_{\nabla} + u_{\operatorname{curl}}$ with $u_{\operatorname{curl}} \in \operatorname{curl} H(\operatorname{curl}, \Omega)$ and $u_{\nabla} \in \nabla H_0^1(\Omega)$. We now want to prove that $u_{\nabla} = 0$. Choosing $v \in H(\operatorname{div}^0, \Omega)^{\perp} \cap H(\operatorname{div}, \Omega)$ in Eq. (3.9), we get

$$\int_{\Omega} (\operatorname{div} u_{\nabla})(\operatorname{div} v) = \int_{\Omega} B \cdot v = 0.$$

Using the Poincaré inequality from Proposition A.2 of Appendix A, we get $u_{\nabla} = 0$, so that $\operatorname{div} u = 0$. As a consequence, Eq. (3.9) gives $\operatorname{curl} A^1(\Omega) = B(\Omega)$.

Finally, since $\operatorname{curl} B(\Omega) = 0$, we simply get by choosing $\tau = B(\Omega)$ in Eq. (3.8)

$$\int_{\Omega} A^1(\Omega) \cdot B(\Omega) = 0,$$

proving Item 3. □

For the second vector potential $A^2(\Omega)$, we first need to introduce the following spaces.

$$\begin{aligned}\mathcal{X}(\Omega) &= \{u \in H(\text{curl}, \Omega) \mid \text{curl } u \cdot n = 0\}, \\ \mathcal{Z}(\Omega) &= \left\{u \in \mathcal{X}(\Omega) \mid \int_{\gamma'} u \cdot t' = 0\right\}.\end{aligned}$$

We then introduce the second vector potential $A^2(\Omega)$, given by the following result proven in [Val19]

Proposition 3.2.2. *The following problem has a unique solution. Find $(A^2(\Omega), u) \in \mathcal{Z}(\Omega) \times \nabla H^1(\Omega)$ such that for all $(\tau, v) \in \mathcal{Z}(\Omega) \times \nabla H^1(\Omega)$*

$$\begin{aligned}\int_{\Omega} \text{curl } A^2(\Omega) \cdot \text{curl } \tau + \int_{\Omega} u \cdot \tau &= \int_{\Omega} B(\Omega) \cdot \text{curl } \tau, \\ \int_{\Omega} A^2(\Omega) \cdot v &= 0.\end{aligned}\tag{3.10}$$

Furthermore, we have $\text{curl } A^2(\Omega) = B(\Omega)$ and $A^2(\Omega) \in H_0(\text{div}^0, \Omega)$.

Of course, the two choices of potential vectors are related to each other. Since $A^1(\Omega)$ and $A^2(\Omega)$ are in $H_0(\text{div}^0, \Omega)$ and have the same curl, we get that $A^1(\Omega) - A^2(\Omega)$ is in $\mathcal{K}(\Omega)$. The fact that $A^2(\Omega)$ has zero circulation along γ' , and that $B(\Omega)$ has a circulation of 1 allows us to find the relation

$$A^2(\Omega) = A^1(\Omega) - \left(\int_{\gamma'} A^1(\Omega) \cdot t'\right) B(\Omega).\tag{3.11}$$

3.3 Harmonic helicity and its shape derivative

As we have seen in the previous section, with each Lipschitz toroidal domain Ω , we are able to associate a normalized harmonic field $B(\Omega)$ and a vector potential of $B(\Omega)$, denoted $A^2(\Omega)$, with zero circulation along γ' . As a consequence of the Bevir–Gray formula Eq. (3.7), the magnetic helicity of $B(\Omega)$ is then given by $\mathcal{H}(B(\Omega)) = \int_{\Omega} B(\Omega) \cdot A^2(\Omega)$. In turn, this allows us to define the helicity of the normalized magnetic field of Ω , which we refer to as the harmonic helicity of Ω for simplicity. As was noted in Remark 2.2.1, $B(\Omega)$ is actually defined as a function of Ω only up to a sign. However, since the helicity is a quadratic form, this sign indetermination is not relevant, and the harmonic helicity is well-defined as a shape functional.

Definition 3.3.1. *Let Ω be a Lipschitz toroidal domain. Then, the harmonic helicity of Ω is defined as*

$$\mathcal{H}(\Omega) = \int_{\Omega} B(\Omega) \cdot A^2(\Omega),$$

where $B(\Omega)$ and $A^2(\Omega)$ are given by the solutions to Eqs. (3.5) and (3.10).

The aim of this section is to study how the harmonic helicity varies as a function of the domain Ω . More precisely, we prove that the harmonic helicity is shape Fréchet differentiable under Lipschitz deformation, and we give a formula for its shape derivative.

Before studying the shape differentiability of \mathcal{H} , we state the following properties of harmonic helicity.

Proposition 3.3.2. *The following scaling and symmetry properties hold:*

- Given $\lambda > 0$, we have $\mathcal{H}(\lambda\Omega) = \lambda\mathcal{H}(\Omega)$.
- Given a planar reflection $R \in O_3$, we have $\mathcal{H}(R\Omega) = -\mathcal{H}(\Omega)$.

Proof. We begin by proving the first point. Let $u(\Omega)$ and $u(\lambda\Omega)$ be the solution to Eq. (3.5) in Ω and $\lambda\Omega$ respectively. Then, it is clear that $u(\lambda\Omega) = u(\Omega)(\cdot/\lambda)$. Therefore, we have $B(\lambda\Omega) = \tilde{\nabla}u_\lambda = \frac{1}{\lambda}B(\Omega)(\cdot/\lambda)$. Similarly, we have $A^2(\lambda\Omega) = \frac{1}{\lambda}A(\Omega)(\cdot/\lambda)$. Writing

$$\begin{aligned}\mathcal{H}(\lambda\Omega) &= \int_{\lambda\Omega} B(\lambda\Omega) \cdot A^2(\lambda\Omega) \\ &= \lambda^3 \int_{\Omega} \left(\frac{1}{\lambda}B(\Omega)\right) \cdot \left(\frac{1}{\lambda}A^2(\Omega)\right) \\ &= \lambda\mathcal{H}(\Omega)\end{aligned}$$

For the second point, let R be a planar reflection. We introduce as in Definition 2.3.1

$$\begin{aligned}\Phi_R^1 u &= R^T u \circ R, \\ \Phi_R^2 u &= (\det R)R^{-1}u \circ R,\end{aligned}$$

for u a vector field of $R\Omega$. One then finds, using identical proofs, that Proposition 2.3.3 and Lemma 2.3.4 remain true for these transformations. Since R is a planar reflection, we have $\det R = -1$ and $R^{-1} = R^T$ so that $\Phi_R^2 u = -\Phi_R^1 u$. Let $u(\Omega)$ and $u(R\Omega)$ be the solutions to Eq. (3.5) in Ω and $R\Omega$ respectively. Then, since R is an isometry, we have

$$u(\Omega) = u(R\Omega) \circ R,$$

so that using the definition of the normalized harmonic field and Proposition 2.3.3, we have $B(\Omega) = \Phi_R^1 B(R\Omega)$. We now prove that $A^2(\Omega) = \Phi_R^2 A^2(R\Omega)$. First, since $\Phi_R^2 = -\Phi_R^1$, it is clear from Proposition 2.3.3 that $\Phi_R^2 A^2(R\Omega)$ is in $H_0(\operatorname{div}^0, \Omega)$. Using once again Proposition 2.3.3, we also have

$$\begin{aligned}\operatorname{curl} \Phi_R^2 A^2(R\Omega) &= -\operatorname{curl} \Phi_R^1 A^2(R\Omega) \\ &= -\Phi_R^2 B(R\Omega) \\ &= \Phi_R^1 B(R\Omega) \\ &= B(\Omega).\end{aligned}$$

Moreover, using Lemma 2.3.4, we know that $\Phi_R^2 A^2(R\Omega) = -\Phi_R^1 A^2(R\Omega)$ is in $\mathcal{Z}(\Omega)$. It is then known (see for example [Val19, Proposition 2]) that $\Phi_R^2 A^2(R\Omega)$ solving

$$\begin{cases} \operatorname{div} (\Phi_R^2 A^2(R\Omega)) = 0 & \text{in } \Omega, \\ \operatorname{curl} (\Phi_R^2 A^2(R\Omega)) = B(\Omega) & \text{in } \Omega, \\ (\Phi_R^2 A^2(R\Omega)) \cdot n = 0, & \text{on } \partial\Omega, \\ \int_{\gamma'} (\Phi_R^2 A^2(R\Omega)) \cdot t' = 0, \end{cases}$$

is equivalent to $\Phi_R^2 A^2(R\Omega)$ solving Eq. (3.10). From unicity, we then obtain $\Phi_R^2 A^2(R\Omega) = A^2(\Omega)$.

Finally, since R is an isometry, we have

$$\begin{aligned}
\mathcal{H}(R\Omega) &= \int_{R\Omega} B(R\Omega) \cdot A^2(R\Omega) \\
&= \int_{\Omega} (R^T B(R\Omega) \circ R) \cdot (R^T A^2(R\Omega) \circ R), \\
&= - \int_{\Omega} \Phi_R^1 B(R\Omega) \cdot \Phi_R^2 A^2(R\Omega) \\
&= -\mathcal{H}(\Omega).
\end{aligned}$$

□

Corollary 3.3.3. *If Ω admits a planar symmetry, we have $\mathcal{H}(\Omega) = 0$. In particular, this is the case if Ω is axisymmetric.*

As was mentioned in the introduction of this chapter, another notion for the helicity of a domain which was studied in [Can+00; Can+99; Val19; Mon23] is the maximal value of the helicity on the unit L^2 sphere for fields in $H_0(\operatorname{div}^0, \Omega)$, that is

$$\tilde{\mathcal{H}}(\Omega) = \sup \{ \mathbf{H}(V) \mid V \in H_0(\operatorname{div}^0, \Omega), \|V\|_{L^2} = 1 \}.$$

Since the helicity is quadratic, it is therefore clear that we have the following inequality

$$\mathcal{H}(\Omega) \leq \|B(\Omega)\|_{L^2}^2 \tilde{\mathcal{H}}(\Omega).$$

To remove the L^2 norm in this inequality, one may normalize the harmonic field using the L^2 norm instead of the circulation. Although this makes the comparison between the two quantities more direct, this normalization is less convenient to work with in our context. We note however that one may easily obtain the shape derivative of $\|B(\Omega)\|_{L^2}^2$ using the methods we will introduce in this section, so that this change of normalization may be done without issues for computing the shape derivative of harmonic helicity. We also note that, although $\tilde{\mathcal{H}}$ is known to be bounded when fixing the volume (see [Can+00, Theorem E]), it is not immediately clear whether this is the case for \mathcal{H} . The optimization problems we will consider numerically will be described more precisely in Section 3.5.

In order to state the shape differentiability result, we recall some notations from Chapter 2. We define

$$\mathcal{B}_1 = \left\{ V \in W^{1,\infty}(\mathbb{R}^3)^3 \mid \|DV\|_{L^\infty} < 1 \right\},$$

so that for all V in \mathcal{B}_1 , $\mathbf{I} + V$ is a Lipschitz diffeomorphism of \mathbb{R}^3 . For Ω a Lipschitz toroidal domain and V in \mathcal{B}_1 , we denote $\Omega_V = (\mathbf{I} + V)(\Omega)$.

In order to write the shape derivative of the harmonic helicity as a surface integral, we need to assume that Ω is s -regular for some $s > 1/2$ [AFW06, Section 7.7], that is we have the continuous embedding

$$H(\operatorname{curl}, \Omega) \cap H_0(\operatorname{div}, \Omega) \hookrightarrow H^s(\Omega). \quad (3.12)$$

Indeed, we need $B(\Omega)$ and $A^2(\Omega)$ to have traces in $L^2(\partial\Omega)^3$. For example Ω being Lipschitz-polyhedral or $\mathcal{C}^{1,1}$ is sufficient [Amr+98, Prop. 3.7 or Th. 2.9].

Theorem 3.3.4. *Let Ω be a Lipschitz toroidal domain. The mapping*

$$\begin{cases} \mathcal{B}_1 \rightarrow \mathbb{R} \\ V \mapsto \mathcal{H}(\Omega_V) \end{cases},$$

is smooth at zero. Furthermore, if Ω is s -regular with $s > 1/2$, its differential is given by

$$\mathcal{H}'(\Omega; V) = 2 \int_{\partial\Omega} (B(\Omega) \cdot A^2(\Omega)) (V \cdot n). \quad (3.13)$$

In order to prove this theorem, we will be using the transformations defined in Section 2.3 to pull vector fields and variational formulations back from Ω_V to Ω . We will also be using the fact that $V \mapsto \Phi_V^2 B(\Omega_V)$ is smooth at zero as proven in Theorem 2.4.1, and prove a similar smoothness property for $V \mapsto \Phi_V^1 A^2(\Omega)$. The rest of the proof then follows easily using once again the transformations defined in Section 2.3 and Lemma 2.3.5 to obtain the necessary properties on the differential of $V \mapsto \Phi_V^2 B(\Omega_V)$.

Let V be in \mathcal{B}_1 and Ω a Lipschitz toroidal domain. Throughout the rest of this section n_V is the unit outward pointing vector field on $\partial\Omega_V$, and we define γ_V , γ'_V , Σ_V and Σ'_V in the deformed domain Ω_V as the image by $I + V$ of the corresponding geometrical constructions given in Section 2.2.1, with tangent and normal vector fields t_V , t'_V , n_{Σ_V} , $n_{\Sigma'_V}$ respectively.

In order to prove Theorem 3.3.4, we will use the smoothness of $V \mapsto \Phi_V^2 B(\Omega_V)$ and $V \mapsto \Phi_V^1 A^2(\Omega_V)$. The former was already proven in Theorem 2.4.1. Indeed, we will use Proposition 2.3.3 to write

$$\Phi_V^3 (B(\Omega_V) \cdot A^2(\Omega_V)) = (\Phi_V^2 B(\Omega_V)) \cdot (\Phi_V^1 A^2(\Omega_V)).$$

Then, since Φ_V^3 preserves volume integrals, the result will follow naturally. We thus still need to prove that $V \mapsto \Phi_V^1 A^2(\Omega_V)$ is smooth, which is given by the following proposition.

Proposition 3.3.5. *Let Ω be a Lipschitz toroidal domain, and for V in \mathcal{B}_1 , let us denote by $A^2(\Omega_V)$ the solution of Eq. (3.10) in $\Omega_V = (I + V)(\Omega)$. Then, the mapping*

$$\begin{cases} \mathcal{B}_1 \mapsto \mathcal{Z}(\Omega) \\ V \mapsto \Phi_V^1 A^2(\Omega_V) \end{cases}$$

is smooth at zero.

Proof. We proceed with an implicit function theorem argument, similar to the one used for Theorem 2.4.1. For V in \mathcal{B}_1 , we know that $A^2(\Omega_V)$ solves the following variational formulation. Find $(A^2(\Omega_V), u(\Omega_V)) \in \mathcal{Z}(\Omega_V) \times \nabla H^1(\Omega_V)$ such that for all $(\tau, v) \in \mathcal{Z}(\Omega_V) \times \nabla H^1(\Omega_V)$

$$\int_{\Omega_V} \text{curl } A^2(\Omega_V) \cdot \text{curl } \tau + \int_{\Omega_V} u(\Omega_V) \cdot \tau = \int_{\Omega_V} B(\Omega_V) \cdot \text{curl } \tau, \quad (3.14)$$

$$\int_{\Omega_V} A^2(\Omega_V) \cdot v = 0. \quad (3.15)$$

First, we note that from Proposition 2.3.3 and Lemma 2.3.4, we get $\Phi_V^1 \mathcal{Z}(\Omega_V) = \mathcal{Z}(\Omega)$, so that the functional spaces of Eqs. (3.14) and (3.15) are preserved by the pullbacks.

Pulling back Eqs. (3.14) and (3.15) onto Ω and using Lemma 2.3.2, we get

$$\begin{aligned} \int_{\Omega} (\alpha(V)^{-1} \Phi_V^2 B(\Omega_V)) \cdot (\operatorname{curl} \Phi_V^1 \tau) &= \int_{\Omega} (\alpha(V)^{-1} \operatorname{curl} \Phi_V^1 A^2(\Omega_V)) \cdot (\operatorname{curl} \Phi_V^1 \tau) \\ &\quad + \int_{\Omega} (\alpha(V) \Phi_V^1 u(\Omega_V)) \cdot (\Phi_V^1 \tau), \\ \int_{\Omega} (\alpha(V) \Phi_V^1 A^2(\Omega_V)) \cdot (\Phi_V^1 v) &= 0. \end{aligned}$$

We therefore define

$$F : \mathcal{B}_1 \times (\mathcal{Z}(\Omega) \times \nabla H^1(\Omega)) \rightarrow (\mathcal{Z}(\Omega) \times \nabla H^1(\Omega))'$$

by

$$\begin{aligned} F(V; \sigma, u)(\tau, v) &= \int_{\Omega} (\alpha(V)^{-1} \operatorname{curl} \sigma) \cdot \operatorname{curl} \tau + \int_{\Omega} (\alpha(V) u) \cdot \tau + \int_{\Omega} (\alpha(V) \sigma) \cdot v \\ &\quad - \int_{\Omega} (\alpha(V)^{-1} \Phi_V^2 B(\Omega_V)) \cdot \operatorname{curl} \tau, \end{aligned}$$

so that $(A^2(\Omega_V), u^2(\Omega_V))$ solving Eqs. (3.14) and (3.15) is equivalent to

$$F(V; \Phi_V^1 A^2(\Omega_V), \Phi_V^1 u(\Omega_V)) = 0.$$

By Lemma 2.3.5, we know that $V \mapsto \alpha(V)$ and $V \mapsto \alpha(V)^{-1}$ are smooth. Furthermore, we know from Theorem 2.4.1 that $V \mapsto \Phi_V^2 B(\Omega_V)$ is smooth. Therefore, by linearity and continuity of F with respect to (σ, u) , we know that F is smooth. We have

$$D_{\sigma, u} F(0; A(\Omega), u(\Omega))(\sigma', u')(\tau, v) = \int_{\Omega} \operatorname{curl} \sigma' \cdot \operatorname{curl} \tau + \int_{\Omega} u' \cdot \tau + \int_{\Omega} \sigma' \cdot v,$$

so that $D_{\sigma, u} F(0; A_0, v_0)$ is an isomorphism by the inf-sup conditions proven in [Val19, Section IV]. This proves, by the implicit function theorem, that for V small enough there is a unique smooth mapping $V \mapsto (\sigma(V), u(V))$ such that $F(V; \sigma(V), u(V)) = 0$. By uniqueness, we get $(\sigma(V), u(V)) = (\Phi_V^1 A(\Omega_V), \Phi_V^1 u(\Omega_V))$. \square

Now that we have proved the smoothness of $V \mapsto \Phi_V^2 B(\Omega_V)$ and $V \mapsto \Phi_V^1 A^2(\Omega_V)$, we can conclude the proof of Theorem 3.3.4. To do so, we simply pullback the integral of $B(\Omega_V)$ against $A^2(\Omega_V)$ onto Ω using Lemma 2.3.2, and use the differentiability results for the harmonic field and the vector potential.

Proof. We have

$$\begin{aligned} \mathcal{H}(\Omega_V) &= \int_{\Omega_V} B(\Omega_V) \cdot A^2(\Omega_V) \\ &= \int_{\Omega} \Phi_V^3(B(\Omega_V)) \cdot A^2(\Omega_V) \\ &= \int_{\Omega} (\Phi_V^2 B(\Omega_V)) \cdot (\Phi_V^1 A^2(\Omega_V)). \end{aligned}$$

From Theorem 2.4.1 and Proposition 3.3.5, we know that $V \mapsto \Phi_V^2 B_V$ and $V \mapsto \Phi_V^1 A_V$ are smooth

at zero, so that $V \mapsto \mathcal{H}(\Omega_V)$ is smooth at zero. Denoting the differentials of $V \mapsto \Phi_V^2 B(\Omega_V)$ and $V \mapsto \Phi_V^1 A^2(\Omega_V)$ by $B'_2(\Omega; V)$ and $A'(\Omega; V)$ respectively, we have

$$\mathcal{H}'(\Omega; V) = \int_{\Omega} B'_2(\Omega; V) \cdot A^2(\Omega) + \int_{\Omega} B(\Omega) \cdot A'(\Omega; V).$$

Since $B(\Omega) = \text{curl } A^2(\Omega)$, and $A^2(\Omega)$ and $A'(\Omega; V)$ are both in $\mathcal{Z}(\Omega)$, we know from [Alo+18, Lemma 7] that

$$\int_{\Omega} B(\Omega) \cdot A'(\Omega; V) = \int_{\Omega} \text{curl } A^2(\Omega) \cdot A'(\Omega; V) = \int_{\Omega} \text{curl } A'(\Omega; V) \cdot A^2(\Omega).$$

Furthermore, since $\text{curl } A^2(\Omega_V) = B(\Omega_V)$ for all V , we get $\text{curl } \Phi_V^1 A^2(\Omega_V) = \Phi_V^2 B(\Omega_V)$. By differentiating, we get $\text{curl } A'(\Omega; V) = B'_2(\Omega; V)$, so that

$$\mathcal{H}'(\Omega; V) = 2 \int_{\Omega} B'_2(\Omega; V) \cdot A^2(\Omega).$$

Now, we know from the proof of Theorem 2.4.1 that we have

$$\int_{\Omega_V} B'_2(\Omega; V) \cdot A^2(\Omega) = \int_{\Omega} (\alpha'(0; V) B(\Omega)) \cdot A^2(\Omega).$$

Assuming that Ω is s -regular for $s > 1/2$, we know from Eq. (2.19) of Lemma 2.3.5 that

$$\begin{aligned} \int_{\Omega} (\alpha'(0; V) B(\Omega)) \cdot A^2(\Omega) &= \int_{\Omega} (\text{div } B(\Omega)) \cdot A^2(\Omega) + \int_{\Omega} (B(\Omega) \times V) \cdot \text{curl } A^2(\Omega) \\ &\quad - \int_{\Omega} (\text{curl } B(\Omega)) \times V \cdot A^2(\Omega) + \int_{\Omega} (B(\Omega) \cdot V) (\text{div } A^2(\Omega)) \\ &\quad + \int_{\partial\Omega} (B(\Omega) \cdot A^2(\Omega)) (V \cdot n) \\ &= \int_{\partial\Omega} (B(\Omega) \cdot A^2(\Omega)) (V \cdot n). \end{aligned}$$

□

3.4 Approximation by finite element exterior calculus

In this section we assume that Ω is a toroidal domain with polyhedral boundary and that $(\mathcal{T}_h)_{h>0}$ is a quasi-uniform and shape regular³ family of tetrahedron meshes of $\bar{\Omega}$, with h the largest diameter of the cells. From [Amr+98, Proposition 3.7], we know that we can choose $s > 1/2$ so that Ω is s -regular. We denote by $\Delta^0(\mathcal{T}_h)$, $\Delta^1(\mathcal{T}_h)$, $\Delta^2(\mathcal{T}_h)$ and $\Delta^3(\mathcal{T}_h)$ the sets of points, edges, faces and cells of the mesh \mathcal{T}_h , respectively. For a k -simplex S of the mesh \mathcal{T}_h , we define $\Delta^i(S)$ as the set of i -simplices which have non-empty intersection with \bar{S} for $i < k$. Moreover, we assume that the cutting surface Σ and toroidal curve γ' introduced in Section 2.2.1 which are used in the variational formulations of the harmonic field are compatible with the mesh, that is, are given by unions of elements of $\Delta^2(\mathcal{T}_h)$ and $\Delta^1(\mathcal{T}_h)$ respectively. Throughout this section, inequality constants denoted by C are independent of h , but may depend on the domain Ω .

3. We refer to [EG21a] for the definition of quasi-uniformity and shape regularity.

Our goal is to provide a finite elements scheme to compute both the harmonic helicity of the domain Ω and its shape gradient. In Section 3.4.1, we recall the main properties of classical families of elements coming from finite element exterior calculus. Then, we recall in Section 3.4.2 some notions related to the discrete version of the de Rham complex, and the related discrete harmonic fields. Afterwards, in Section 3.4.3 we prove the convergence of the numerical harmonic helicity. Finally, we prove in Section 3.4.4 that the numerical shape gradient converges to the continuous one.

3.4.1 Classical finite element exterior calculus families

Here, we introduce some classical families in finite element exterior calculus. The main idea is to define a discretized version of each functional space in the de Rham complex, and stable projections onto these spaces which commute with the differential operators. All these notions were first introduced in [RT77; Ned80], and later generalized for differential forms in [AFW06]. We also recall that a short introduction to the subject was given in Section 1.3.4.

For r an integer and T a tetrahedral domain in \mathbb{R}^3 , we define $\mathcal{P}_r(T)$ as the set of polynomials on T with degree at most r , and $\tilde{\mathcal{P}}_r(T)$ the set of homogeneous polynomials on T of degree r . Then, $\mathcal{P}_r^{-,\text{curl}}(T)$ and $\mathcal{P}_r^{-,\text{div}}$ are defined as

$$\begin{aligned}\mathcal{P}_r^{-,\text{curl}}(T) &= \mathcal{P}_{r-1}(T)^3 \oplus \{p \in \tilde{\mathcal{P}}_r(T)^3 \mid p \cdot \mathbf{x} = 0\}, \\ \mathcal{P}_r^{-,\text{div}}(T) &= \mathcal{P}_{r-1}(T)^3 \oplus \{\mathbf{x}p \mid p \in \tilde{\mathcal{P}}_{r-1}(T)\}.\end{aligned}$$

For r positive, we then define the discretizations

$$\begin{aligned}V_h^0(\Omega) &= \{u \in H^1(\Omega) \mid u|_K \in \mathcal{P}_r(T) \ \forall T \in \mathcal{T}_h\}, \\ V_h^1(\Omega) &= \{u \in H(\text{curl}, \Omega) \mid u|_K \in \mathcal{P}_r^{-,\text{curl}}(T) \ \forall T \in \mathcal{T}_h\}, \\ V_h^2(\Omega) &= \{u \in H(\text{div}, \Omega) \mid u|_K \in \mathcal{P}_r^{-,\text{div}}(T) \ \forall T \in \mathcal{T}_h\}, \\ V_h^3(\Omega) &= \{u \in L^2(\Omega) \mid u|_K \in \mathcal{P}_{r-1}(T) \ \forall T \in \mathcal{T}_h\}.\end{aligned}$$

We then obtain the following sequence

$$V_h^0(\Omega) \xrightarrow{\nabla} V_h^1(\Omega) \xrightarrow{\text{curl}} V_h^2(\Omega) \xrightarrow{\text{div}} V_h^3(\Omega).$$

These finite element spaces correspond respectively to the Lagrange P^r elements, the Nedelec first kind elements of order r , the Raviart Thomas elements of order r , and the discontinuous P^{r-1} elements.

One can check easily, using integration by parts, that u is in $V_h^1(\Omega)$ if and only if the tangential trace of u is continuous along all shared faces of Ω . More precisely, if T_1 and T_2 are in $\Delta^3(\mathcal{T}_h)$ and S_1, S_2 are in $\Delta^2(K_1)$ and $\Delta^2(K_2)$ respectively with $T_1 \cap T_2 = S_1 = S_2$, we have

$$u \times n_{S_1} + u \times n_{S_2} = 0.$$

Similarly, we have that u is in $V_h^2(\Omega)$ if and only the normal trace of u is continuous along all shared faces of Ω .

We also introduce the discrete affine space V_h^{aff} to solve Eq. (3.5) numerically. It is defined by

$$V_h^{\text{aff}}(\Omega) = \{v \in H^1(\Omega \setminus \Sigma) \mid v|_T \in \mathcal{P}_r(T) \ \forall T \in \mathcal{T}_h, \text{ and } \llbracket v \rrbracket_\Sigma = 1\},$$

where $\llbracket v \rrbracket_\Sigma$ denotes the jump of v across Σ . The corresponding linear space is $V_h^0(\Omega)$.

We also use the smoothed quasi interpolators built for example in [AFW06, Section 5.4.] for differential forms and [EG21a, Chapter 23] for vector fields. The usual quasi interpolators are denoted by Π_h^k , and the trace preserving quasi interpolators by $\Pi_{h,0}^k$. It is known that these quasi interpolators are stable, and that they make the following diagram commute

$$\begin{array}{ccccccc} H^1(\Omega) & \xrightarrow{\nabla} & H(\text{curl}, \Omega) & \xrightarrow{\text{curl}} & H(\text{div}, \Omega) & \xrightarrow{\text{div}} & L^2(\Omega) \\ \Pi_h^0 \downarrow & & \Pi_h^1 \downarrow & & \Pi_h^2 \downarrow & & \Pi_h^3 \downarrow \\ V_h^0(\Omega) & \xrightarrow{\nabla} & V_h^1(\Omega) & \xrightarrow{\text{curl}} & V_h^2(\Omega) & \xrightarrow{\text{div}} & V_h^3(\Omega) \end{array},$$

with a similar diagram for the traceless spaces. We then have the following approximation estimates on the quasi interpolators (see for example [EG18, Theorem 2.2. and 2.3.]).

Proposition 3.4.1. *We have, for all k between 0 and 3 and $u \in H^s$ regular,*

$$\begin{aligned} \|u - \Pi_h^k u\|_{L^2} &\leq Ch^s |u|_{H^s}, \\ \|u - \Pi_{h,0}^k u\|_{L^2} &\leq Ch^s |u|_{H^s}. \end{aligned}$$

3.4.2 Discretization of the de Rham complex

In this section we state some results about the discretization of the de Rham complex. We borrow here most of our notations and lemmas from [AFW06]. We begin by defining discrete equivalents of closed and exact fields, which allow us to define the discrete harmonic fields. This then allows us to derive Hodge decompositions in the discrete setting, and uniform Poincaré inequalities. We then state some lemmas which will be useful for the coming convergence results.

First, we use some notations from the differential forms setting to unify some definitions and results. We denote

$$H\Lambda^0(\Omega) = H^1(\Omega), \quad H\Lambda^1(\Omega) = H(\text{curl}, \Omega), \quad H\Lambda^2(\Omega) = H(\text{div}, \Omega), \quad \text{and} \quad H\Lambda^3(\Omega) = L^2(\Omega),$$

as well as

$$d^0 = \nabla, \quad d^1 = \text{curl}, \quad \text{and} \quad d^2 = \text{div}.$$

We also denote $d^k = 0$ when k is negative or larger than 2. The corresponding traceless spaces are denoted $\mathring{H}\Lambda^k(\Omega)$, and the discrete traceless spaces are given by $\mathring{V}_h^k(\Omega) = V_h^k(\Omega) \cap \mathring{H}\Lambda^k(\Omega)$.

We are now able to define the discrete harmonic fields. We denote

$$\mathcal{B}_h^k(\Omega) = d^{k-1}V_h^{k-1}(\Omega), \quad \mathcal{Z}_h^k(\Omega) = \{u \in V_h^k(\Omega) \mid d^k u = 0\},$$

and

$$\mathcal{K}_h^k(\Omega) = \mathcal{Z}_h^k(\Omega) \cap \mathcal{B}_h^k(\Omega)^\perp.$$

Similarly, we define for traceless spaces

$$\mathring{\mathcal{B}}_h^k(\Omega) = d^{k-1}\mathring{V}_h^{k-1}(\Omega), \quad \mathring{\mathcal{Z}}_h^k(\Omega) = \{u \in \mathring{V}_h^k(\Omega) \mid d^k u = 0\},$$

and

$$\mathring{\mathcal{K}}_h^k(\Omega) = \mathring{\mathcal{Z}}_h^k(\Omega) \cap \mathring{\mathcal{B}}_h^k(\Omega)^\perp.$$

From the equivalence of discrete and continuous de Rham cohomology (see e.g. [AFW10, Section 5.6]), we get

$$\mathcal{K}_h^0(\Omega) \cong \mathbb{R}, \quad \mathcal{K}_h^1(\Omega) \cong \mathbb{R}, \quad \mathcal{K}_h^2(\Omega) \cong 0 \quad \text{and} \quad \mathcal{K}_h^3(\Omega) \cong 0.$$

Similarly, from the equivalence of discrete and continuous de Rham cohomology with boundary condition, and Poincaré duality, we get

$$\mathring{\mathcal{K}}_h^0(\Omega) \cong 0, \quad \mathring{\mathcal{K}}_h^1(\Omega) \cong 0, \quad \mathring{\mathcal{K}}_h^2(\Omega) \cong \mathbb{R} \quad \text{and} \quad \mathring{\mathcal{K}}_h^3(\Omega) \cong \mathbb{R}.$$

Remark 3.4.2. *In the continuous case, we defined the harmonic fields as $\mathcal{K}(\Omega) = H(\text{curl}^0, \Omega) \cap H_0(\text{div}^0, \Omega)$. By using $H_0(\text{div}^0, \Omega) = \nabla H^1(\Omega)^\perp$ and $H(\text{curl}^0, \Omega) = \text{curl} H_0(\text{curl}, \Omega)^\perp$ from Proposition A.3 of Appendix A, we recover two expressions for $\mathcal{K}(\Omega)$ which are similar to the discrete ones. However, in the discrete case, the two spaces $\mathcal{K}_h^1(\Omega)$ and $\mathring{\mathcal{K}}_h^2(\Omega)$ do not coincide. Indeed, elements of $\mathcal{K}_h^1(\Omega)$ are curl free but only weakly divergence free and tangent to the boundary meaning that they are not orthogonal to $\nabla H^1(\Omega)$ but only to the finite dimensional space $\nabla V_h^0(\Omega)$. On the other hand, elements of $\mathring{\mathcal{K}}_h^2(\Omega)$ are divergence free and tangent to the boundary, but only weakly curl free, that is, not orthogonal to $\text{curl} H_0(\text{curl}^0, \Omega)$ but to $\text{curl} \mathring{V}_h^1(\Omega)$.*

From these definitions, it is now straightforward to find the discrete Hodge decompositions.

$$\begin{aligned} V_h^k(\Omega) &= \mathcal{Z}_h^k(\Omega)^\perp \oplus \mathcal{K}_h^k(\Omega) \oplus \mathcal{B}_h^k(\Omega), \\ \mathring{V}_h^k(\Omega) &= \mathring{\mathcal{Z}}_h^k(\Omega)^\perp \oplus \mathring{\mathcal{K}}_h^k(\Omega) \oplus \mathring{\mathcal{B}}_h^k(\Omega). \end{aligned}$$

There is also an equivalent of the Poincaré inequality in the discrete case which is given in [AFW06][Lemma 5.11].

Proposition 3.4.3. *There exists a constant C , independent of h , such that for all u in $\mathcal{Z}_h^k(\Omega)^\perp$*

$$\|u\|_{L^2} \leq C \|d^k u\|_{L^2}.$$

We will also be using the following lemma for the proof of convergence of the harmonic field. This lemma is proven in [AFW06][Lemma 5.9] for harmonic forms.

Lemma 3.4.4. *For all u_h in $\mathcal{K}_h^1(\Omega)$ there exists u in $\mathcal{K}(\Omega)$ such that $\|u\| \leq \|u_h\|$ and*

$$\|u_h - u\|_{L^2} \leq \|u - \Pi_h^1 u\|_{L^2}.$$

3.4.3 Numerical convergence of the harmonic helicity

We begin by studying the approximation of the harmonic field. As we have seen in Section 2.2.2, there are two different variational formulations for the harmonic fields. Although they give the same fields in the continuous case, this will not be true at the discrete level. As we will see, the classical Poisson formulation will give a discrete harmonic field in $\mathcal{K}_h^1(\Omega)$, and the mixed formulation will give a discrete harmonic field in $\mathring{\mathcal{K}}_h^2(\Omega)$. Since the domain Ω is fixed throughout this section, we denote $B(\Omega)$, $A^2(\Omega)$ and $A^1(\Omega)$ as B , A^1 and A^2 respectively.

Before studying the convergence of the numerical solutions, we state their well-posedness.

Proposition 3.4.5. *There exists a unique solution to the following variational formulation. Find $u_h \in V_h^{\text{aff}}(\Omega)$ such that, for all $v_h \in V_h^0(\Omega)$,*

$$\int_{\Omega} \nabla u_h \cdot \nabla v_h = 0. \tag{3.16}$$

Furthermore, $B_h^{\text{curl}} = \nabla u_h$ is in $\mathcal{K}_h^1(\Omega)$.

Proof. We denote by u the solution to Eq. (3.5), and $B = \nabla u$ the normalized harmonic field of Ω . First, we notice that for all h there exists a function φ_h in $V_h^{\text{aff}}(\Omega)$ such that $\|\varphi_h\|_{H^1(\Omega \setminus \Sigma)} \leq C\|u\|_{H^1(\Omega \setminus \Sigma)}$. This may for example be obtained by taking the H^1 orthogonal projection of u onto $V_h^{\text{aff}}(\Omega)$. We then notice that there is a unique solution to the following variational problem. Find $\tilde{u}_h \in V_h^0(\Omega)$ with zero average such that for all $v_h \in V_h^0(\Omega)$

$$\int_{\Omega} \nabla \tilde{u}_h \cdot \nabla v_h = - \int_{\Omega} \nabla \varphi_h \cdot \nabla v_h. \quad (3.17)$$

Indeed, this problem is a classical discretization of a Poisson equation, so that the Lax–Milgram theorem applies.

Now, define $u_h = \tilde{u}_h + \varphi_h$. Since $\nabla u_h = \nabla \tilde{u}_h + \nabla \varphi_h$, and φ_h is in $V_h^{\text{aff}}(\Omega)$, we notice that u_h is solution to Eq. (3.16) if and only if \tilde{u}_h is solution to Eq. (3.17). As a consequence, Eq. (3.16) is also well-posed.

We now prove that ∇u_h is in $V_h^1(\Omega)$. It is straightforward that interelement continuity will be verified on all surfaces which are not included in Σ_h . Therefore, we take $S \in \Delta^2(\mathcal{T}_h)$ included in Σ_h . We know that there exist two cells T_1 and T_2 in $\Delta^3(\mathcal{T}_h)$ such that $S \in \Delta^2(T_1) \cap \Delta^2(T_2)$. We then denote $S = S_1$ when seen as an element of $\Delta^2(T_1)$, and $S = S_2$ when seen as an element of $\Delta^2(T_2)$, and order T_1 and T_2 so that the exterior normal of T_1 on S_1 is n_{Σ_h} . Since u_h is in $V_h^{\text{aff}}(\Omega)$, we have $u_h|_{S_2} - u_h|_{S_1} = 1$, so that $\nabla u_h \times n_{\Sigma_h|S_2} = \nabla u_h \times n_{\Sigma_h|S_1}$. As a consequence, interelement continuity is verified across S , so that $B_h^{\text{curl}} = \nabla u_h$ is in $V_h^1(\Omega)$.

Finally, we prove that B_h^{curl} is in $\mathcal{K}_h^1(\Omega)$. The fact that B_h^{curl} is in $\mathcal{B}_h^1(\Omega)^\perp$ is given directly by Eq. (3.16). Now, we take T in $\Delta^3(\mathcal{T}_h)$. Since $B_h^{\text{curl}}|_T = \nabla u_h|_T$, we have $B_h^{\text{curl}}|_T \in \mathcal{B}_h^1(T)$. Now, using that $\mathcal{B}_h^1(T)$ is a subset of $\mathcal{Z}_h^1(T)$, and that B_h^{curl} is in $\mathcal{Z}_h^1(\Omega)$ if and only if $B_h^{\text{curl}}|_T$ is in $\mathcal{Z}_h^1(T)$ for all T , we are able to conclude. \square

Proposition 3.4.6. *There exists a unique solution to the following variational formulation. Find $(B_h^{\text{div}}, u_h) \in \mathring{V}_h^2(\Omega) \times (V_h^3(\Omega) \cap L_0^2(\Omega))$ such that, for all $(\tau_h, v_h) \in \mathring{V}_h^2(\Omega) \times V_h^3(\Omega)$*

$$\begin{aligned} \int_{\Omega} (\text{div } B_h^{\text{div}}) v_h &= 0, \\ \int_{\Omega} B_h^{\text{div}} \cdot \tau_h + \int_{\Omega} u_h (\text{div } \tau_h) &= \int_{\Sigma} \tau_h \cdot n_{\Sigma}. \end{aligned} \quad (3.18)$$

Furthermore, B_h^{div} is in $\mathring{\mathcal{K}}_h^2(\Omega)$.

Proof. The well-posedness comes from the exact same arguments as in the continuous case, by replacing the Poincaré inequalities and Hodge decompositions by their discrete counterparts.

We now prove that B_h^{div} is in $\mathring{\mathcal{K}}_h^2(\Omega)$. The fact that B_h^{div} is in $\mathring{\mathcal{Z}}_h^2(\Omega)$ comes directly from the first equation of (3.18). Now, taking $\tau_h = \text{curl } \rho_h$ in the second equation for $\rho_h \in \mathring{V}_h^1(\Omega)$, we get

$$\begin{aligned} \int_{\Omega} B_h^{\text{div}} \cdot \text{curl } \rho_h &= \int_{\Sigma} \text{curl } \rho_h \cdot n_{\Sigma} \\ &= \int_{\gamma'} \rho_h \cdot t' \\ &= 0, \end{aligned}$$

so that B_h^{div} is in $\mathring{\mathcal{B}}_h^2(\Omega)^\perp$. \square

We now prove the two following approximation results.

Proposition 3.4.7. *There exists a constant C independent of h such that*

$$\begin{aligned}\|B_h^{\text{curl}} - B\|_{L^2} &\leq Ch^s \|B\|_{L^2}, \\ \|B_h^{\text{div}} - B\|_{L^2} &\leq Ch^s \|B\|_{L^2}.\end{aligned}$$

Proof. We begin by proving the convergence for B_h^{curl} . From Lemma 3.4.4, we know there exists \tilde{B}_h in $\mathcal{K}(\Omega)$ such that

$$\|\tilde{B}_h - B_h^{\text{curl}}\|_{L^2} \leq \|\tilde{B}_h - \Pi_h^1 \tilde{B}_h\|_{L^2}.$$

From the continuity of the circulation along γ with respect to the $H\text{curl}$ norm, we have

$$\begin{aligned}\left| \int_{\gamma} (\tilde{B}_h - B) \cdot t \right| &= \left| \int_{\gamma} (\tilde{B}_h - B_h^{\text{curl}}) \cdot t \right| \\ &\leq C \|\tilde{B}_h - B_h^{\text{curl}}\|_{H\text{curl}} \\ &\leq C \|\tilde{B}_h - B_h^{\text{curl}}\|_{L^2} \\ &\leq C \|\tilde{B}_h - \Pi_h^1 \tilde{B}_h\|_{L^2}.\end{aligned}$$

Since B and \tilde{B}_h are in $\mathcal{K}(\Omega)$, we get from [Val19, Lemma 5] that

$$\begin{aligned}\|\tilde{B}_h - B\|_{L^2} &\leq C \left(\|\text{div } \tilde{B}_h - \text{div } B\|_{L^2} + \|\text{curl } \tilde{B}_h - \text{curl } B\|_{L^2} + \left| \int_{\gamma} (\tilde{B}_h - B) \cdot t \right| \right) \\ &\leq C \|\tilde{B}_h - \Pi_h^1 \tilde{B}_h\|_{L^2}.\end{aligned}$$

We then get by triangle inequality

$$\begin{aligned}\|B_h^{\text{curl}} - B\|_{L^2} &\leq \|B_h^{\text{curl}} - \tilde{B}_h\|_{L^2} + \|\tilde{B}_h - B\|_{L^2} \\ &\leq C \|\tilde{B}_h - \Pi_h^1 \tilde{B}_h\|_{L^2}.\end{aligned}$$

Finally, using Proposition 3.4.1 and the continuous injection of $H(\text{curl}, \Omega) \cap H_0(\text{div}, \Omega)$ into $H^s(\Omega)^3$, we get

$$\begin{aligned}\|B_h^{\text{curl}} - B\|_{L^2} &\leq Ch^s |\tilde{B}_h|_{H^s} \\ &\leq Ch^s \|\tilde{B}_h\|_{L^2} \\ &\leq Ch^s \|B_h\|_{L^2} \\ &\leq Ch^s \|B\|_{L^2},\end{aligned}$$

where we used the inequality $\|\tilde{B}_h\|_{L^2} \leq \|B_h\|_{L^2}$ from Lemma 3.4.4. We now prove the convergence of B_h^{div} to B . Using Eqs. (2.15) and (3.18), we have

$$\begin{aligned}\int_{\Omega} B \cdot \tau + \int_{\Omega} u (\text{div } \tau_h) &= \int_{\Sigma} \tau_h \cdot n_{\Sigma}, \\ \int_{\Omega} B_h^{\text{div}} \cdot \tau + \int_{\Omega} u_h (\text{div } \tau_h) &= \int_{\Sigma} \tau_h \cdot n_{\Sigma},\end{aligned}$$

for all τ_h in $\dot{V}_h^2(\Omega)$. As a consequence, for all τ_h in $\dot{Z}_h^2(\Omega)$, we get

$$\int_{\Omega} (B_h^{\text{div}} - B) \cdot \tau_h = 0.$$

Since both B_h^{div} and $\Pi_{h,0}^2 B$ are in $\mathring{Z}_h^2(\Omega)$, we have

$$\int_{\Omega} (B_h^{\text{div}} - B) \cdot (B_h^{\text{div}} - B) = \int_{\Omega} (B_h^{\text{div}} - B) \cdot (\Pi_{h,0}^2 B - B),$$

so that

$$\|B_h^{\text{div}} - B\|_{L^2} \leq \|\Pi_{h,0}^2 B - B\|_{L^2}.$$

Using again Proposition 3.4.1 and the fact that Ω is s -regular, we get the desired result

$$\|B_h^{\text{div}} - B\|_{L^2} \leq Ch^s \|B\|_{L^2}.$$

□

We now study the well-posedness and the convergence of the vector potentials of B . A first remark is that the vector potential orthogonal to B is well studied in the literature via the Hodge Laplacian (see for example [AFW06]). As such, we study the approximation of such vector potentials which we denote A_h^1 , and recover A_h^2 , the one which is circulation free, by the discrete counterpart of Eq. (3.11)

$$A_h^2 = A_h^1 - \left(\int_{\gamma'} A_h^1 \cdot t' \right) B_h^{\text{curl}}. \quad (3.19)$$

Proposition 3.4.8. *There exists a unique solution to the following variational formulation. Find $(A_h^1, u_h) \in V_h^1(\Omega) \times V_h^2(\Omega)$ such that, for all $(\tau_h, v_h) \in V_h^1(\Omega) \times V_h^2(\Omega)$,*

$$\begin{aligned} \int_{\Omega} A_h^1 \cdot \tau_h &= \int_{\Omega} \text{curl } \tau_h \cdot u_h, \\ \int_{\Omega} \text{curl } A_h^1 \cdot v_h + \int_{\Omega} (\text{div } u_h) (\text{div } v_h) &= \int_{\Omega} B_h^{\text{div}} \cdot v_h. \end{aligned} \quad (3.20)$$

Furthermore, we have $\text{curl } A_h^1 = B_h^{\text{div}}$.

Proof. The well-posedness is proven in the exact same way as in the continuous case Proposition 3.2.1, by replacing the Hodge decomposition and Poincaré inequality by their discrete counterparts. The fact that $\text{curl } A_h^1 = B_h^{\text{div}}$ is also proven in a similar way as in Proposition 3.2.1. Using $\mathcal{K}_h^2(\Omega) = 0$, and the discrete Hodge decomposition (see Section 3.4.2), we have

$$V_h^2(\Omega) = \mathcal{Z}_h^2(\Omega)^\perp \oplus \mathcal{B}_h^2(\Omega),$$

so that $u_h = u_h^\nabla + u_h^{\text{curl}}$ with $\int_{\Omega} u_h^\nabla \cdot v_h = 0$ for all v_h in $V_h^2(\Omega)$ with $\text{div } v_h = 0$, and $\text{div } u_h^{\text{curl}} = 0$. Therefore, taking $v_h = u_h^{\text{curl}}$ in the second equation of Eq. (3.20), we get

$$\int_{\Omega} (\text{div } u_h) (\text{div } u_h^\nabla) = 0,$$

so that, since $\text{div } u_h^{\text{curl}} = 0$, we obtain $\text{div } u_h^\nabla = \text{div } u_h = 0$. From this, we get $\int_{\Omega} A_h^1 \cdot v_h = \int_{\Omega} B_h^{\text{div}} \cdot v_h$ for all $v_h \in V_h^2(\Omega)$, and $B_h^{\text{div}} \in V_h^2(\Omega)$ implies the desired equality. □

Proposition 3.4.9. *There exists a constant C independent of h such that*

$$\|A_h^1 - A^1\|_{L^2} \leq Ch^s \|B\|_{L^2}.$$

Proof. Define $(\tilde{A}_h^1, \tilde{u}_h)$ as the solution to the following variational problem. Find $(\tilde{A}_h^1, \tilde{u}_h) \in V_h^1(\Omega) \times V_h^2(\Omega)$ such that, for all $(\tau_h, v_h) \in V_h^1(\Omega) \times V_h^2(\Omega)$,

$$\begin{aligned} \int_{\Omega} \tilde{A}_h^1 \cdot \tau_h &= \int_{\Omega} \operatorname{curl} \tau_h \cdot \tilde{u}_h, \\ \int_{\Omega} \operatorname{curl} \tilde{A}_h^1 \cdot v_h + \int_{\Omega} (\operatorname{div} \tilde{u}_h) (\operatorname{div} v_h) &= \int_{\Omega} B \cdot v_h. \end{aligned}$$

The well-posedness of this equation is obtained in the same way as for A_h^1 . Furthermore, by continuity of the resolvent, and independence of the discrete Poincaré inequality constants in h , we get

$$\|\tilde{A}_h^1 - A_h^1\|_{L^2} \leq C \|B - B_h^{\operatorname{div}}\|_{L^2}.$$

Furthermore, we obtain from of [AFW06, Theorem 7.9] that

$$\|\tilde{A}_h^1 - A^1\|_{L^2} \leq Ch^s \|B\|_{L^2}.$$

We then get the desired result from a triangle inequality and Proposition 3.4.7. \square

As we have seen in Section 3.2.1, there are two ways of computing the harmonic helicity of Ω . The first one is done by computing circulations of A^1 , and the second by taking the L^2 product of B and A^2 . As we shall see in the following results, we can also recover the numerical harmonic helicity in two similar ways. To do this, we first need to establish convergence of the circulation of A_h^1 , which is given by the following lemma.

Lemma 3.4.10. *We have*

$$\left| \int_{\gamma'} (A_h^1 - A^1) \cdot t' \right| \leq Ch^s \|B\|_{L^2}.$$

Proof. From Proposition 3.4.8, we have

$$\begin{aligned} \|A_h^1 - A^1\|_{H_{\operatorname{curl}}}^2 &= \|A_h^1 - A^1\|_{L^2}^2 + \|\operatorname{curl} A_h^1 - \operatorname{curl} A^1\|_{L^2}^2 \\ &= \|A_h^1 - A^1\|_{L^2}^2 + \|B_h^{\operatorname{div}} - B\|_{L^2}^2, \end{aligned}$$

so that by Propositions 3.4.7 and 3.4.9, we get

$$\|A_h^1 - A^1\|_{H_{\operatorname{curl}}} \leq Ch^s \|B\|_{L^2}.$$

Now, since $\operatorname{curl} A_h^1 = B_h^{\operatorname{div}}$, which is in $H_0(\operatorname{div}, \Omega)$, the circulation of A_h^1 along γ' is well-defined by Eq. (2.13), and this circulation is bounded by the $H(\operatorname{curl}, \Omega)$ norm. We therefore have

$$\left| \int_{\gamma'} (A_h^1 - A^1) \cdot t \right| \leq Ch^s \|B\|_{L^2}.$$

\square

Corollary 3.4.11. *Defining A_h^2 as in Eq. (3.19), we get*

$$\|A_h^2 - A^2\|_{L^2} \leq Ch^s \|B\|_{L^2}.$$

Proof. We get this result by writing

$$A_h^2 - A^2 = A_h^1 - A^1 - \left(\int_{\gamma'} (A_h^1 - A^1) \cdot t \right) B_h^{\text{curl}} + \left(\int_{\gamma'} A^1 \cdot t \right) (B - B_h^{\text{curl}}).$$

We are then able to conclude using Propositions 3.4.7 and 3.4.9 and Lemma 3.4.10. \square

Theorem 3.4.12 (Convergence of harmonic helicity). *We have*

$$|\mathcal{H}(\Omega) - \mathbb{H}(B_h^{\text{div}})| \leq Ch^s \|B\|_{L^2}^2,$$

where $\mathbb{H}(B_h^{\text{div}})$ can be either computed as

$$\mathbb{H}(B_h^{\text{div}}) = - \left(\int_{\gamma'} A_h^1 \cdot t' \right) \left(\int_{\gamma} A_h^1 \cdot t \right),$$

or as

$$\mathbb{H}(B_h^{\text{div}}) = \int_{\Omega} B_h^{\text{div}} \cdot A_h^2.$$

Proof. We use the formulation of the helicity through A_h^2 , the other one being a simple consequence of the Bevir–Gray formula. To obtain the desired estimate, we write

$$\int_{\Omega} B_h^{\text{div}} \cdot A_h^2 - \mathcal{H}(\Omega) = \int_{\Omega} (B_h^{\text{div}} - B) \cdot A_h^2 + \int_{\Omega} B \cdot (A_h^2 - A^2).$$

The conclusion then follows from Proposition 3.4.7 and Corollary 3.4.11. \square

3.4.4 Convergence of the Shape Gradient

In this section, we aim to prove the convergence of the numerical shape gradient to the continuous one. This is given by the following theorem.

Theorem 3.4.13. *Let B_h be either B_h^{curl} or B_h^{div} as defined in Section 3.4.3, and A_h^2 as defined by Eq. (3.19). Then, for all V in \mathcal{B}_1 , we have*

$$\left| 2 \int_{\partial\Omega} (B_h \cdot A_h^2) (V \cdot n) - \mathcal{H}'(\Omega; V) \right| \leq Ch^{s-1/2} \|B\|_{L^2}^2 \|V \cdot n\|_{L^\infty(\partial\Omega)}$$

The idea of the proof is to estimate the L^2 error for B_h and A_h^2 on faces of \mathcal{T}_h which are on the boundary of Ω . In order to do so, we begin by noting that for each such face F in $\Delta^2(\mathcal{T}_h)$, there exists a unique cell T in $\Delta^3(\mathcal{T}_h)$ such that F is in $\Delta^2(T)$. For a cell T , we also denote its diameter as h_T . From quasi-uniformity of the mesh, we know that there exists $C > 0$ such that for all T in $\Delta^3(\mathcal{T}_h)$, we have $h_T \geq Ch$. Furthermore, using shape regularity, we know that there exists $C > 0$ such that $|T| \geq Ch_T^3$.

In order to prove Theorem 3.4.13, we use the following Lemmas from [EG21a, Chapter 12]. The author also notes that the proof of Theorem 3.4.13 was suggested by Alexandre Ern.

Lemma 3.4.14 (Remark 12.19 in [EG21a]). *Let T be in $\Delta^3(\mathcal{T}_h)$ and F be in $\Delta^2(T)$. Then, there exists $C > 0$ such that for all v in $H^s(T)$*

$$\|v\|_{L^2(F)} \leq C \left(h_T^{-1/2} \|v\|_{L^2(T)} + h_T^{s-1/2} |v|_{H^s(T)} \right).$$

Lemma 3.4.15 (Lemma 12.8 in [EG21a]). *Let T be in $\Delta^3(\mathcal{T}_h)$ and F be in $\Delta^2(T)$. Then, there exists $C > 0$ such that for all v in $\mathcal{P}_r(T)$*

$$\|v\|_{L^2(F)} \leq Ch_T^{-1/2} \|v\|_{L^2(T)}.$$

Lemma 3.4.16 (Lemma 12.12 in [EG21a]). *Let T be in $\Delta^3(\mathcal{T}_h)$. Then, there exists $C > 0$ such that for all v in $H^s(T)$*

$$\|v - \bar{v}_T\|_{L^2(T)} \leq h_T^s \left(\frac{h_T^d}{|T|} \right)^{1/2} |v|_{H^s(T)},$$

where \bar{v}_T is the average of v on T .

In order to prove Theorem 3.4.13, we prove the following local estimate.

Proposition 3.4.17. *Let T be in $\Delta^3(\mathcal{T}_h)$ and F in $\Delta^2(T)$. Then, for all v in $H^s(T)$ and v_h in $\mathcal{P}_r(T)$, we have*

$$\|v_h - v\|_{L^2(F)} \leq C \left(h_T^{-1/2} \|v_h - v\|_{L^2(T)} + h_T^{s-1/2} |v|_{H^s(T)} \right).$$

Proof. We begin by writing

$$\|v_h - v\|_{L^2(F)} \leq \|v_h - \bar{v}_T\|_{L^2(F)} + \|\bar{v}_T - v\|_{L^2(F)}. \quad (3.21)$$

Then, using Lemma 3.4.14 and the fact that $|\bar{v}_T - v|_{H^s(T)} = |v|_{H^s(T)}$, we obtain

$$\|\bar{v}_T - v\|_{L^2(F)} \leq C \left(h_T^{-1/2} \|\bar{v}_T - v\|_{L^2(T)} + h_T^{s-1/2} |v|_{H^s(T)} \right).$$

Moreover, using Lemma 3.4.16 and shape regularity, we obtain

$$\|\bar{v}_T - v\|_{L^2(T)} \leq Ch_T^s |v|_{H^s(T)},$$

so that

$$\|\bar{v}_T - v\|_{L^2(F)} \leq Ch_T^{s-1/2} |v|_{H^s(T)}. \quad (3.22)$$

Now, for the first term of Eq. (3.21), we use Lemma 3.4.15 to obtain

$$\begin{aligned} \|v_h - \bar{v}_T\|_{L^2(F)} &\leq Ch_T^{-1/2} \|v_h - \bar{v}_T\|_{L^2(T)} \\ &\leq Ch_T^{-1/2} (\|v_h - v\|_{L^2(T)} + \|v - \bar{v}_T\|_{L^2(T)}) \\ &\leq C \left(h_T^{-1/2} \|v_h - v\|_{L^2(T)} + h_T^{s-1/2} |v|_{H^s(T)} \right), \end{aligned} \quad (3.23)$$

where Lemma 3.4.16 was once again used for the last inequality. Combining Eq. (3.22) and Eq. (3.23) in Eq. (3.21), we obtain the desired result. \square

Corollary 3.4.18. *We have*

$$\begin{aligned} \|B_h^{\text{curl}} - B\|_{L^2(\partial\Omega)} &\leq Ch^{s-1/2} \|B\|_{L^2(\Omega)}, \\ \|B_h^{\text{div}} - B\|_{L^2(\partial\Omega)} &\leq Ch^{s-1/2} \|B\|_{L^2(\Omega)}, \\ \|A_h^2 - A^2\|_{L^2(\partial\Omega)} &\leq Ch^{s-1/2} \|B\|_{L^2(\Omega)}. \end{aligned}$$

Proof. We only prove the first inequality, the latter two being proven in the same way. Using Proposition 3.4.17 on the components of B_h and B , we obtain

$$\|B_h^{\text{curl}} - B\|_{L^2(F)} \leq C \left(h_T^{-1/2} \|B_h^{\text{curl}} - B\|_{L^2(T)} + h_T^{s-1/2} |B|_{H^s(T)} \right)$$

for all F in $\Delta^2(\mathcal{T}_h)$ such that $F \subset \partial\Omega$, and T the cell in $\Delta^3(\mathcal{T}_h)$ such that F is in $\Delta^2(T)$. Summing over all such faces, we then obtain

$$\begin{aligned} \|B_h^{\text{curl}} - B\|_{L^2(\partial\Omega)} &= \sum_{\substack{F \in \Delta^2(\mathcal{T}_h), \\ F \subset \partial\Omega}} \|B_h^{\text{curl}} - B\|_{L^2(F)} \\ &\leq C \sum_{\substack{T \in \Delta^3(\mathcal{T}_h), \\ \bar{T} \cap \partial\Omega \neq \emptyset}} \left(h_T^{-1/2} \|B_h^{\text{curl}} - B\|_{L^2(T)} + h_T^{s-1/2} |B|_{H^s(T)} \right) \\ &\leq C \sum_{T \in \Delta^3(\mathcal{T}_h)} \left(h_T^{-1/2} \|B_h^{\text{curl}} - B\|_{L^2(T)} + h_T^{s-1/2} |B|_{H^s(T)} \right) \\ &\leq C \left(h^{-1/2} \|B_h^{\text{curl}} - B\|_{L^2(\Omega)} + h^{s-1/2} |B|_{H^s(\Omega)} \right), \end{aligned}$$

where we used quasi-uniformity of the mesh for the last inequality. Finally, from Proposition 3.4.7 and s -regularity of the domain, we obtain the desired result. \square

Proof of Theorem 3.4.13. For V in \mathcal{B}_1 , we write

$$\int_{\partial\Omega} (B \cdot A^2)(V \cdot n) - \int_{\partial\Omega} (B_h \cdot A_h^2)(V \cdot n) = \int_{\partial\Omega} (B - B_h) \cdot A^2(V \cdot n) + \int_{\partial\Omega} B_h \cdot (A^2 - A_h^2)(V \cdot n).$$

The result is then a simple consequence of Corollary 3.4.18 together with the expression of the shape derivative of \mathcal{H} given in Theorem 3.3.4. \square

3.5 Numerical implementation and results

3.5.1 Specificity of simulations for stellarators

For both historical and practical considerations, it is frequently advantageous for the surfaces under examination to exhibit specific symmetries. In particular, a majority of stellarators are invariant under discrete rotations along the Oz axis, with an angle of $2\pi/N_p$, where N_p takes values of 3 (as in the case of NCSX [Zar+01]) or 5 (as observed in W7X [War+17]). Additionally, stellarators commonly exhibit invariance under the continuous symmetry known as stellarator symmetry, as discussed in detail in [IPW20, Section 12.3] and [DH98]. In practice, these surfaces are represented by a set of coefficients $(R_{m,n}), (Z_{m,n})$ for $m \in \mathbb{N}$ and $n \in \mathbb{Z}$ which define the functions

$$R(u, v) = \sum_{m \geq 0} \sum_{n \in \mathbb{Z}} R_{m,n} \cos(2\pi(mu + nv)), \quad (3.24)$$

$$Z(u, v) = \sum_{m \geq 0} \sum_{n \in \mathbb{Z}} Z_{m,n} \sin(2\pi(mu + nv)). \quad (3.25)$$

Note the absence of sin terms for R and cos terms for Z due to the imposition of stellarator symmetry. The surface is then parametrized in cylindrical coordinates by $\left(R(u, v), \frac{2\pi v}{N_p}, Z(u, v)\right)$ where N_p stands for the discrete symmetry imposed.

For the numerical simulation, we truncate the number of Fourier components in (3.24) and (3.25).

3.5.2 Implementation

Using the symmetries of the system, we only work with one section of the stellarator, characterized by the coefficients $(R_{m,n}, Z_{m,n})$. Our first step is to use Gmsh [GR09] to mesh the interior of a polyhedral approximation of the surface.

Then we use the finite element library FEniCSx ([Scr+22b; Scr+22a; Aln+14]) to assemble the finite element problems Eqs. (3.16), (3.18) and (3.20) to obtain B_h^{div} , B_h^{curl} and A_h^1 . We implemented both first or second order FEEC elements defined in Section 3.4.1 with adequate periodic conditions at the cuts of our section. To solve the linear system required to get B_h^{curl} , that is a Poisson equation, we use the solver MUMPS: MULTifrontal Massively Parallel sparse direct Solver [Ame+01; Ame+06]. B_h^{div} and A_h^1 are more expensive and complex to solve as both are defined in mixed formulations. Both are solved using the iterative Krylov method GMRES [SS86] applied after a careful preconditioning. More precisely, we use the block diagonal preconditioner proposed by Arnold et al. in [AFW06, Section 10.2] for Hodge-Laplacian problems. The preconditioning problems are solved using MUMPS. We believe that using an Auxiliary-space Maxwell (AMS) Solver [HX07] instead⁴ of a direct solver for the preconditioner would improve the efficiency and scalability of our method when using more than a few million degrees of freedom.

3.5.3 Numerical tests

Once we have computed B_h^{div} , B_h^{curl} and A_h^1 that are represented in Fig. 3.1, we compute the harmonic helicity and its shape gradient. As was stated in Corollary 3.3.3, we know that axisymmetric tori have zero harmonic helicity. Numerically, we have found in this case a value of 10^{-9} . This was computed with a major and minor radius of 1 and 0.1 respectively, second order elements, and h equal to 0.025. For more interesting shapes, as NCSX's plasma, we do not have a reference. As mentioned in Section 3.5.1, we have a continuous description of the shape (i.e. not a polyhedral one), thus we perform two tests.

1. On the left side of Fig. 3.2, we perform a better and better approximation of the continuous shape. To this aim we provide finer and finer grid description of the surface to the mesher. Hence, variation of the obtained magnetic helicity are due both to variations of the domain and to the finite element approximation error.
2. On the right side of Fig. 3.2, we fix at the beginning a polyhedral shape that is an approximation of the continuous surface described by the set of coefficients $(R_{m,n}, Z_{m,n})$ and use finer and finer meshes of this fixed polyhedral shape as h goes to 0. Hence, variations of the magnetic helicity are only due to the numerical approximation of the fields. This is the situation described by the theoretical analysis in Section 3.4. The reference solution was obtained on a high-performance computing cluster using a mesh size of $h = 0.025$ with second-order finite elements. This resulted in linear systems with approximately 5 million degrees of freedom, which were solved in a matter of minutes.

Except for the reference solution, all simulations can be conveniently performed on a laptop with 32 GB of RAM.

4. We had issues porting AMS hypre [FY02] solvers to the background sparse linear library Petsc [Bal+98]

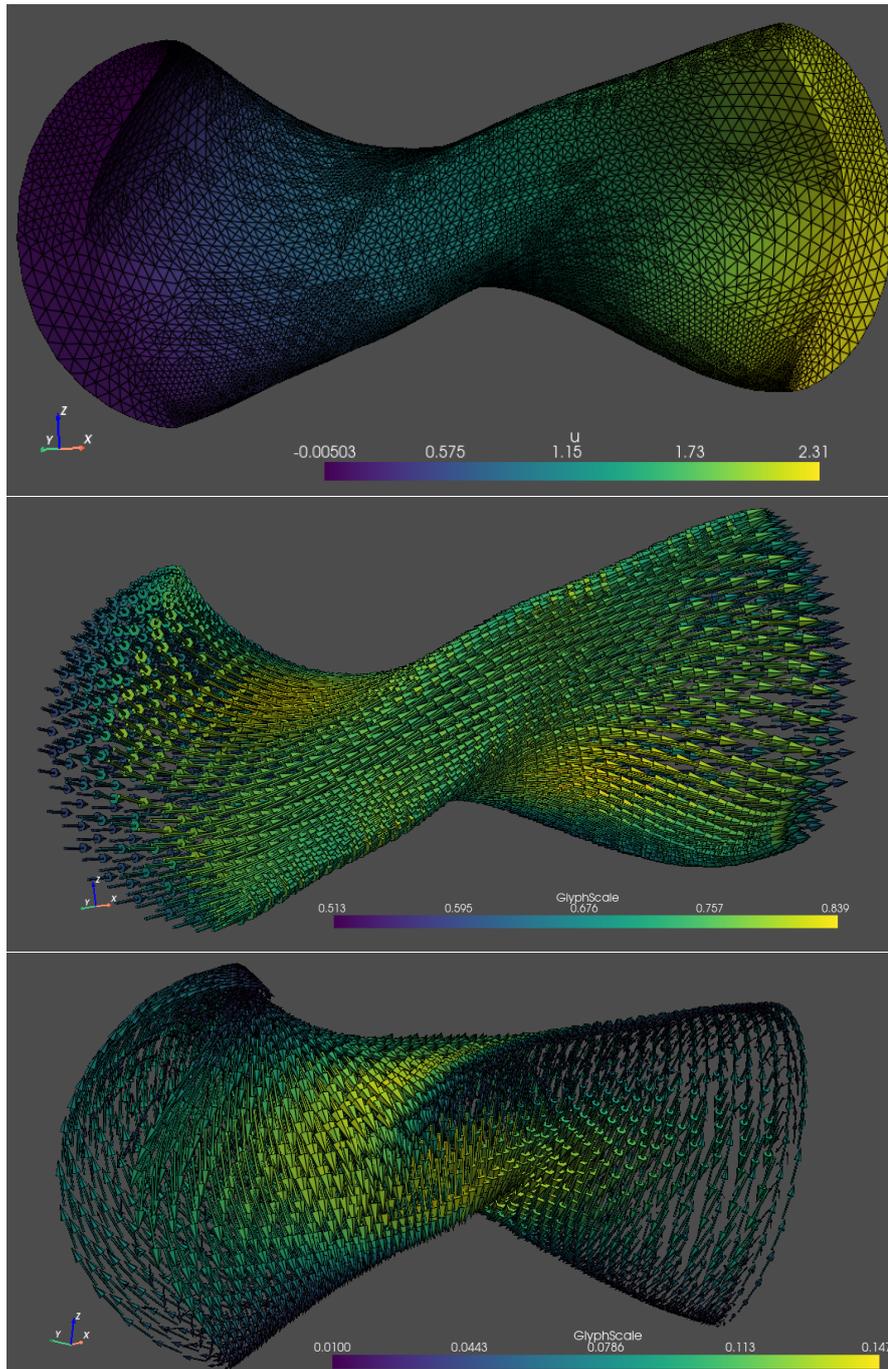


Figure 3.1 – One section (i.e. one third) of NCSX plasma. In the upper plot, we represent the function u_h of Eq. (3.16). Its gradient B_h^{curl} is shown in the middle figure. The bottom figure is a representation of A_h^2 which is computed from A_h^1 and B_h^{curl} using Eq. (3.19).

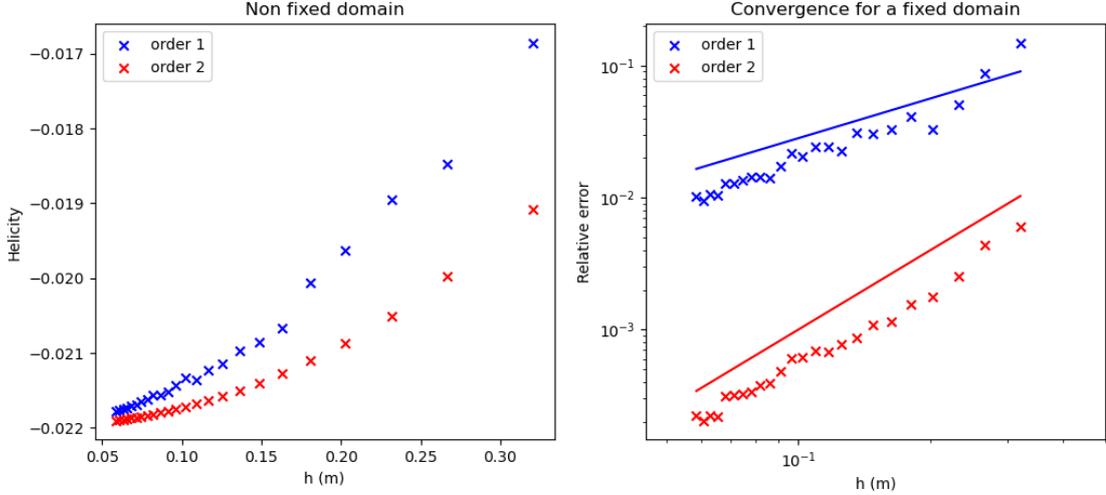


Figure 3.2 – On the left, we provide better and better approximations of the surface to the mesher. We then plot the characteristic size of an element versus the harmonic helicity. On the right, we mesh with different characteristic size h the same polyhedral approximation of the continuous surface and compare it to a reference solution obtained with second order elements and $h = 0.025$. The two lines are merely indicative as their slopes correspond to theoretical first order (blue) and second order (red) convergence rates.

The shape gradient is shown in Fig. 3.3. As mentioned in Section 3.4.4, we have not exactly proven that this numerical approximation converges toward the correct shape gradient, but that it is the case for a regularized version of the numerical solutions. This regularization step is not performed numerically, so that we have no guaranty of convergence. However, we performed numerical tests using finite differences on the Fourier coefficients of the surface, which were consistent with the numerical shape gradient computed with A_h^2 and B_h^{curl} .

3.5.4 Two optimization programs

As the harmonic helicity of NCSX plasma is a negative quantity⁵, we are interested in minimizing it. Indeed, we recall that in a stellarator, one generates a magnetic field that is in first approximation a harmonic field in the plasma domain Ω . As the stability of the plasma is related to the twisting of the magnetic field, we are trying to increase the absolute value of the harmonic helicity to search for interesting and hopefully more stable plasma configurations.

As proved in Proposition 3.3.2, the harmonic helicity scales as $\mathcal{H}(\lambda\Omega) = \lambda\mathcal{H}(\Omega)$ for $\lambda > 0$. For this reason we impose an upper bound either on the volume of Ω or on the area of $\partial\Omega$. Under one of these constraints, it is unclear whether an optimal shape exists. Hence, we add the condition that $\partial\Omega$ satisfies a uniform ball condition. This imposes a strong regularity constraint on the surface and ensures existence of an optimal shape among these regular shapes, we refer for example to [PRS24; Ger23a]. Numerically, we set the uniform ball condition by imposing a lower limit on the minimal curvature radius everywhere on the surface $\partial\Omega$. These three constraints, namely upper bound on the volume Ω or on the area of $\partial\Omega$ and lower bound on the minimal curvature radii on $\partial\Omega$, along with their corresponding shape gradients, can be efficiently computed

5. Using a planar symmetry, we could also choose to take a positive value, see Proposition 3.3.2.

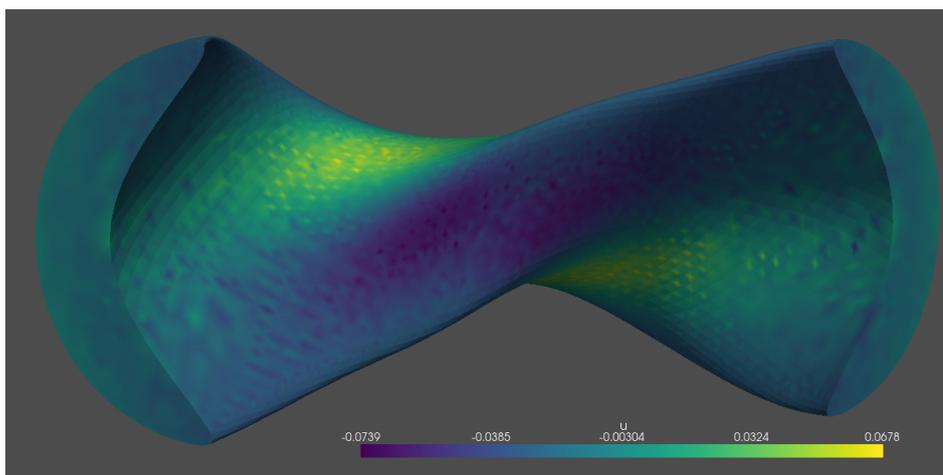


Figure 3.3 – One section of NCSX plasma. The plot shows the shape gradient $2A_h^2 \cdot B_h^{\text{curl}}$ on the boundary. NCSX plasma configuration has a negative harmonic helicity. Improving our criterion implies following the opposite of the shape gradient.

using the smooth parametrization of the surface outlined in Eqs. (3.24) and (3.25) and performing quadrature across either $\partial\Omega$ or Ω .

Subsequently, we introduce smooth non-linear costs that blow up to guarantee the fulfillment of the specified constraints. Once all the costs are assembled, we apply the Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization algorithm from the scipy library [Vir+20] on the Fourier components of the description of the surface.

Bounded Perimeter and Curvature (BPC) We initially focus on optimization with a bounded perimeter, employing a soft threshold set at 25 m^2 to ensure comparability with the NCSX plasma shape. Our goal also involves achieving a minimal inverse curvature radius of 50 m^{-1} , surpassing the regularity of the NCSX reference. The results of this simulation are depicted in Fig. 3.4 and summarized in Table 3.1. Notably, we observe a remarkable 30-fold improvement in harmonic helicity. While the shape appears to collapse toward the Oz axis, this effect is restrained by the imposed curvature constraints. This behavior may be attributed to our normalization choice for the harmonic field; as proximity to the Oz axis increases, the magnitude rises, given our fixed toroidal circulation.

Bounded Volume and Curvature (BVC) We also perform the optimization using a constraint on the volume instead of the perimeter. We apply an upper bound at 3 m^3 along with the same curvature constraints. This time, we achieve more than a 3-fold improvement, and the shape does not seem to collapse toward the Oz axis. The shape is more intricate than the initial plasma shape of NCSX.

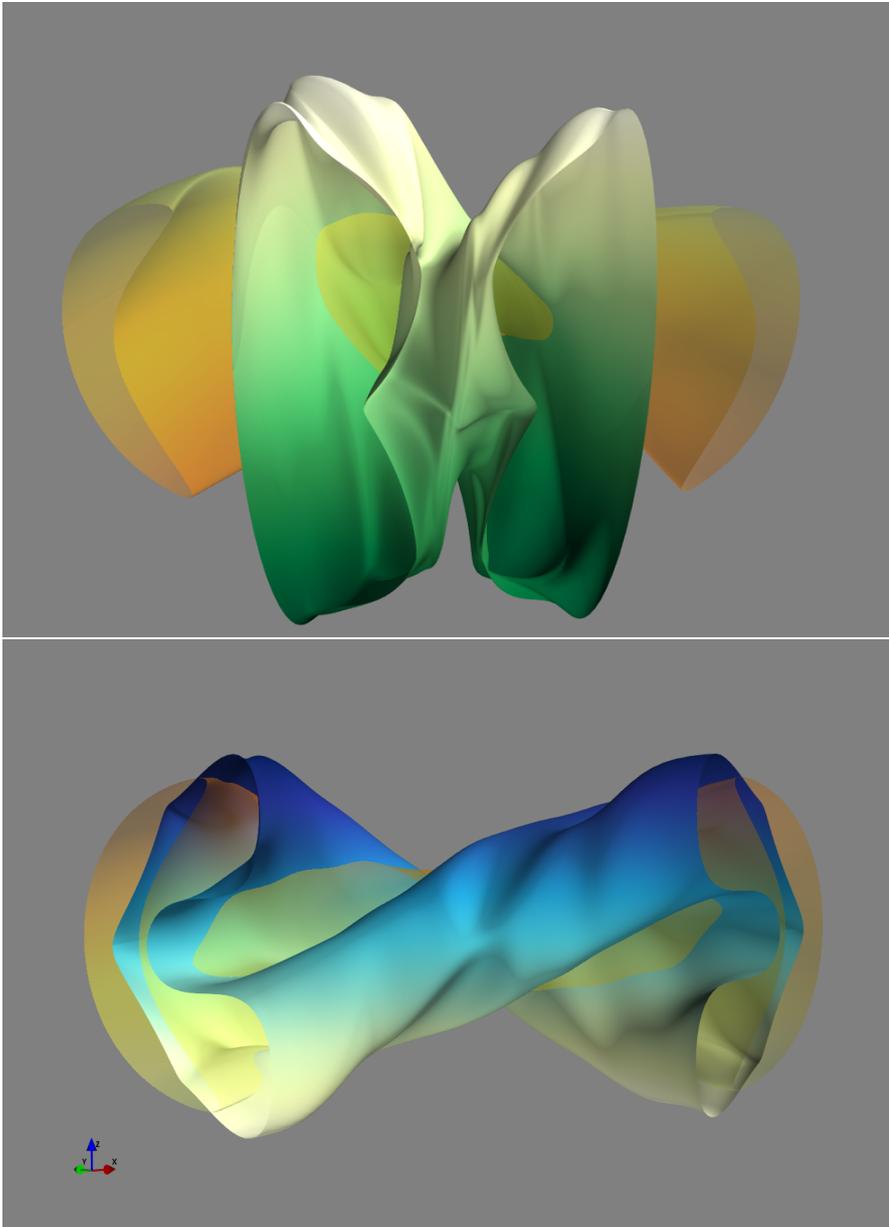


Figure 3.4 – The results of the two optimization problems, BPC (shown in green above) and BVC (shown in blue below). The associated costs are reported in Table 3.1. Additionally, the reference NCSX plasma is plotted in transparent orange.

Plasma shape	Perimeter (m^2)	Volume (m^3)	max curvature (m^{-1})	Harmonic helicity
NCSX (ref)	24.52	2.96	119.3	-0.0220
BPC	25.02	5.45	53.0	-0.6427
BVC	33.5	2.99	50.0	-0.0726

Table 3.1 – harmonic helicity and geometric properties of the optimized shapes in Fig. 3.4. As we aim to compare the optimized shapes with the NCSX reference, for BPC we penalized the area of the surface $\partial\Omega$ above $25 m^2$, whereas for BVC we penalized the volume of Ω above $3 m^3$. In both cases, we targeted a minimal curvature radius of $2 cm$; thus a more regular shape than the reference NCSX plasma shape.

3.6 Conclusion and perspectives

Conclusion We introduced a new shape functional for toroidal domains capturing the linkage of the corresponding harmonic field. We then introduced variational formulations in order to obtain this quantity from the solution of PDEs. Then, using careful differential form pullbacks, we have been able to prove its shape differentiability and obtain a formula for the shape derivative. We also showed that this functional can be efficiently computed numerically. We illustrated this using finite element exterior calculus and applied it to a stellarator device for magnetic confinement in nuclear fusion.

It seems to us that the pure optimization of harmonic helicity provides degenerate shapes, which appear to be less usable for applications in magnetic confinement. However, given the very significant potential gain (factors of 3 and 30 in our two simulations), studying multi-objective optimization with more conventional costs could yield interesting results.

Perspective First, we showed that the harmonic helicity shape functional is smooth at Lipschitz domains under Lipschitz deformations. However, we only gave a formula for the first order shape derivative. A first thing that could thus be studied in the future is how to obtain higher order shape derivatives. In particular, an explicit formula for the shape hessian could give necessary conditions for optimal shapes. For example, some simple arguments which we choose to omit here for conciseness allow to find that, in the case of an axisymmetric torus, $A^2(\Omega)$ is everywhere orthogonal to $B(\Omega)$. Therefore, from the expression of the shape derivative of harmonic helicity, we find that axisymmetric tori are critical shapes. However, from the planar symmetry of such domains, we conjecture that they are in fact saddle points. Indeed, if there exists a deformation field V such that

$$\mathcal{H}''(\Omega; V, V) > 0,$$

then, using Proposition 3.3.2, we find that

$$\mathcal{H}''(\Omega; RV, RV) < 0,$$

for a planar symmetry R leaving Ω invariant. We thus conclude that the shape hessian is either zero for all deformation fields, or neither positive nor negative. This argument could be generalized for all critical domains exhibiting a planar symmetry. However, in order to complete such an argument, one would need to have an explicit enough expression for the shape hessian. Although we believe that this task may be attainable, we expect the expressions for the second order shape derivatives of harmonic fields to be trickier to obtain, and it is complicated to predict in advance if one may obtain a simple enough expression of the shape hessian in order to deduce explicit results. The regularity assumptions on the domain in order to obtain such a formula are also still

unclear to the author.

Finally, we have mentioned that adding a reach constraint for such shape optimization problems often leads to existence of optimal shapes, and we do believe that such a result would also hold in our case. However, we expect that studying the existence of optimal toroidal shapes in the Lipschitz context should be a much harder task. We do note that the numerical results we have obtained when removing the curvature constraint suggest that the shape optimization problem in the Lipschitz case may not have optimal shapes, but this is only a conjecture.

Data availability statement The code created for this chapter is openly accessible through the GitLab repository <https://plmlab.math.cnrs.fr/rrobin/helicity>.

Shape differentiation for Poincaré maps of harmonic fields

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4.1 Introduction

When designing magnetic fields for confinement in fusion reactors, such as tokamaks or stellarators, dynamical properties of the field lines play a key role in the stability properties of the plasma. In this context, spatial variations of the magnetic field magnitude lead to a drift of charged particles. However, as was discussed in Section 1.2.3, introducing a twist in the magnetic field lines is known to average out the drift along the trajectories of charged particles. We also refer to [IPW20, Chapter 5][Lit83][HS05, Chapter 7]. To quantify this notion of twist, an important object in reactor design is the so-called rotational transform [IPW20][Chapter 7]. Assuming the plasma domain foliates into tori tangent to the magnetic field, the rotational transform is defined on each leaf by the average ratio of poloidal turns and toroidal turns along the field lines. Mathematically, this is given by the rotation number of the Poincaré map on each leaf.

In addition to giving information on the stability of charged particles in the plasma, the rotational transform is also useful in studying the topological and dynamical stability of the

magnetic field itself. Indeed, due to errors arising from the coil design and fluctuations in the plasma, the actual magnetic field inside a reactor will be a perturbation of the theoretical one. Loosely speaking, KAM theory and Hamiltonian representations of magnetic fields lead to non-degenerate leaves of the magnetic field with a diophantine rotational transform being preserved after perturbations, whereas leaves with rational rotational transform may lead to chaotic regions and magnetic islands [IPW20, Chapter 10][LHL90].

Mathematically, however, the assumption of a foliated magnetic field leads to complications. Indeed, the existence of such foliated magnetic fields is still closely linked to open questions. As was discussed in Section 1.3.3, the most notable problem related to existence of foliations is Grad's conjecture [Gra67], which states that foliated smooth MHD equilibria with non-constant pressure should be axisymmetric. Theoretical results as well as a solid mathematical framework are therefore scarce when it comes to the study of rotational transform profiles. We still refer to a series of articles by Enciso, Luque and Peralta-Salas [EP15; ELP20; ELP22], also discussed in Section 1.3.3, which study the dynamical properties of Beltrami fields. These articles develop a thorough theory to study Poincaré maps of Beltrami fields with small eigenvalue in thin toroidal tubes, and deduce several interesting results from this, such as the construction of non-trivial stepped pressure MHD equilibria in [ELP22].

In this chapter, we are more specifically interested in the study of harmonic fields. Given a domain Ω of \mathbb{R}^3 , we say that a vector field on Ω is harmonic if it is divergence free, curl free, and tangent to the boundary. When Ω has the topology of a full torus, the space of harmonic fields is one dimensional, and we may therefore single out a generator of this space by picking a normalization criterion, such as the circulation along a toroidal loop. We refer to Section 1.3.1 for the justification of this normalization using concepts from differential geometry and algebraic topology. From a physical point of view, harmonic fields are important in the design of stellarators, which aim to stabilize plasma without inducing current inside it. This therefore leads to magnetic fields with small curl inside the plasma domain, which may be approximated by harmonic fields. The fact that one may assign a harmonic field to each toroidal domain can lead to stellarator design using shape optimization techniques.

Although, to the author's knowledge, there is no clearly established conjecture in this direction, there seems to be no result on the existence of non-trivial foliated harmonic fields. We still refer to Section 1.3.3 for the construction of a family of non-axisymmetric harmonic fields which are foliated. However, this construction leads to harmonic fields with trivial dynamics. To simplify things, we therefore choose to study the Poincaré maps of harmonic fields on the boundary only. Indeed, since harmonic fields of Ω are by definition tangent to the boundary, they define a flow on $\partial\Omega$. Therefore, if Ω is a toroidal domain, the Poincaré map of the harmonic field restricted to the boundary is a circle diffeomorphism, to which we may associate a rotation number. Since one may assign a harmonic field to each toroidal domain, the approach of this chapter is to investigate properties of the Poincaré maps of harmonic fields on the boundary using a shape differentiation approach, that is, to study how variations of the domain may lead to variations of the Poincaré map in the space of diffeomorphisms of the circle. To avoid technicalities related to regularity, we choose to work in the C^∞ -smooth category throughout the chapter. We will therefore only be working with smooth domains, use smooth functions and vector fields, and prove smoothness of the studied objects when needed.

4.1.1 General approach and main results

Before discussing the contributions of the chapter, we give a formal introduction to the main objects we will study. The precise definitions will be given in Section 4.2. Let Ω be a smooth toroidal domain, that is, a smooth open set of \mathbb{R}^3 such that $\bar{\Omega}$ is diffeomorphic to the full torus

$S^1 \times D^2$, where D^2 is the closed unit disk of \mathbb{R}^2 , and $S^1 = \mathbb{R}/\mathbb{Z}$. Given a curve γ' which generates the first homology group of $\bar{\Omega}$ with unit tangent vector field t' , there exists a unique harmonic field $B(\Omega)$ verifying

$$\int_{\gamma'} B(\Omega) \cdot t' = 1.$$

As was explained in Section 1.3.1, this can be seen by identifying harmonic fields as representatives of the first de Rham cohomology space of Ω , and using de Rham's theorem. In order to define the Poincaré map of $B(\Omega)$ on the boundary as a diffeomorphism of the circle, we need the following data:

- γ' , a generator of the first homology group of $\bar{\Omega}$,
- P , a poloidal cut of $\partial\Omega$,
- Coordinates on P , that is, a diffeomorphism between S^1 and P .

Furthermore, Σ needs to be a Poincaré cut of $B(\Omega)|_{\partial\Omega}$. All the required data and assumptions will be given by the notion of admissible embeddings of the torus in \mathbb{R}^3 , which we denote $\text{Emb}_{\text{ad}}(\mathbb{T}^2; \mathbb{R}^3)$ (see Definition 4.2.1). We are thus able to consider the mapping

$$\Pi : \text{Emb}_{\text{ad}}(\mathbb{T}^2; \mathbb{R}^3) \rightarrow \text{Diff}(S^1),$$

which associates with each admissible embedding the Poincaré map of $B(\Omega)$, where Ω is the smooth toroidal domain whose boundary is the image of the embedding. We also note that we model S^1 as \mathbb{R}/\mathbb{Z} throughout the paper, so that S^1 is equipped with canonical coordinates inherited from \mathbb{R} .

Although Π is not, strictly speaking, a shape function (as it also depends on the coordinates on the boundary), the techniques we will use to study it are largely inspired by shape differentiation. Let \mathcal{E} be an admissible embedding, and $t \mapsto P_t$ a smooth path of smooth diffeomorphisms of \mathbb{R}^3 with $P_0 = \text{I}$. Let V in $\text{Vec}(\mathbb{R}^3)$, the set of smooth vector fields of \mathbb{R}^3 , be the derivative of $t \mapsto P_t$ at time $t = 0$. As will be further explained later in the chapter, $\mathcal{E}_t := P_t \circ \mathcal{E}$ is then admissible as well for t small enough. Our goal is then to study the derivative of $t \mapsto \Pi(\mathcal{E}_t)$ in the space of circle diffeomorphisms. More precisely, we will show that there exist a linear map $V \mapsto \Pi'(\mathcal{E}; V)$ such that

$$\Pi(\mathcal{E}_t) = \Pi(\mathcal{E}) + t\Pi'(\mathcal{E}; V) + o(t).$$

We refer to $\Pi'(\mathcal{E}; V)$ as the shape derivative of the Poincaré map at \mathcal{E} in the direction V .

In this chapter, we establish this shape differentiability result and we study the image of the map $V \mapsto \Pi'(\mathcal{E}; V)$ in specific cases. The first case we will study is the one where \mathcal{E} is the usual embedding of the standard axisymmetric torus. In this case, we will show that $\Pi'(\mathcal{E}; V)$ actually vanishes for all V . This result is given in Theorem 4.4.1. Then, we will study the case where $\Pi(\mathcal{E})$ is a diophantine rotation. In this case, we will show that under an additional assumption on the geometry of the domain, the mapping $V \mapsto \Pi'(\mathcal{E}; V)$ is surjective. This result is given in Theorem 4.5.1.

4.1.2 Outline of the chapter

The chapter is organized as follows.

- In Section 4.2, we give a proper definition of the objects we will study throughout the paper. Firstly, we recall some properties of harmonic fields in toroidal domains given in Sections 1.3.1 and 2.2.2. We then define the notion of Poincaré map we will be studying. This is done first by defining a notion of admissible embeddings of the torus in \mathbb{R}^3 which provides the necessary data, and then by describing how we construct the Poincaré map

from an admissible embedding.

- In Section 4.3, we study the general shape differentiability of the Poincaré map of harmonic fields. We first use a shape differentiation result from Chapter 2, which we adapt to our context. This gives us a shape differentiability result for harmonic fields in the smooth category which is well suited to describe the dynamics of the field lines. In Section 4.3.2, we then obtain the shape derivative of the Poincaré map. We also provide a useful formula for the case in which the coordinates on the boundary linearize the harmonic field, which will be used in Sections 4.4 and 4.5.
- In Section 4.4, we study the particular case of a standard axisymmetric torus. For axisymmetric domains the harmonic field is explicitly known, greatly simplifying the computations. We prove in Theorem 4.4.1 that, in this case, the shape derivative of the Poincaré map always vanishes. This implies that around these domains, it is necessary to go to second-order in order to find local information about the Poincaré map of harmonic fields. The geometry of the domain plays a role in two steps of the proof. First through the explicit expression of the harmonic field and its relation with the curvature of the boundary, and second, through symmetries of the solution to a PDE which appears in the expression of the shape derivative of the harmonic field.
- In Section 4.5, we study the case where the Poincaré map has diophantine rotation number. Under an additional assumption relating the curvature of the boundary and the harmonic field, we prove Theorem 4.5.1, which states that the shape derivative of the Poincaré map can be any smooth function of the circle if we choose a correct perturbation of the embedding. For this, we use cohomological equations to prove that the shape derivative of the Poincaré map can be any zero average function of the circle, and a specific normal perturbation to generate the last remaining dimension.

4.1.3 Notations

- $S_\ell^1 = \mathbb{R}/(\ell\mathbb{Z})$ and $S^1 = S_1^1$. We also define $\mathbb{T}^2 = \mathbb{R}^2/\mathbb{Z}^2 \cong S^1 \times S^1$ and denote the closed unit disk of \mathbb{R}^2 as D^2 .
- For two vectors u and v in \mathbb{R}^3 , $u \cdot v$ is their Euclidean scalar product.
- Given a smooth manifold M with (possibly empty) smooth boundary and k in $\mathbb{N} \cup \{\infty\}$, $\mathcal{C}^k(M)$ is the space of real valued k times differentiable functions on M , and $\text{Vec}(M)$ is the set of smooth vector fields of M .
- Given a smooth manifold M and a continuous family of vector fields $s \in \mathbb{R} \mapsto X_s \in \text{Vec}(M)$, we denote

$$\overrightarrow{\text{exp}} \int_0^t X_s ds,$$

as the flow of $s \mapsto X_s$ at time t when it is well-defined. That is, if $x(\cdot)$ is the solution to

$$\begin{cases} \dot{x}(t) = X_t(x(t)), \\ x(0) = x_0, \end{cases}$$

then $\overrightarrow{\text{exp}} \int_0^t X_s ds(x_0) := x(t)$. In our case, the manifold will always be compact without boundary, so that there is global existence of flow.

- Let X, Y be topological spaces and $f : X \rightarrow Y$ a continuous function. For k in \mathbb{N} , $H_k(X)$ is the k -th singular homology group of X , and $f_* : H_k(X) \rightarrow H_k(Y)$ is the group morphism associated to f . We refer to [Hat02][Chapter 2] for the precise definitions of these objects. We note however that only basic homological notions will be used so that an intuitive

understanding of singular homology and its relation with de Rham cohomology will be sufficient to understand its use in the paper.

- Suppose Ω is a smooth toroidal domain of \mathbb{R}^3 , that is an open set such that $\bar{\Omega}$ is smoothly diffeomorphic to $S^1 \times D^2$, and $(\phi, \theta) : \partial\Omega \rightarrow \mathbb{T}^2$ are smooth coordinates on $\partial\Omega$.
 - n is the unit normal outward pointing vector field on $\partial\Omega$.
 - $\operatorname{div}_\Gamma$ is the divergence on $\partial\Omega$, and ∇_Γ the tangential gradient. Both are defined using the metric on $\partial\Omega$ inherited from the Euclidean metric on \mathbb{R}^3 .
 - \sqrt{g} is the square root of the determinant of the metric matrix in the (ϕ, θ) coordinates. As such, the surface form on $\partial\Omega$ is given by $\sqrt{g}d\phi d\theta$.
 - Given $\vec{\omega} = (\omega_1, \omega_2)$ in \mathbb{R}^2 and f in $\mathcal{C}^\infty(\partial\Omega)$, we denote $\langle \vec{\omega}, \nabla_{\mathbb{T}^2} f \rangle = \omega_1 \partial_\phi f + \omega_2 \partial_\theta f$.
 - Given a tangent vector u on $\partial\Omega$, $u^\perp := n \times u$.
- Given a Riemannian manifold M and an oriented one codimensional submanifold N with unit normal vector field n , the second fundamental form of N is defined as

$$\mathbb{III} : \begin{cases} \operatorname{Vec}(N) \times \operatorname{Vec}(N) \rightarrow \mathcal{C}^\infty(N) \\ (X, Y) \mapsto \nabla_X \tilde{Y} \cdot n \end{cases}.$$

Here, \tilde{Y} is a smooth extension of Y to M , and $\nabla_X \tilde{Y}$ is the covariant derivative of \tilde{Y} along X using the Riemannian metric on M . It is then known that $\mathbb{III}(X, Y)$ is independent of the choice of extension of Y , that \mathbb{III} is a tensor, that is, a bilinear form on $\operatorname{Vec}(N)$ as a $\mathcal{C}^\infty(N)$ -module, and that it is symmetric. We refer to [Lee18, Section 8] for more information on this definition of the second fundamental form.

In the particular case where $N \subset \mathbb{R}^3$ is a surface defined via an embedding $\mathcal{E} : \mathbb{T}^2 \mapsto \mathbb{R}^3$, the fact that the Christoffel symbols vanish in Cartesian coordinates and that ∂_ϕ (resp. ∂_θ) is given in coordinates by $\partial_\phi \mathcal{E}$ (resp. $\partial_\theta \mathcal{E}$) implies the usual formula

$$\begin{aligned} \mathbb{III}(\partial_i, \partial_j) &= \nabla_{\partial_i} \partial_j \cdot n \\ &= \partial_i \partial_j \mathcal{E} \cdot n, \end{aligned}$$

where i and j are either ϕ or θ .

4.2 Definitions

In this section, we wish to define a notion of Poincaré maps for harmonic fields in toroidal domains. First, we give a few reminders on the notions of harmonic fields (see Section 1.3.1 and Section 2.2.2 for more details.)

We recall that, given a bounded Lipschitz domain Ω of \mathbb{R}^3 , the set of harmonic vector fields is given by

$$\mathcal{K}(\Omega) = \{u \in L^2(\Omega)^3 \mid \operatorname{curl} u = 0, \operatorname{div} u = 0 \text{ and } u \cdot n = 0\},$$

and that its dimension is equal to the first Betti number of $\bar{\Omega}$. If $\bar{\Omega}$ is smoothly diffeomorphic to the full torus, its first Betti number is equal to one. One therefore finds that, given a generator γ' of the first singular Homology group $H_1(\bar{\Omega})$, there is a unique vector field $B(\Omega)$ such that

$$\int_{\gamma'} B(\Omega) \cdot t' = 1.$$

We note that, $\bar{\Omega}$ having a smooth boundary implies that elements of $\mathcal{K}(\Omega)$ are smooth up to the boundary so that the above circulation may be defined in the usual way (see [Sch95, Theorem

2.2.2]). We also note that $B(\Omega)$ in fact also depends on the choice of generator γ' . However, since $H_1(\Omega)$ is isomorphic to \mathbb{Z} , changing the generator may change $B(\Omega)$ only by a sign. We therefore choose to omit this dependence in our notations for convenience.

We now wish to define the Poincaré maps of harmonic fields on the boundary of toroidal domains. In order to do so, we proceed by specifying coordinates on the boundary. Indeed, having such coordinates allows us to define a Poincaré cut and coordinates on this Poincaré cut, which is the required data to obtain the Poincaré map as a diffeomorphism of S^1 . This is done by working with the set of smooth embeddings of \mathbb{T}^2 into \mathbb{R}^3 , which we denote by $\text{Emb}(\mathbb{T}^2; \mathbb{R}^3)$. We recall that, with an element \mathcal{E} of $\text{Emb}(\mathbb{T}^2; \mathbb{R}^3)$, we can associate an isomorphism \mathcal{E}_* between the singular homology groups of \mathbb{T}^2 and the ones of $\mathcal{E}(\mathbb{T}^2)$. We denote by γ_ϕ and γ_θ the canonical generators of the homology group $H_1(\mathbb{T}^2)$. In order to be able to define the Poincaré map, we need to make some further assumptions on the embedding which are given by the following definition.

Definition 4.2.1. *Let \mathcal{E} be in $\text{Emb}(\mathbb{T}^2; \mathbb{R}^3)$. We say \mathcal{E} is admissible if it satisfies the following conditions.*

- $\mathcal{E}(\mathbb{T}^2)$ bounds a smooth toroidal domain Ω in \mathbb{R}^3 .
- \mathcal{E} is toroidal, that is
 - $\mathcal{E}_*\gamma_\phi$ is trivial in $H_1(\Omega^c)$ and generates $H_1(\bar{\Omega})$,
 - $\mathcal{E}_*\gamma_\theta$ is trivial in $H_1(\bar{\Omega})$ and generates $H_1(\Omega^c)$.
- \mathcal{E} is transverse, that is, if $B(\Omega) = B(\Omega)^\phi \partial_\phi + B(\Omega)^\theta \partial_\theta$ is the harmonic field of Ω associated to the generator $\mathcal{E}_*\gamma_\phi$ where $(\phi, \theta) = \mathcal{E}^{-1}$ are the coordinates induced on $\partial\Omega$ by \mathcal{E} , then $B(\Omega)^\phi$ is positive on $\partial\Omega$.

We denote by $\text{Emb}_{\text{ad}}(\mathbb{T}^2; \mathbb{R}^3)$ the set of admissible embeddings of \mathbb{T}^2 into \mathbb{R}^3 .

Remark 4.2.2. *Here are a few remarks which may help the reader to interpret the definition of admissible embeddings:*

- The first condition of Definition 4.2.1 is not redundant. Indeed, although a smoothly embedded torus in S^3 always bounds a full torus, this result is not true for embeddings in \mathbb{R}^3 . We refer to [Arn10][Definition 3] for a description of such domains, referred to as knotted anti-tori, as well as [CDG02][Figure 13] for an illustration of such embedded tori.
- The second condition of Definition 4.2.1 essentially states that $(\phi, \theta) = \mathcal{E}^{-1}$ define toroidal and poloidal coordinates respectively on the boundary of Ω . Although it is only necessary to assume that $\mathcal{E}_*\gamma_\phi$ generates $H_1(\bar{\Omega})$ to define the Poincaré map, the additional assumptions are here to ensure that the Poincaré map we will construct corresponds to what we may expect geometrically. For example, the assumption that $\mathcal{E}_*\gamma_\theta$ is trivial in $H_1(\bar{\Omega})$ means that curves of constant ϕ correspond to poloidal cuts of $\partial\Omega$.
- The last condition of Definition 4.2.1 ensures that $B(\Omega)$ is transverse to poloidal cuts, that is, nowhere tangent to curves of constant ϕ . Therefore, its Poincaré map may be defined on such cuts.

We now explain how we can define the Poincaré maps of harmonic fields. Let \mathcal{E} be an admissible embedding, Ω be the toroidal domain such that $\partial\Omega = \mathcal{E}(\mathbb{T}^2)$, $B(\Omega)$ the harmonic field of Ω associated to the generator $\mathcal{E}_*\gamma_\phi$, and (ϕ, θ) the coordinates on $\partial\Omega$ associated with \mathcal{E} . First, to define the Poincaré map, we need to normalize the harmonic field. This is done by defining the following vector field on $\partial\Omega$:

$$X(\mathcal{E}) = \frac{B(\Omega)}{B(\Omega)^\phi}. \quad (4.1)$$

From this definition, and the fact that $B(\Omega)^\phi$ is positive, we know that the field lines of $X(\mathcal{E})$ correspond to the ones of $B(\Omega)$ up to an order-preserving reparametrization of time. Furthermore,

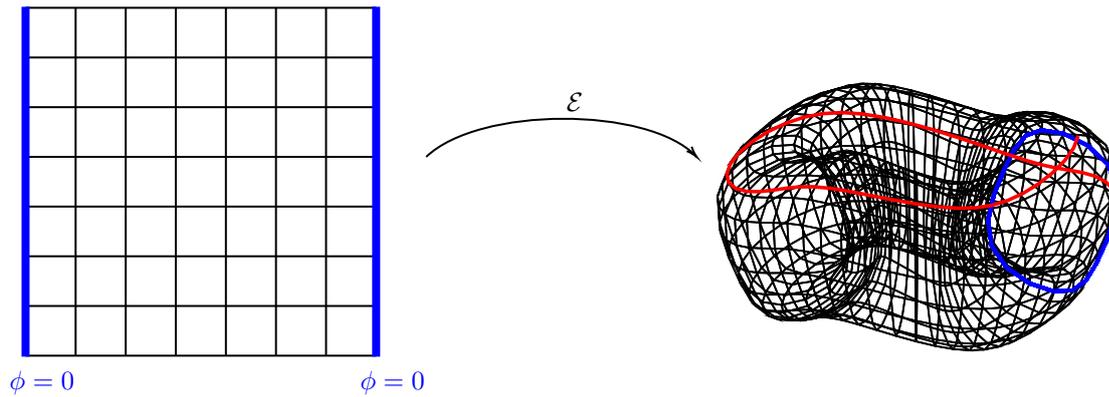


Figure 4.1 – Example of an admissible embedding with Poincaré cut in blue and field line in red.

we get that $X(\mathcal{E})^\phi = 1$, so that the field lines of $X(\mathcal{E})$ evolve linearly in ϕ . This implies that if a field line starts on the poloidal cut $\phi = 0$ at time $t = 0$, it will return to the same cut at time $t = 1$, which is precisely what we need for the Poincaré map.

We may therefore define the Poincaré map of $B(\Omega)$ as the one time flow of $X(\mathcal{E})$ restricted to the cut $\phi = 0$. However, it is more convenient to work on the fixed space S^1 in order to study variations of the Poincaré map. This can be done once again using the (ϕ, θ) coordinates associated with \mathcal{E} . Let $S^1 \ni \phi \mapsto X_\phi(\mathcal{E}) \in \text{Vec}(S^1)$ be the one-parameter family of vector fields given by

$$X_\phi(\mathcal{E})(\theta) = X(\mathcal{E})^\theta(\phi, \theta)e_\theta, \quad (4.2)$$

where e_θ is the canonical unit vector field of S^1 . We then define the Poincaré map $\Pi(\mathcal{E})$ as

$$\Pi(\mathcal{E}) = \overrightarrow{\text{exp}} \int_0^1 X_\phi(\mathcal{E}) d\phi, \quad (4.3)$$

which is a diffeomorphism of the circle. It will also prove to be useful to define the same flow at time ϕ , which we denote by $\Pi^\phi(\mathcal{E})$.

Remark 4.2.3. *Since $\phi \mapsto \Pi^\phi(\mathcal{E})$ defines a homotopy between the identity on S^1 and $\Pi(\mathcal{E})$, there is a canonical choice of lift for the Poincaré map. This implies in particular that the rotation number of $\Pi(\mathcal{E})$ may be seen as a real number, and not just an element of S^1 .*

4.3 Shape differentiation

In this section, we consider an admissible embedding \mathcal{E} , Ω its corresponding domain, and $t \mapsto P_t$ a differentiable family of diffeomorphisms of \mathbb{R}^3 with $P_0 = id$. We denote

$$V := \left. \frac{d}{dt} \right|_{t=0} P_t,$$

which is a smooth vector field of \mathbb{R}^3 . Denoting $\mathcal{E}_t = P_t \circ \mathcal{E}$, our goal is to prove that $t \mapsto \Pi(\mathcal{E}_t)$ is differentiable in $\text{Diff}(S^1)$. More precisely, we will identify a linear map $V \mapsto \Pi'(\mathcal{E}; V)$ such that

$$\Pi(\mathcal{E}_t) = \Pi(\mathcal{E}) + t\Pi'(\mathcal{E}; V) + o(t).$$

In order to obtain shape differentiability results, we need to mention the topologies we will be using. Given a manifold M , we equip $\mathcal{C}^\infty(M)$ with its natural Fréchet structure (see for example [AS02, Section 2.2]). In this topology, convergence is equivalent to convergence in every \mathcal{C}^k norm in every compact subset. Given an open set Ω of \mathbb{R}^3 , we may identify $\text{Vec}(\Omega)$ with $\mathcal{C}^\infty(\bar{\Omega})^3$, so that the corresponding topology comes naturally. Since, in the context of Poincaré maps, we are working with specific lifts, we may identify $\text{Diff}(S^1)$ as a subset of $\mathcal{C}^\infty(\mathbb{R})$. This therefore equips $\text{Diff}(S^1)$ with a natural Fréchet topology. Importantly, since convergence in \mathcal{C}^∞ spaces is equivalent to convergence in \mathcal{C}^k spaces for all k , proving differentiability in \mathcal{C}^∞ topologies is equivalent to proving differentiability in the corresponding \mathcal{C}^k topologies for all k . We will often be using this fact throughout the section without further mention.

4.3.1 Shape differentiation of harmonic fields in the smooth category

In order to differentiate $t \mapsto \Pi_t := \Pi(\mathcal{E}_t)$, we first need to differentiate $t \mapsto B_t := B(\Omega_t)$, where $\Omega_t = P_t(\Omega)$ and Ω is the domain associated to \mathcal{E} . This is given in the sense of the main results of Chapter 2. Recalling the definitions of the pullbacks given in Section 2.3, we denote $\Phi_{1-P_t}^1$ as $(P_t)_1^*$. Theorem 2.5.1 then implies that $t \mapsto (P_t)_1^* B_t$ is smooth at $t = 0$ in \mathcal{C}^k for all k and that its derivative is given by

$$\nabla(V \cdot B(\Omega)) + \nabla u_V,$$

where u_V solves

$$\begin{cases} \Delta u_V = 0, & \text{in } \Omega, \\ \nabla u_V \cdot n = \text{div}_\Gamma(B(\Omega)(V \cdot n)). \end{cases} \quad (4.4)$$

However, we are here interested in the dynamics of the field lines of B_t . It is therefore more relevant to consider $(P_t^{-1})_* B_t$ rather than $(P_t)_1^* B_t$ as the former transformation preserves the field lines of B_t . Indeed, the field lines of $(P_t^{-1})_* B_t$ are equal to the ones of B_t up to composition with P_t^{-1} . We recall that, given a smooth vector field X , $(P_t^{-1})_* X$ is given by

$$(P_t^{-1})_* X = (DP_t)^{-1} X \circ P_t,$$

and that

$$\left. \frac{d}{dt} \right|_{t=0} (P_t^{-1})_* X = [V, X].$$

In order to differentiate $t \mapsto (P_t^{-1})_* B_t$, we prove the following lemma.

Lemma 4.3.1. *Let X be a vector field in $\text{Vec}(\bar{\Omega})$. We have*

$$\left. \frac{d}{dt} \right|_{t=0} (P_t^{-1})_* ((P_t^{-1})_1^* X) = [V, X] - \nabla(V \cdot X) - \text{curl } X \times V.$$

Proof. First, we extend X to a smooth vector field of \mathbb{R}^3 , which we also denote X . Now, we compute

$$(P_t^{-1})_1^* X = D(P_t^{-1})^T X \circ P_t^{-1}.$$

We have

$$\begin{aligned} X \circ P_t^{-1} &= X - t(DX)V + o(t), \\ D(P_t^{-1})^T &= I - tDV^T + o(t), \end{aligned}$$

so that

$$(P_t^{-1})_* X = X - t((DV^T)X + (DX)V) + o(t).$$

Now, combining the identities

$$\begin{aligned}\nabla(V \cdot X) &= (DV^T)X + (DX^T)V, \\ \operatorname{curl} X \times V &= (DX - DX^T)V,\end{aligned}$$

we obtain

$$(P_t^{-1})_* X = X - t(\nabla(V \cdot X) + \operatorname{curl} X \times V) + o(t).$$

Finally, defining $Y_t = (P_t^{-1})_* X$ and using

$$(P_t^{-1})_* Y_t = Y_t + t[V, Y_t] + o(t),$$

we obtain the desired formula. \square

We now prove the following proposition

Proposition 4.3.2. *The mapping*

$$\begin{cases} \mathbb{R} \rightarrow \operatorname{Vec}(\bar{\Omega}) \\ t \mapsto (P_t^{-1})_* B_t \end{cases}$$

is smooth at zero, and its derivative is given by

$$B'(\Omega; V) = [V, B(\Omega)] + \nabla u_V, \quad (4.5)$$

where u_V solves Eq. (4.4)

Remark 4.3.3. *Using the notations introduced in Chapter 2, this notion of shape derivative of the harmonic field should be denoted $B'_{\text{vf}}(\Omega; V)$. However, since this is the only notion of shape derivative of the harmonic field we will use in the rest of this chapter, we will keep the notation $B'(\Omega; V)$ for convenience.*

Proof.

$$(P_t^{-1})_* B_t = (P_t^{-1})_* ((P_t^{-1})_*^{-1} (P_t)_* B_t).$$

Using Theorem 2.5.1 and Lemma 4.3.1, we thus know that $t \mapsto (P_t^{-1})_* B_t$ is smooth at zero in \mathcal{C}^k for all k . Furthermore, its derivative is given by

$$\begin{aligned}\frac{d}{dt}\Big|_{t=0} (P_t^{-1})_* B_t &= \frac{d}{dt}\Big|_{t=0} (P_t)_* B_t + [V, B(\Omega)] - \nabla(V \cdot B(\Omega)) - \operatorname{curl} B(\Omega) \times V \\ &= \nabla u_V + \nabla(V \cdot B(\Omega)) + [V, B(\Omega)] - \nabla(V \cdot B(\Omega)) \\ &= [V, B(\Omega)] + \nabla u_V,\end{aligned}$$

as claimed. \square

4.3.2 Shape differentiation of the Poincaré map

Now that we have obtained the shape differentiability of the harmonic field, we proceed to compute the shape derivative of its Poincaré map. We denote with an additional t subscript

all the objects defined in Section 4.2 associated with the embedding $\mathcal{E}_t = P_t \circ \mathcal{E}$. We recall in particular that $X_t \in \text{Vec}(\partial\Omega_t)$ is defined as

$$X_t = \frac{B_t}{B_t^{\phi_t}},$$

where $(\phi_t, \theta_t) = \mathcal{E}_t^{-1}$.

Proposition 4.3.4. *For $|t| < \varepsilon$ sufficiently small, \mathcal{E}_t is admissible and the mapping*

$$\begin{cases} (-\varepsilon, \varepsilon) \rightarrow \text{Vec}(\partial\Omega) \\ t \mapsto (P_t^{-1})_* X_t \end{cases}$$

is smooth at zero. Furthermore, if $(\partial_\phi, \partial_\theta)$ is positively oriented, the θ component of its derivative is given by

$$(X'_V)^\theta = \frac{1}{\sqrt{g} (B_0^\phi)^2} B'(\Omega; V) \cdot B(\Omega)^\perp, \quad (4.6)$$

and we obtain the same formula with opposite sign if the orientation of the coordinates is reversed.

Before proving Proposition 4.3.4, we introduce some geometrical notations for vector fields on the boundary. We denote by $\nabla_\Gamma \phi$ (resp. $\nabla_\Gamma \theta$) the vector field of $\partial\Omega$ dual to $d\phi$ (resp. $d\theta$). These are therefore defined by the relations

$$\nabla_\Gamma \phi \cdot v = d\phi(v), \quad \nabla_\Gamma \theta \cdot v = d\theta(v),$$

for all vectors v which are tangent to $\partial\Omega$. Contrary to what the notations may suggest, these vector fields are not gradient vector fields, but are only curl $_\Gamma$ -free. This is similar to the fact that $d\phi$ and $d\theta$ are not differentials of global functions, but are closed one-forms. In coordinates, we have

$$\nabla_\Gamma \phi = g^{\phi\phi} \partial_\phi + g^{\phi\theta} \partial_\theta, \quad \nabla_\Gamma \theta = g^{\theta\phi} \partial_\phi + g^{\theta\theta} \partial_\theta. \quad (4.7)$$

By definition, it is clear that $\nabla_\Gamma \phi$ is orthogonal to ∂_θ , and that $\nabla_\Gamma \theta$ is orthogonal to ∂_ϕ . Furthermore, if $(\partial_\phi, \partial_\theta)$ is a positively oriented frame on $\partial\Omega$, a straightforward computation in coordinates shows that

$$\partial_\phi^\perp = \sqrt{g} \nabla_\Gamma \theta, \quad \partial_\theta^\perp = -\sqrt{g} \nabla_\Gamma \phi, \quad (4.8)$$

with opposite signs if the orientation of the coordinates is reversed. Because of this dependence on orientation for the sign of orthogonal vectors in coordinates, we will often only treat the case where $(\partial_\phi, \partial_\theta)$ is positively oriented. Treating the other case is however a straightforward process, so we will often omit this technicality when writing the main results.

Proof of Proposition 4.3.4. For the first point of the proposition, we observe that $\mathcal{E}_t = P_t \circ \mathcal{E}$ automatically verifies the first two assumptions of Definition 4.2.1. We therefore only need to prove that $B_t^{\phi_t}$ is positive on $\partial\Omega$ for t small enough. To do so, we note that since $\mathcal{E}_t = P_t \circ \mathcal{E}$, we have $\phi_t = \phi \circ P_t^{-1}$, so that

$$B_t^{\phi_t} = ((P_t^{-1})_* B_t)^\phi \circ P_t^{-1}. \quad (4.9)$$

We then deduce from the differentiability of $t \mapsto (P_t^{-1})_* B_t$ in $\text{Vec}(\bar{\Omega})$ and the admissibility of \mathcal{E} that $B_t^{\phi_t}$ is positive for small enough t , so that \mathcal{E}_t is admissible.

Now, using Eq. (4.9), we obtain

$$\begin{aligned} (P_t^{-1})_* X_t &= (P_t^{-1})_* \left(\frac{B_t}{B_t^{\phi_t}} \right) \\ &= \frac{(P_t^{-1})_* B_t}{((P_t^{-1})_* B_t)^\phi}. \end{aligned}$$

Therefore, from the differentiability of $t \mapsto (P_t^{-1})_* B_t$ given by Proposition 4.3.2 and the fact that $((P_t^{-1})_* B_t)^\phi$ is nowhere zero for small enough t , we obtain that $t \mapsto (P_t^{-1})_* X_t$ is differentiable in $\text{Vec}(\partial\Omega)$ at $t = 0$, and its derivative at zero is given by

$$X'_V = \frac{1}{(B(\Omega)^\phi)^2} \left(B(\Omega)^\phi B'(\Omega; V) - (B'(\Omega; V))^\phi B(\Omega) \right).$$

Now, using the fact that $(\partial_\phi, \partial_\theta)$ is positively oriented and Eq. (4.8), we obtain

$$B(\Omega)^\perp = \sqrt{g} (B(\Omega)^\phi \nabla_\Gamma \theta - B(\Omega)^\theta \nabla_\Gamma \phi),$$

so that

$$\begin{aligned} (X'_V)^\theta &= \frac{1}{(B(\Omega)^\phi)^2} \left(B(\Omega)^\phi (B'(\Omega; V))^\theta - (B'(\Omega; V))^\phi B(\Omega)^\theta \right) \\ &= \frac{1}{(B(\Omega)^\phi)^2} (B(\Omega)^\phi \nabla_\Gamma \theta - B(\Omega)^\theta \nabla_\Gamma \phi) \cdot \left((B'(\Omega; V))^\phi \partial_\phi + (B'(\Omega; V))^\theta \partial_\theta \right) \\ &= \frac{1}{\sqrt{g} (B(\Omega)^\phi)^2} B(\Omega)^\perp \cdot B'(\Omega; V). \end{aligned}$$

□

We are now able to prove that the Poincaré map is shape differentiable.

Theorem 4.3.5. *The mapping*

$$\begin{cases} (-\varepsilon, \varepsilon) \rightarrow \text{Diff}(S^1) \\ t \mapsto \Pi_t \end{cases}$$

is smooth at zero, and its derivative is given by

$$\Pi'(\mathcal{E}; V)(\theta) = \int_0^1 \mathcal{T}(\phi, \theta) (X'_V)^\theta(\phi, \Pi_0^\phi(\theta)) d\phi,$$

where

$$\mathcal{T}(\phi, \theta) = \exp \left(\int_\phi^1 \partial_\theta X_0^\theta(\phi', \Pi_0^{\phi'}(\theta)) d\phi' \right).$$

Proof. Let $x_t(\cdot)$ be the solution to

$$\frac{d}{d\phi} x_t(\phi) = X_t^{\theta_t}(\phi, x_t(\phi)), \quad (4.10)$$

with $x_t(0) = \theta \in S^1$, so that $\Pi_t^\phi(\theta) = x_t(\phi)$. Using $\theta_t = \theta \circ P_t^{-1}$, we get

$$X_t^{\theta_t} = ((P_t^{-1})_* X_t)^\theta,$$

so that from Proposition 4.3.4, $t \mapsto X_t^{\theta_t}$ is smooth at $t = 0$ in $\mathcal{C}^\infty(\mathbb{T}^2)$. As a consequence, $t \mapsto x_t(\cdot)$ is also smooth at $t = 0$, and we can write

$$\begin{aligned} x_t(\phi) &= x^{(0)}(\phi) + tx^{(1)}(\phi) + o(t), \\ X_t^{\theta_t}(\phi, \theta) &= X_0^\theta(\phi, \theta) + t(X'_V)^\theta(\phi, \theta) + o(t), \end{aligned}$$

Where $o(t)$ is here a shorthand for a function whose \mathcal{C}^k norms on all compact subsets are $o(t)$. Since $\Pi_t(\theta) = x_t(1)$, we obtain that $t \mapsto \Pi_t$ is smooth at $t = 0$, and its derivative is given by $\Pi'(\mathcal{E}; V) = x^{(1)}(1)$. Inserting the expansions for $X_t^{\theta_t}$ and x_t in Eq. (4.10), we obtain

$$\begin{aligned} \frac{d}{d\phi}x^{(0)}(\phi) + t\frac{d}{d\phi}x^{(1)}(\phi) &= X_0^\theta(\phi, x^{(0)}(\phi)) \\ &+ t\left[\partial_\theta X_0^\theta(\phi, x^{(0)}(\phi))x^{(1)}(\phi) + (X'_V)^\theta(\phi, x^{(0)}(\phi))\right] + o(t), \end{aligned}$$

so that $x^{(1)}(\cdot)$ solves the following linear equation with a drift term

$$\frac{d}{d\phi}x^{(1)}(\phi) = \partial_\theta X_0^\theta(\phi, \Pi_0^\phi(\theta))x^{(1)}(\phi) + (X'_V)^\theta(\phi, \Pi_0^\phi(\theta)),$$

with $x^{(1)}(0) = 0$. Using Duhamel's formula, we thus obtain

$$x^{(1)}(1) = \int_0^1 e^{\int_\phi^1 \partial_\theta X_0^\theta(\phi', \Pi_0^{\phi'}(\theta))d\phi'} (X'_V)^\theta(\phi, \Pi_0^\phi(\theta))d\phi,$$

which is the desired result. \square

In the case where $B(\Omega)$ is linearized in the (ϕ, θ) coordinates, that is, $(B(\Omega))|_{\partial\Omega} = \chi(\partial_\phi + \omega\partial_\theta)$ where χ is a smooth function of $\partial\Omega$ and ω is in \mathbb{R} , we have the following formulas for $(X'_V)^\theta$ and $\Pi'(\mathcal{E}; V)$. We note that, in such coordinates, we have $B(\Omega)^\phi = \chi$ and $\omega = B(\Omega)^\theta/B(\Omega)^\phi$ is a constant number characterizing the slope of the field lines in the (ϕ, θ) coordinates.

Proposition 4.3.6. *Suppose there exist χ in $\mathcal{C}^\infty(\partial\Omega)$ positive and a real number ω such that $(B(\Omega))|_{\partial\Omega} = \chi(\partial_\phi + \omega\partial_\theta)$ with $(\partial_\phi, \partial_\theta)$ positively oriented. Let \tilde{n} be a smooth extension of n to \mathbb{R}^3 and $\vec{\omega} = (1, \omega)^T$. Decomposing $V \in \text{Vec}(\mathbb{R}^3)$ as $V = f\tilde{n} + V_\Gamma$ where $(V_\Gamma)|_{\partial\Omega}$ is tangent to $\partial\Omega$, we have*

$$(X'_V)^\theta = f\frac{2\text{III}(B(\Omega), B(\Omega)^\perp)}{\sqrt{g}\chi^2} + \left\langle \vec{\omega}, \nabla_{\mathbb{T}^2}(\omega V_\Gamma^\phi - V_\Gamma^\theta) \right\rangle + \frac{1}{\sqrt{g}\chi^2}B(\Omega)^\perp \cdot \nabla_\Gamma u_V, \quad (4.11)$$

where III is the second fundamental form of $\partial\Omega$. Furthermore, we also have

$$\Pi'(\mathcal{E}; V)(\theta) = \int_0^1 (X'_V)^\theta(\phi, \theta + \omega\phi)d\phi.$$

Proof. From Proposition 4.3.2 and Proposition 4.3.4, we have

$$\begin{aligned} (X'_V)^\theta &= \frac{1}{\sqrt{g}\chi^2} B(\Omega)^\perp \cdot B'(\Omega; V) \\ &= \frac{1}{\sqrt{g}\chi^2} B(\Omega)^\perp \cdot ([V, B(\Omega)] + \nabla u_V) \\ &= \frac{1}{\sqrt{g}\chi^2} B(\Omega)^\perp \cdot [f\tilde{n}, B(\Omega)] + \frac{1}{\sqrt{g}\chi^2} B(\Omega)^\perp \cdot [V_\Gamma, B(\Omega)] + \frac{1}{\sqrt{g}\chi^2} B(\Omega)^\perp \cdot \nabla_\Gamma u_V. \end{aligned} \quad (4.12)$$

For the first term of Eq. (4.12), we have

$$[f\tilde{n}, B(\Omega)] = f[\tilde{n}, B(\Omega)] - (B(\Omega) \cdot \nabla f) \tilde{n},$$

so that

$$B(\Omega)^\perp \cdot [f\tilde{n}, B(\Omega)] = fB(\Omega)^\perp \cdot [\tilde{n}, B(\Omega)].$$

We note that since $B(\Omega)$ is in $\text{Vec}(\bar{\Omega})$ and Ω is a smooth domain, we may extend $B(\Omega)$ and $B(\Omega)^\perp$ to smooth vector fields of \mathbb{R}^3 when necessary. Now, denoting by $\nabla_X Y$ the covariant derivative of a vector field Y in the direction X in \mathbb{R}^3 , and using the fact that the Levi–Civita connection is torsion free, we have

$$[\tilde{n}, B(\Omega)] = \nabla_{\tilde{n}} B(\Omega) - \nabla_{B(\Omega)} \tilde{n}.$$

We also have

$$\nabla(B(\Omega) \cdot \tilde{n}) = \nabla_{\tilde{n}} B(\Omega) + \nabla_{B(\Omega)} \tilde{n} + \tilde{n} \times \text{curl} B(\Omega) + B(\Omega) \times \text{curl} \tilde{n}.$$

It is straightforward to see that the tangential part of $[\tilde{n}, B(\Omega)]$ does not depend on the choice of extension of the normal, so that we may choose \tilde{n} in a specific way. Since $\partial\Omega$ is smooth, we know that the signed distance to $\partial\Omega$ (which we denote $\sigma_{\partial\Omega}$) is smooth in a neighborhood U of $\partial\Omega$. Let K be a compact subset of U containing a neighborhood of $\partial\Omega$, and η be a smooth positive function which is equal to one in K , and has support included in U . Then, $\tilde{n} := \eta \nabla \sigma_{\partial\Omega}$ is smooth extension of the normal, and $\text{curl} \tilde{n} = 0$ in K . Therefore, we have $\text{curl} \tilde{n} = 0$ on $\partial\Omega$. Furthermore, we also have $\text{curl} B(\Omega) = 0$ in $\bar{\Omega}$. As such, using that $B(\Omega)^\perp$ is tangent to $\partial\Omega$, and that $B(\Omega) \cdot \tilde{n}$ is equal to zero on $\partial\Omega$, we have

$$B(\Omega)^\perp \cdot \nabla_{\tilde{n}} B(\Omega) + B(\Omega)^\perp \cdot \nabla_{B(\Omega)} \tilde{n} = B(\Omega)^\perp \cdot \nabla(B(\Omega) \cdot \tilde{n}) = 0,$$

so that

$$B(\Omega)^\perp \cdot [\tilde{n}, B(\Omega)] = -2B(\Omega)^\perp \cdot \nabla_{B(\Omega)} \tilde{n}.$$

Now, using the fact that the Levi–Civita is compatible with the metric, we write

$$B(\Omega) \cdot \nabla(B(\Omega)^\perp \cdot \tilde{n}) = \nabla_{B(\Omega)} B(\Omega)^\perp \cdot \tilde{n} + B(\Omega)^\perp \cdot \nabla_{B(\Omega)} \tilde{n}.$$

Therefore, since $B(\Omega) \cdot \nabla(B(\Omega)^\perp \cdot \tilde{n})$ vanishes on $\partial\Omega$, we have

$$\begin{aligned} B(\Omega)^\perp \cdot \nabla_{B(\Omega)} \tilde{n} &= -\nabla_{B(\Omega)} B(\Omega)^\perp \cdot \tilde{n} \\ &= -\text{III}(B(\Omega), B(\Omega)^\perp). \end{aligned}$$

We refer to [Lee18][Section 8] for the definition of the second fundamental form of 1-codimensional

manifolds using the Levi-Civita connection. As a consequence, the first term of Eq. (4.12) is given by

$$\frac{1}{\sqrt{g}\chi^2}[f\tilde{n}, B(\Omega)] = f \frac{2\text{III}(B(\Omega), B(\Omega)^\perp)}{\sqrt{g}\chi^2}.$$

Now, we compute the second term of Eq. (4.12). Since V_Γ and $B(\Omega)$ are tangent vector fields, the tangential part of $[V_\Gamma, B(\Omega)]$ is given by the Lie bracket of V_Γ and $B(\Omega)$ as vector fields of $\partial\Omega$, which we denote $[V_\Gamma, B(\Omega)]_{\partial\Omega}$. We have $B(\Omega) = \chi(\partial_\phi + \omega\partial_\theta) = \chi X_0$, so that

$$[V_\Gamma, B(\Omega)]_{\partial\Omega} = V_\Gamma \cdot (\nabla_\Gamma \chi) X_0 + \chi [V_\Gamma, X_0]_{\partial\Omega}.$$

Since X_0 is collinear to $B(\Omega)$ it is orthogonal to $B(\Omega)^\perp$ which implies

$$B(\Omega)^\perp \cdot [V_\Gamma, B(\Omega)] = \chi B(\Omega)^\perp \cdot [V_\Gamma, X_0]_{\partial\Omega}.$$

Now, we write in coordinates

$$\begin{aligned} X_0 &= \partial_\phi + \omega\partial_\theta, \\ V_\Gamma &= V_\Gamma^\phi \partial_\phi + V_\Gamma^\theta \partial_\theta, \end{aligned}$$

which gives us

$$[V_\Gamma, X_0]_{\partial\Omega} = -(\partial_\phi V_\Gamma^\phi + \omega\partial_\theta V_\Gamma^\phi)\partial_\phi - (\partial_\phi V_\Gamma^\theta + \omega\partial_\theta V_\Gamma^\theta)\partial_\theta.$$

Finally, using $B(\Omega)^\perp = \sqrt{g}\chi(\nabla_\Gamma\theta - \omega\nabla_\Gamma\phi)$, we get

$$\begin{aligned} B(\Omega)^\perp \cdot [V_\Gamma, B(\Omega)] &= -\sqrt{g}\chi^2(\nabla_\Gamma\theta - \omega\nabla_\Gamma\phi) \cdot \left[(\partial_\phi V_\Gamma^\phi + \omega\partial_\theta V_\Gamma^\phi)\partial_\phi + (\partial_\phi V_\Gamma^\theta + \omega\partial_\theta V_\Gamma^\theta)\partial_\theta \right] \\ &= -\sqrt{g}\chi^2 \left(\partial_\phi V_\Gamma^\theta + \omega\partial_\theta V_\Gamma^\theta - \omega\partial_\phi V_\Gamma^\phi - \omega^2\partial_\theta V_\Gamma^\phi \right), \\ &= \sqrt{g}\chi^2 \left\langle \vec{\omega}, \nabla_{\mathbb{T}^2} \left(\omega V_\Gamma^\phi - V_\Gamma^\theta \right) \right\rangle, \end{aligned}$$

which completes the proof of the first statement. The second result is then a simple consequence of Theorem 4.3.5 and the fact that, since $(X_0)|_{\partial\Omega} = \partial_\phi + \omega\partial_\theta$, we have $\Pi^\phi(\theta) = \theta + \omega\phi$ and $\mathcal{T}(\phi, \theta) = 1$. \square

4.4 The axisymmetric case

In this section, we consider the embedding of the standard axisymmetric torus defined in Cartesian coordinates by

$$\mathcal{E}(\phi, \theta) = ((R_T + r_P \cos(2\pi\theta)) \cos(2\pi\phi), (R_T + r_P \cos(2\pi\theta)) \sin(2\pi\phi), r_P \sin(2\pi\theta)), \quad (4.13)$$

where R_T and r_P are the major and minor radius respectively with $r_P < R_T$. We also denote

$$R(\theta) = R_T + r_P \cos(2\pi\theta),$$

which is the distance of the point $\mathcal{E}(\phi, \theta)$ to the z -axis. The aim of this section is to prove the following theorem.

Theorem 4.4.1. *Let \mathcal{E} be as described above. We have for all V in $\text{Vec}(\mathbb{R}^3)$*

$$\Pi'(\mathcal{E}; V) = 0.$$

Although we are working with a torus with circular cross-section for simplicity, it will be clear during the proof that one may choose any smooth axisymmetric torus. We begin by computing the relevant geometric objects associated with this embedding. The basis vectors of the coordinates (ϕ, θ) are given by

$$\begin{aligned}\partial_\phi &= -2\pi R(\theta) \sin(2\pi\phi) \partial_x + 2\pi R(\theta) \cos(2\pi\phi) \partial_y, \\ \partial_\theta &= -2\pi r_P \sin(2\pi\theta) \cos(2\pi\phi) \partial_x - 2\pi r_P \sin(2\pi\theta) \sin(2\pi\phi) \partial_y + 2\pi r_P \cos(2\pi\theta) \partial_z,\end{aligned}$$

so that

$$g = 4\pi^2 R(\theta)^2 d\phi^2 + 4\pi^2 r_P^2 d\theta^2.$$

We also deduce $\sqrt{g} = 4\pi^2 r_P R(\theta)$. One also verifies that

$$n = \cos(2\pi\theta) \cos(2\pi\phi) \partial_x + \cos(2\pi\theta) \sin(2\pi\phi) \partial_y + \sin(2\pi\theta) \partial_z.$$

Computing the second-order derivatives of \mathcal{E} , we get

$$\begin{aligned}\partial_\phi^2 \mathcal{E} &= -4\pi^2 R(\theta) \cos(2\pi\phi) \partial_x - 4\pi^2 R(\theta) \sin(2\pi\phi) \partial_y, \\ \partial_\phi \partial_\theta \mathcal{E} &= 4\pi^2 r_P \sin(2\pi\theta) \sin(2\pi\phi) \partial_x - 4\pi^2 r_P \sin(2\pi\theta) \cos(2\pi\phi) \partial_y, \\ \partial_\theta^2 \mathcal{E} &= -4\pi^2 r_P \cos(2\pi\theta) \cos(2\pi\phi) \partial_x - 4\pi^2 r_P \cos(2\pi\theta) \sin(2\pi\phi) \partial_y - 4\pi^2 r_P \sin(2\pi\theta) \partial_z,\end{aligned}$$

so that

$$\begin{aligned}\text{III} &= (\partial_\phi^2 \mathcal{E} \cdot n) d\phi^2 + 2 (\partial_\phi \partial_\theta \mathcal{E} \cdot n) d\phi d\theta + (\partial_\theta^2 \mathcal{E} \cdot n) d\theta^2, \\ &= -4\pi^2 R(\theta) \cos(2\pi\theta) d\phi^2 - 4\pi^2 r_P d\theta^2.\end{aligned}\tag{4.14}$$

We now turn to the underlying domain Ω , and the associated harmonic field. $\mathcal{E}(\mathbb{T}^2)$ bounds the domain

$$\Omega = \{((R_T + r_P x) \cos(2\pi\phi), (R_T + r_P x) \sin(2\pi\phi), r_P y) \in \mathbb{R}^3 \mid (\phi, x, y) \in S^1 \times D^2\}.$$

In this case, the harmonic field of Ω is explicitly known, and is given by the formula

$$B(\Omega) = \frac{1}{2\pi} \left(-\frac{y}{x^2 + y^2} \partial_x + \frac{x}{x^2 + y^2} \partial_y \right),$$

where the $1/2\pi$ constant ensures that $B(\Omega)$ has unit circulation along positively oriented toroidal loops. Moreover, the restriction of $B(\Omega)$ to the boundary is given by

$$B(\Omega)|_{\partial\Omega} = \frac{1}{4\pi^2 R(\theta)^2} \partial_\phi.\tag{4.15}$$

It is then clear that \mathcal{E} is indeed an admissible embedding. We are now able to prove the following lemma.

Proposition 4.4.2. *Let \mathcal{E} , $B(\Omega)$ and (ϕ, θ) be as defined above. We then have*

- $X(\mathcal{E}) = \partial_\phi$,
- $\Pi(\mathcal{E}) = id$,
- $\text{III}(B(\Omega), B(\Omega)^\perp) = 0$.

Proof. The first two statements are straightforward using Eq. (4.15). As for the third statement, using the fact that the coordinates (ϕ, θ) are orthogonal, we know that $B(\Omega)^\perp$ is colinear to ∂_θ .

Furthermore, we know from Eq. (4.14) that the second fundamental form is diagonalized in the coordinates (ϕ, θ) , which gives us the desired result. \square

Corollary 4.4.3. *Let \mathcal{E} and Ω be as defined above, and u_V be the solution to Eq. (4.4). Then*

$$\Pi'(\mathcal{E}; V)(\theta) = \frac{R(\theta)^2}{r_P^2} \int_0^1 \partial_\theta u_V(\phi, \theta) d\phi.$$

Proof. Using Proposition 4.4.2, we know that we can apply Proposition 4.3.6 with $\omega = 0$. We decompose $V \in \text{Vec}(\mathbb{R}^3)$ as $V = f\tilde{n} + V_\Gamma$, where \tilde{n} is a smooth extension of n to \mathbb{R}^3 , and V_Γ is tangent to $\partial\Omega$. Since $(\partial_\phi, \partial_\theta)$ is positively oriented, we know from Proposition 4.3.6 and Proposition 4.4.2 that

$$(X'_V)^\theta = -\partial_\phi V_\Gamma^\theta + \frac{1}{\sqrt{g}(B(\Omega)^\phi)^2} B(\Omega)^\perp \cdot \nabla_\Gamma u_V.$$

Using the fact that $v \mapsto v^\perp$ is an isometry on each tangent plane of $\partial\Omega$ and that $(v^\perp)^\perp = -v$, we find

$$\begin{aligned} B(\Omega)^\perp \cdot \nabla_\Gamma u_V &= -B(\Omega) \cdot (\nabla_\Gamma u_V)^\perp \\ &= - (B(\Omega)^\phi \partial_\phi) \cdot \left(\frac{1}{\sqrt{g}} \partial_\phi u_V \partial_\theta - \frac{1}{\sqrt{g}} \partial_\theta u_V \partial_\phi \right) \\ &= B(\Omega)^\phi \partial_\theta u_V \frac{g_{\phi\phi}}{\sqrt{g}}, \end{aligned}$$

where we used $\nabla_\Gamma u_V = \partial_\phi u_V \nabla_\Gamma \phi + \partial_\theta u_V \nabla_\Gamma \theta$, as well as $\nabla_\Gamma \phi^\perp = 1/\sqrt{g} \partial_\theta$ and $\nabla_\Gamma \theta^\perp = -1/\sqrt{g} \partial_\phi$, which are simple consequences of Eqs. (4.7) and (4.8). Therefore, we obtain

$$\begin{aligned} (X'_V)^\theta &= -\partial_\phi V_\Gamma^\theta + \frac{g_{\phi\phi}}{(\det g) B(\Omega)^\phi} \partial_\theta u_V \\ &= -\partial_\phi V_\Gamma^\theta + \frac{R(\theta)^2}{r_P^2} \partial_\theta u_V. \end{aligned}$$

Using once again Proposition 4.3.6, we obtain

$$\begin{aligned} \Pi'(\mathcal{E}; V) &= \int_0^1 (X'_V)^\theta(\phi, \theta) d\phi \\ &= \frac{R(\theta)^2}{r_P^2} \int_0^1 \partial_\theta u_V(\phi, \theta) d\phi. \end{aligned}$$

\square

The proof of Theorem 4.4.1 follows from Corollary 4.4.3 taking into account suitable symmetry properties described in the following lemmas.

Lemma 4.4.4. *Let Ω be as defined above and u_V be a solution to Eq. (4.4). Then, for all θ in S^1 , we have*

$$\int_0^1 \nabla u_V(\phi, \theta) \cdot n d\phi = 0. \quad (4.16)$$

Proof. We recall that u_V is a harmonic function of Ω satisfying the boundary condition

$$\nabla u_V \cdot n = \operatorname{div}_\Gamma(B(\Omega)(V \cdot n)).$$

A quick computation in coordinates shows that $\operatorname{div}_\Gamma(B(\Omega)) = 0$, so that

$$\operatorname{div}_\Gamma(B(\Omega)(V \cdot n)) = B(\Omega) \cdot \nabla_\Gamma(V \cdot n).$$

Furthermore, since $B(\Omega) = 1/(4\pi^2 R(\theta)^2) \partial_\phi$, we have $B(\Omega) \cdot \nabla_\Gamma(V \cdot n) = 1/(4\pi^2 R(\theta)^2) \partial_\phi(V \cdot n)$. Finally, we deduce

$$\begin{aligned} \int_0^1 \nabla u_V(\phi, \theta) \cdot n d\phi &= \frac{1}{4\pi^2 R(\theta)^2} \int_0^1 \partial_\phi(V \cdot n)(\phi, \theta) d\phi \\ &= 0. \end{aligned}$$

□

Since u_V is harmonic in Ω , we know that $\nabla u_V \cdot n$ must be of zero average on $\partial\Omega$. Lemma 4.4.4 then tells us that $\nabla u_V \cdot n$ must moreover be of zero average along any toroidal loop. In particular, u_V may not be any harmonic function of $\bar{\Omega}$ and its trace may not be any smooth function of $\partial\Omega$. This fact is then used to prove the following lemma, for which we introduce the notation

$$\int_{\partial\Omega} f = \frac{\int_{\partial\Omega} f}{|\partial\Omega|} = \frac{\int_{\partial\Omega} f}{\int_{\partial\Omega} 1},$$

where f is an integrable function on $\partial\Omega$.

Lemma 4.4.5. *Let Ω be as defined above and u_V be as in Eq. (4.4). Let f be a smooth function on $\partial\Omega$ such that $\partial_\phi f = 0$. We have*

$$\int_{\partial\Omega} f u_V = \int_{\partial\Omega} f \int_{\partial\Omega} u_V. \quad (4.17)$$

Proof. First, suppose that f has zero average on $\partial\Omega$. We then define v as the zero average solution to

$$\begin{cases} \Delta v = 0 & \text{in } \Omega, \\ \nabla v \cdot n = f & \text{on } \partial\Omega. \end{cases}$$

We now show that $\partial_\phi v = 0$. Indeed, call R_Φ the rotation of angle Φ around the z -axis. We then get that $v \circ R_\Phi$ satisfies

$$\Delta(v \circ R_\Phi) = (\Delta v) \circ R_\Phi = 0,$$

because R_Φ is an isometry, and

$$\nabla(v \circ R_\Phi) \cdot n = (\nabla v \cdot n) \circ R_\Phi = f,$$

because R_Φ is an isometry which leaves Ω unchanged and $\partial_\phi f = 0$. Therefore, v and $v \circ R_\Phi$ satisfy the same PDE, and have the same average. As a consequence, $v \circ R_\Phi = v$ for all Φ , meaning that $\partial_\phi v = 0$.

Now, using the equations satisfied by u_V and v , and Lemma 4.4.4, we get

$$\begin{aligned}
\int_{\partial\Omega} f u_V &= \int_{\partial\Omega} (\nabla v \cdot n) u_V \\
&= \int_{\Omega} \nabla v \cdot \nabla u_V \\
&= \int_{\partial\Omega} v (\nabla u_V \cdot n) \\
&= 4\pi^2 r_P \int_0^1 R(\theta) v(\theta) \int_0^1 \nabla u_V \cdot n(\phi, \theta) d\phi d\theta \\
&= 0.
\end{aligned}$$

Finally, if we now take any f in $C^\infty(\partial\Omega)$, we can repeat the procedure with $f - \int_{\partial\Omega} f$, and get

$$\int_{\partial\Omega} \left[\left(f - \int_{\partial\Omega} f \right) u_V \right] = 0,$$

which gives us our desired result. \square

We now have all the ingredients to prove Theorem 4.4.1.

Proof of Theorem 4.4.1. To prove that $\Pi'(\mathcal{E}; V)$ vanishes, we use Lemma 4.4.5 on approximations of δ_{θ_0} . We define $\tilde{f}_{\theta_0, \varepsilon} \in C^\infty(S^1)$ so that $4\pi^2 r_P R \tilde{f}_{\theta_0, \varepsilon}$ is a family of smooth approximations of the Dirac at θ_0 . We may take for example

$$R(\theta) \tilde{f}_{\theta_0, \varepsilon}(\theta) = C_\varepsilon \sum_{k \in \mathbb{Z}} \exp\left(-\frac{\varepsilon^2(\theta - \theta_0 - k)^2}{2}\right),$$

with C_ε chosen so that

$$\int_0^1 4\pi^2 r_P R(\theta) \tilde{f}_{\theta_0, \varepsilon}(\theta) d\theta = 1.$$

Then, defining $f_{\theta_0, \varepsilon}(\phi, \theta) = \tilde{f}_{\theta_0, \varepsilon}(\theta)$ and using $\sqrt{g} = 4\pi^2 r_P R(\theta)$, we get

$$\begin{aligned}
\int_{\partial\Omega} f_{\theta_0, \varepsilon} u_V &= \int_0^1 \int_0^1 4\pi^2 r_P R(\theta) \tilde{f}_{\theta_0, \varepsilon}(\theta) u_V(\phi, \theta) d\theta d\phi \\
&\xrightarrow{\varepsilon \rightarrow 0} \int_0^1 u_V(\phi, \theta_0) d\phi.
\end{aligned}$$

On the other hand, Lemma 4.4.5 gives us

$$\begin{aligned}
\int_{\partial\Omega} f_{\theta_0, \varepsilon} u_V &= \int_{\partial\Omega} f_{\theta_0, \varepsilon} \int_{\partial\Omega} u_V \\
&= \int_{\partial\Omega} u_V.
\end{aligned}$$

As a consequence, we have for all θ in S^1

$$\int_0^1 u_V(\phi, \theta) d\phi = \int_{\partial\Omega} u_V,$$

and thus

$$\int_0^1 \partial_\theta u_V(\phi, \theta) d\phi = 0.$$

We then conclude using the formula of $\Pi'(\mathcal{E}; V)$ given in Corollary 4.4.3. \square

4.5 The diophantine case

In this section, we suppose that \mathcal{E} is an admissible embedding such that, in the corresponding coordinates (ϕ, θ) , we have $B|_{\partial\Omega} = \chi(\partial_\phi + \omega\partial_\theta)$, where χ is a smooth function on the boundary and ω is a diophantine number, that is, there exist C, τ positive constants such that, for all $p/q \in \mathbb{Q}$

$$|\omega - p/q| \geq C|q|^{-(\tau+1)}. \quad (4.18)$$

We note that this definition of diophantine numbers implies two other inequalities which will be used in this section. The first one, which is generally used for cohomological equations in the continuous context, is the following. For all $n \neq 0$ in \mathbb{Z}^2 , we have

$$|\vec{\omega} \cdot n| \geq C|n|^{-\tau}, \quad (4.19)$$

with $\vec{\omega} = (1, \omega)^T$. The second one, which is generally more common in discrete contexts, is the following. For all $q \neq 0$ in \mathbb{Z} , we have

$$|e^{2\pi i\omega q} - 1| \geq C|q|^{-\tau}, \quad (4.20)$$

where C is not necessarily the same constant as before. To obtain this inequality, we write using Eq. (4.18)

$$\inf_{p \in \mathbb{Z}} |\omega q - p| \geq C|q|^{-\tau}.$$

The quantity on the right-hand side of this inequality is the distance between ωq and 0 in $S^1 = \mathbb{R}/\mathbb{Z}$ using the quotient metric induced from the usual metric on \mathbb{R} . This metric is then equivalent to the metric on S^1 when seen as the unit circle in \mathbb{C} , which gives us Eq. (4.20).

In this section, we prove the following theorem

Theorem 4.5.1. *Suppose \mathcal{E} is an admissible embedding with associated domain Ω and coordinates (ϕ, θ) verifying the following hypotheses.*

1. *There exists χ in $C^\infty(\partial\Omega)$ and a diophantine number ω such that $B(\Omega)|_{\partial\Omega} = \chi(\partial_\phi + \omega\partial_\theta)$.*
2. *$\mathbb{I}(B(\Omega), B(\Omega)^\perp)$ vanishes nowhere on $\partial\Omega$.*

Then, the mapping $V \mapsto \Pi'(\mathcal{E}; V)$ is surjective from $\text{Vec}(\mathbb{R}^3)$ to $C^\infty(S^1)$.

Remark 4.5.2. *For a point x of $\partial\Omega$, the second fundamental form \mathbb{I}_x at x is related to the shape operator S_x by $\mathbb{I}_x(u, v) = S_x(u) \cdot v$. Since \mathbb{I}_x is a symmetric bilinear form, S_x is self adjoint and there exist two orthonormal eigenvectors E_1 and E_2 of $T_x\partial\Omega$ with associated eigenvalues κ_1 and κ_2 . E_i are the principal directions at x , and κ_i the related principal curvatures. We can also assume that (E_1, E_2) is positively oriented on $T_x\partial\Omega$. If we decompose $B(\Omega)$ at x as*

$$B(\Omega) = \alpha_1 E_1 + \alpha_2 E_2,$$

then

$$\mathbb{I}_x(B(\Omega), B(\Omega)^\perp) = \alpha_1 \alpha_2 (\kappa_2 - \kappa_1).$$

Therefore, we find that $\mathbb{I}(B(\Omega), B(\Omega)^\perp)$ does not vanish at x if and only if two conditions are met:

- x is not an umbilical point of $\partial\Omega$, that is $\kappa_1 \neq \kappa_2$.
- $B(\Omega)$ is not in a principal direction at x .

The proof of Theorem 4.5.1 comes in two steps. First, we prove that by choosing V tangent to the boundary, we can generate any $\Pi'(\mathcal{E}; V)$ which is of zero average on S^1 . This result is not surprising as having V tangent to the boundary amounts to changing the coordinates on $\partial\Omega$, which in turn changes the Poincaré map by a conjugation by a diffeomorphism on S^1 . As such, tangent deformations do not generate a change in the rotation number, and the only possible changes in Π_t have zero average at first-order in t . Then, the image of $V \mapsto \Pi(\mathcal{E}; V)$ has co-dimension at most one in $\mathcal{C}^\infty(S^1)$, and one only needs to find a normal deformation which generates $\Pi'(\mathcal{E}; V)$ with nonzero average. This is achieved using the assumption on $\mathbb{I}(B(\Omega), B(\Omega)^\perp)$.

Proposition 4.5.3. *For all μ in $\mathcal{C}^\infty(S^1)$ such that*

$$\int_{S^1} \mu = 0,$$

there exists V_Γ in $\text{Vec}(\mathbb{R}^3)$ such that $(V_\Gamma)|_{\partial\Omega}$ is tangent to $\partial\Omega$ and $\Pi'(\mathcal{E}; V_\Gamma) = \mu$.

Proof. Let μ in $\mathcal{C}^\infty(S^1)$ be given in Fourier basis by

$$\mu(\theta) = \sum_{n \in \mathbb{Z}} \hat{\mu}_n e^{2\pi i n \theta},$$

with $\hat{\mu}_0 = 0$. Since μ is real-valued, we have $(\hat{\mu}_{-n})^* = \hat{\mu}_n$. We define $\hat{\Phi}_n = (2\pi i n \omega) / (e^{2\pi i n \omega} - 1) \hat{\mu}_n$ for $n \neq 0$, and

$$\Phi(\phi, \theta) = \sum_{n \in \mathbb{Z} \setminus \{0\}} \hat{\Phi}_n e^{2\pi i n \theta}.$$

Using the discrete diophantine condition on ω given by Eq. (4.20), we get

$$\begin{aligned} \left| \frac{2\pi i n \omega}{e^{2\pi i n \omega} - 1} \hat{\mu}_n \right| &\leq C |e^{2\pi i n \omega} - 1|^{-1} |n| |\hat{\mu}_n|, \\ &\leq C |n|^{\tau+1} |\hat{\mu}_n|, \end{aligned}$$

so that Φ is smooth on \mathbb{T}^2 . Furthermore, using the symmetries of $\hat{\mu}_n$, it is straightforward that Φ is also real-valued. Now, define V_Γ as a smooth extension of $-\varphi \partial_\theta$ to \mathbb{R}^3 , where φ is the zero average solution to

$$\langle \vec{\omega}, \nabla_{\mathbb{T}^2} \varphi \rangle = \Phi.$$

This solution is known to exist using the continuous diophantine condition given by Eq. (4.19) and the fact that Φ has zero average on \mathbb{T}^2 (see for example [Lla03]). Moreover, we have $V_\Gamma \cdot n = 0$ so that the solution u_{V_Γ} to Eq. (4.4) is constant. Using Proposition 4.3.6, we get

$$\begin{aligned} (X'_{V_\Gamma})^\theta &= \left\langle \vec{\omega}, \nabla_{\mathbb{T}^2} \left(\omega V_\Gamma^\phi - V_\Gamma^\theta \right) \right\rangle \\ &= \langle \vec{\omega}, \nabla_{\mathbb{T}^2} \varphi \rangle \\ &= \Phi. \end{aligned}$$

Now, we compute using Proposition 4.3.6

$$\begin{aligned}
\Pi'(\mathcal{E}; V_\Gamma)(\theta) &= \int_0^1 (X'_{V_\Gamma})^\theta(\phi, \theta + \omega\phi) d\phi \\
&= \int_0^1 \Phi(\phi, \theta + \omega\phi) d\phi \\
&= \sum_{n \in \mathbb{Z} \setminus \{0\}} \hat{\Phi}_n \int_0^1 e^{2\pi i n(\theta + \omega\phi)} d\phi \\
&= \sum_{n \in \mathbb{Z} \setminus \{0\}} \hat{\Phi}_n \frac{e^{2\pi i n \omega} - 1}{2\pi i n} e^{2\pi i n \theta} \\
&= \sum_{n \in \mathbb{Z}} \hat{\mu}_n e^{2\pi i n \theta} \\
&= \mu(\theta).
\end{aligned}$$

□

Proof of Theorem 4.5.1. From Proposition 4.5.3, we know that the image of $V \mapsto \Pi'(\mathcal{E}; V)$ contains all the smooth zero average functions on S^1 . By linearity, we therefore only need to find one deformation which produces a derivative of the Poincaré map with nonzero average. This is done by picking $V = 1/(\sqrt{g}\chi)\tilde{n}$, where \tilde{n} is an extension of the normal. Indeed, this verifies $V \cdot n = 1/(\sqrt{g}\chi)$, so that

$$\begin{aligned}
\operatorname{div}_\Gamma(B(\Omega)(V \cdot n)) &= \frac{1}{\sqrt{g}} \left(\partial_\phi \left(\sqrt{g} \frac{\chi}{\chi\sqrt{g}} \right) + \partial_\theta \left(\sqrt{g} \frac{\omega\chi}{\chi\sqrt{g}} \right) \right) \\
&= 0.
\end{aligned}$$

As a consequence, the solution u_V of Eq. (4.4) is constant, and by Proposition 4.3.6 $(X'_V)^\theta$ is given by

$$(X'_V)^\theta = \frac{2\text{III}(B(\Omega), B(\Omega)^\perp)}{(\det g)\chi^3}.$$

Since we assume that $\text{III}(B(\Omega), B(\Omega)^\perp)$ vanishes nowhere, it is either positive or negative on $\partial\Omega$. As a consequence

$$\theta \mapsto \int_0^1 (X'_V)^\theta(\phi, \theta + \omega\phi) d\phi,$$

is also either positive or negative on S^1 , and has therefore a nonzero average. □

4.6 Conclusion and perspectives

Conclusion In this chapter, we have established a shape differentiability result for the Poincaré maps of harmonic fields, and studied some properties of the shape derivative in specific cases. The proof of shape differentiability in the general case followed from an easy adaptation of the shape differentiation result of harmonic fields given in Section 2.5 in the smooth category. We then studied the case of axisymmetric domains, for which we found that the shape derivative of the Poincaré map of harmonic fields always vanishes. After that, we have found that when the domain has a Poincaré map which is a diophantine rotation on the boundary, the shape derivative

may be any smooth function of the circle under an additional assumption relating the curvature of the boundary and the harmonic field.

Perspectives First, we defined the Poincaré map of harmonic fields Π using the notion of admissible embeddings of the torus into \mathbb{R}^3 . As such, the map that we obtain is not technically speaking a shape function. One may then wonder how changing the embedding of the torus may change the Poincaré map when fixing the shape of the corresponding domain. Indeed, if Π were a true shape functional, such changes in embeddings would not affect the Poincaré map. However, although the coordinates in which we consider the Poincaré map changes, the underlying dynamics of the harmonic field does not. What we expect to find is that, if the embedding preserves a certain notion of orientation, the change of embedding would lead to a change in the Poincaré map given by a conjugation in the group of diffeomorphisms of the circle. In the other case, we expect to find that the Poincaré map associated to the modified embedding would be the inverse of the original Poincaré map up to conjugation. Indeed, changing orientation would intuitively lead to reversing the direction of time for the flow of the harmonic field.

Second, we saw in Section 4.4 that the shape derivative of the Poincaré map of the harmonic field is always zero in the case of the standard torus. One could then naturally ask if the second order derivative may in this case produce changes in the Poincaré map, and in particular, changes in the rotation number. For this, one would need to find an expression for this shape derivative. Although the author has made some preliminary computations in this direction, it seems that the formulas we obtain are much more difficult to deal with than in the first order case so that coming up with deformations of the domain leading to changes in the Poincaré map at second order is not an easy task.

Finally, we believe that the main result of Section 4.5 leads to two questions which we leave open. First, it is not still clear to the author if the assumption relating the harmonic field and the second fundamental form in Theorem 4.5.1 is often realized in practice. The author attempted to study this assumption in the case of the thin toroidal domains from [EP15], but it seems that this assumption is not verified in this case. In fact, we found that the approximate harmonic field denoted as h_0 in [EP15, Section 5] is exactly aligned with the lowest principal curvature direction of the boundary, and that taking some finer approximations leads to changes in sign for the quantity used in the assumption. Although this fact is interesting in itself, it means that the additional assumption used for Theorem 4.5.1 is not satisfied for thin toroidal domains (see Remark 4.5.2). One could then try to find other domains for which the assumption is satisfied, but this does not seem like an easy task. Another thing one may try to do is to weaken the curvature assumption used in Theorem 4.5.1. Indeed, we see when studying the proof that only the first two terms of the shape derivative given by Eq. (4.11) are used to prove surjectivity so that also using the third term may lead to weaker assumptions. Second, we believe that Theorem 4.5.1 may lead to interesting local properties of Π around embeddings where it applies. Indeed, if we were working in the simpler case of Banach spaces, we would obtain that Π is locally surjective around such domains. As a consequence, we would find that generic perturbations of such domains would lead to Morse–Smale diffeomorphisms of the circle, and thus rational rotation numbers¹. However, surjectivity of the differential does not imply local surjectivity in Fréchet spaces, so that this result is harder to establish. We refer the reader to [Ham82] for a local surjectivity theorem in Fréchet spaces, but we do not expect that the assumptions would be verified in our case.

1. See for example [OS98] for the notion of Morse–Smale diffeomorphisms of the circles and some of their properties.

Appendix A

Translation from differential forms and Hodge decomposition

It is common in the literature to find the types of problems we are studying in the language of differential forms. Although this approach deals with more abstract mathematical objects, it allows the use of a unique framework. This approach can notably be found in [AFW06], and is relatively common in the finite element exterior calculus literature.

Since results using the differential forms language are quite often referenced in this manuscript, we choose to write a small appendix to explain how to translate expressions from the language of differential forms to the one of functions and vector fields in three dimensional manifolds. This is done using usual identifications from Riemannian geometry and Hodge theory, that is, the musical isomorphisms and Hodge star operator (see Section 1.3.1). In the case of a three-dimensional manifold, these identifications work perfectly to equate 0 and 3 forms with functions, 1 and 2 forms with vector fields, and to translate the exterior derivatives and coderivatives with the usual differential operators of electromagnetism. These identifications are then summed up in the following commutative diagram, and table.

$$\begin{array}{ccccccc}
 H\Lambda^0(\Omega) & \xrightarrow{d} & H\Lambda^1(\Omega) & \xrightarrow{d} & H\Lambda^2(\Omega) & \xrightarrow{d} & H\Lambda^3(\Omega) \\
 \text{id} \downarrow & & \# \downarrow & & \#* \downarrow & & * \downarrow \\
 H^1(\Omega) & \xrightarrow{\nabla} & H(\text{curl}, \Omega) & \xrightarrow{\text{curl}} & H(\text{div}, \Omega) & \xrightarrow{\text{div}} & L^2(\Omega)
 \end{array} \tag{A.1}$$

	$H\Lambda^k(\Omega)$	$H^*\Lambda^k(\Omega)$	d	δ	$\text{Tr}(u)$	$\iota_V u$	$\mathcal{L}_V u$
$k = 0$	$H^1(\Omega)$	$L^2(\Omega)$	∇	0	$u _{\partial\Omega}$	0	$\nabla u \cdot V$
$k = 1$	$H(\text{curl}, \Omega)$	$H(\text{div}, \Omega)$	curl	$-\text{div}$	$u \times n$	$u \cdot V$	$\text{curl } u \times V + \nabla(u \cdot V)$
$k = 2$	$H(\text{div}, \Omega)$	$H(\text{curl}, \Omega)$	div	curl	$u \cdot n$	$u \times V$	$(\text{div } u)V + \text{curl}(u \times V)$
$k = 3$	$L^2(\Omega)$	$H^1(\Omega)$	0	$-\nabla$	-	uV	$\text{div}(uV)$

Figure A.1 – Table of correspondence between differential forms language and vector calculus language

Here, $H\Lambda^k(\Omega)$ denotes the set of square integrable k -forms whose exterior derivative is square

integrable, $H^* \Lambda^k(\Omega)$ the set of square integrable k -forms whose exterior coderivative is square integrable, d the exterior derivative, δ the exterior coderivative, $*$ the Hodge star operator, $\#$ the musical isomorphism taking 1-forms to vector fields, $\text{Tr}(\omega)$ the trace of a differential form ω defined by the pullback of ω onto $\partial\Omega$ by the inclusion map $i : \partial\Omega \rightarrow \bar{\Omega}$, ι_V is the interior product with a vector field V and \mathcal{L}_V is the Lie derivative in the direction of a vector field V .

We now give three proposition which are used throughout the manuscript. Proposition A.1 is a vectorial Hodge decomposition, Proposition A.2 gives Poincaré type inequalities, and Proposition A.3 gives L^2 orthogonality relations between functional spaces. We also note that similar results may be found directly in the vectorial context for example in [EG23], although the notations and approaches used here are slightly different.

Proposition A.1. *Let Ω be a Lipschitz toroidal domain as defined in Section 2.2.1. We have the following L^2 orthogonal decompositions*

$$L^2(\Omega)^3 = \text{curl } H_0(\text{curl}, \Omega) \oplus^\perp \mathcal{K}(\Omega) \oplus^\perp \nabla H^1(\Omega), \quad (\text{A.2})$$

$$L^2(\Omega)^3 = \text{curl } H(\text{curl}, \Omega) \oplus^\perp \nabla H_0^1(\Omega). \quad (\text{A.3})$$

Proof. This is a simple consequence of the Hodge decomposition given in [AFW06, Section 2], in the cases $k = 1$ and $k = 2$ respectively. The reason no harmonic term appears in Eq. (A.3) is that the second de Rham cohomology space vanishes in Ω , and thus, that the set of harmonic two forms is trivial. \square

Proposition A.2. *There exists C such that for all $u_1 \in H(\text{curl}^0, \Omega)^\perp \cap H(\text{curl}, \Omega)$, $u_2 \in H(\text{div}^0, \Omega)^\perp \cap H(\text{div}, \Omega)$*

$$\|u_1\| \leq C \|\text{curl } u_1\|,$$

$$\|u_2\| \leq C \|\text{div } u_2\|.$$

Proof. This is given by [AFW06, Eq. (2.17)] in the cases $k = 1$ and $k = 2$. \square

Proposition A.3. *We have the following orthogonality relations in $L^2(\Omega)^3$*

$$\nabla H^1(\Omega)^\perp = H_0(\text{div}^0, \Omega), \quad (\text{A.4})$$

$$\text{curl } H(\text{curl}, \Omega)^\perp = H_0(\text{curl}^0, \Omega), \quad (\text{A.5})$$

$$\nabla H_0^1(\Omega)^\perp = H(\text{div}^0, \Omega), \quad (\text{A.6})$$

$$\text{curl } H_0(\text{curl}, \Omega)^\perp = H(\text{curl}^0, \Omega). \quad (\text{A.7})$$

Furthermore, all these linear subspaces are L^2 closed, so that the relations are still correct by taking the orthogonal to the other side.

Proof. Eqs. (A.4) to (A.7) are given by [AFW06, Eqs. (2.15) and (2.16)] in the cases $k = 1$ and $k = 2$. The fact that all the subspaces are L^2 closed is given by the continuity of $\text{div} : H(\text{div}, \Omega) \rightarrow L^2(\Omega)$ and $\text{curl} : H(\text{curl}, \Omega) \rightarrow L^2(\Omega)^3$ on the right-hand sides of Eqs. (A.4) to (A.7), and by [AFW06, Th. 2.3.] for the left-hand side. \square

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