Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering

Variational problems on optimal geometry in physics

Variační problémy na optimální geometrii ve fyzice

Bachelor's Degree Project

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Author's declaration:
I declare that this Bachelor's Degree Project is entirely my own work and I have listed all the used sources in the bibliography.

Prague, July 4, 2017 Jan Šmejkal

Název práce:

Variační problémy na optimální geometrii ve fyzice

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Abstrakt: Tato práce si klade za cíl poskytnout vhled do metod tvarové optimalizace. Tři problémy, jeden z elektrostatiky, druhý z kvantové mechaniky a třetí z dynamiky kontinua jsou uvažovány. Představíme objem zachovávající transformaci, která může být interpretována jako kroucení a ohýbání. Užitím variačních metod je ukázáno, že pokud je koaxiální kondenzátor mírně zkroucen či ohnut, pak jeho kapacita naroste. Dále aplikujeme speciální, kroutící, případ oné transformace na válcový kvantový vlnovod a prostřednictvím spektrální teorie dokážeme, že válcový vlnovod má nižší energii základního stavu, než kterýkoliv zkroucený. Též provedeme porovnání dvou matematických modelů ustáleného viskózního proudění tekutiny v trubce od různých autorů. V jednom modelu válcová trubka optimalizuje disipaci energie, v druhém však nikoliv.

Klíčová slova: Hardyho nerovnosti, kondenzátor, kvantový vlnovod, proudění tekutin, variační počet

Title:

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Abstract: This work aims to provide insight into shape optimization methods. Three problems, one in electrostatics, second in quantum mechanics and the third in contiuum dynamics, are tackled. We introduce a volume-preserving transformation, which can be interpreted as twisting and bending. Using variational methods, it is shown that if a coaxial capacitor is slightly twisted or bent then its capacitance increases. Next, we apply a special, twisting, case of the transformation to a cylindrical quantum waveguide and prove via spectral theory that the cylindrical waveguide has a lower energy of the ground state than any twisted waveguide. We also offer a comparison of two mathematical models of steady viscous fluid motion in a pipe by different authors. In one model, the cylidrical pipe optimizes dissipated energy, in the other, however, it does not.

Key words: calculus of variations, capacitor, fluid dynamics, Hardy's inequalities, quantum waveguide

Contents

Introduction

As modern technology proceeds in its inevitable progress, driven by the use of the scientific method, the range of possibilities for practical realizations derived from one theoretical concept extends beyond the prospect of actualization of every distinct variation into the real world.

One then often faces the dilemma, as to which of the manifold options theoretically available should be invested in and produced into a tangible material form. Undoubtedly, it is the preference of optimality over mediocrity, or in the extreme, pessimality, that motivates this choice.

In this work, we tackle such problems, more specifically, we study the influence of geometrical configuration, or in simple terms – shape, on certain criteria that are regarded as fundamental to the issue at hand.

The incitement for this thesis is that we believe the overall topic to be of great significance, inasmuch as it establishes a connection between abstract principles and concrete purposes.

There are altogether three chapters (if Introduction and Conclusion are not included) and three appendices forming this work. Those are then divided into sections and the sections are further partitioned into subsections.

The first chapter will deal with a question in electrostatics. A coaxial capacitor will be considered and its shape deformed by a class of certain perturbations. With the help of the calculus of variations, we shall study what effect these perturbations have on the capacitance of the capacitor.

The second chapter will examine a quantum mechanical waveguide. We shall begin with a waveguide of cylindrical geometry and then apply a twisting transformation. The ground-state energy of the waveguide is of the interest, and we will analyze it by the means of spectral theory. In addition, the article [10] on similar, yet more general, twisting and bending of a quantum waveguide, is outlined and some Hardy's inequalities therefrom are quoted.

The third chapter will present the Navier-Stokes equations and then will proceed with an overview of two papers, [6] and [15], both of which analyze the steady motion of a viscous fluid. The former claims that the usual technical solution, a cylindrical pipe, is not the most convenient choice in terms of energy dissipation. The latter offers a counterstatement and insist on the optimality of the cylinder. We shall provide a comparison of the proposed mathematical models.

Next will be the conclusion, wherein we shall summarize our results and state some open questions raised by this thesis.

In the first appendix, our notation will be explained.

In the second appendix, we shall introduce basic elements of the calculus of variations. A simple case of the Euler-Lagrange equations will be discussed and the Dirichlet's principle will be presented. We will also propose a modified version of this principle, which is used in the first chapter.

Lastly, in the third appendix, foundations of spectral theory will be laid out for the purpose of their use in the second chapter. We shall begin with the notion of linear operators and thereto closely associated sesquilinear forms, next, Sobolev spaces are defined and some important results such as the minimax theorem are included.

Chapter 1

Shape Perturbation of an Electrostatic Capacitor

1.1 Introduction

This chapter aims to examine how the capacitance of a coaxial capacitor changes when its shape is perturbed while maintaining constant volume. Due to the complexity of the problem in general, we shall only consider a certain class of perturbating transformations that includes, but is not limited to, such that can be interpreted as twisting and bending.

In particular, we shall begin with a coaxial capacitor, introduce the shape transformation and then study the first and second variation of its capacitance under the perturbation.

1.2 Unperturbed Case

A capacitor is a device that utilizes the difference of electrostatic potential (voltage) to store electrical energy. More specifically, the potential differential is achieved by charging two disconnected conductors (called electrodes) with opposite charges (*cf.* [4, 2.5]).

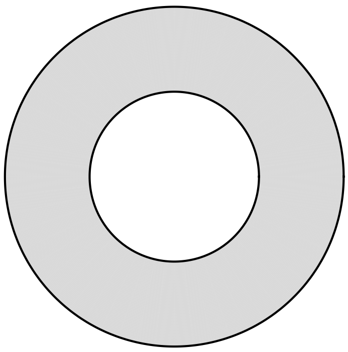
A cylindrical coaxial capacitor is a capacitor of a particular shape. It consists of two disconnected coaxial cylindrical surfaces of radii $R, r \in \mathbb{R}, R > r$. The usual mathematical model of a cylindrical capacitor is such that its length is prescribed as infinite, which in reality corresponds to the notion that it is much longer than it is wide and so the effect of the electrostatic field on the extremes can be neglected.

The transverse cross-section of a cylindrical capacitor (that is, its intersection with a plane perpendicular to axis along its length) is, of course, an annulus. For our purposes, nevertheless, the geometry of the capacitor cross-section can be generalized to a broader family of shapes. One can, in fact, consider instead of an annulus the image thereof by a continuously differentiable injective map $\Upsilon : \overline{\hat{\omega}} \to \mathbb{R}^2$, where $\hat{\omega}$ is the aforementioned (open) annulus. If we denote the new transverse cross-section $\omega := \Upsilon(\hat{\omega})$ then the new capacitor shall be defined as $\Omega_{\mathbb{R}} := \mathbb{R} \times \omega$. We also define the outer and inner electrode as $\partial_R\Omega_{\mathbb{R}} := \mathbb{R} \times \Upsilon(\partial\hat{\omega} \cap \{\mathbf{x}' \in \mathbb{R}^2 : |\mathbf{x}'| = R\})$, $\partial_r\Omega_{\mathbb{R}} := \mathbb{R} \times \Upsilon(\partial\hat{\omega} \cap \{\mathbf{x}' \in \mathbb{R}^2 : |\mathbf{x}'| = r\})$, respectively.

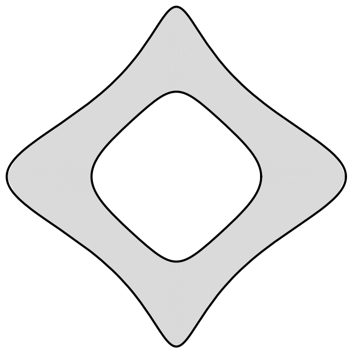
Figure 1.1 shows some possible shapes for ω, which result from the use of the following transformations: (Images are not to scale, however, aspect ratio is preserved.)

$$(1.1a) : (x_2, x_3) \mapsto (x_2, x_3)$$
$$(1.1b) : (x_2, x_3) \mapsto (x_2(1 + x_3^2)^{-1}, x_3)$$
$$(1.1c) : (x_2, x_3) \mapsto (\arctan x_2 + \pi, \arctan x_3 + \pi)$$
$$(1.1d) : (x_2, x_3) \mapsto (x_2, x_3) \mapsto (x_2 \exp x_3, x_3)$$

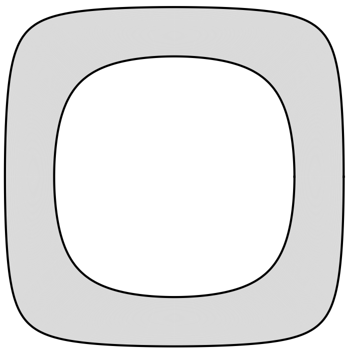
Figure 1.1: Some possible cross-sections



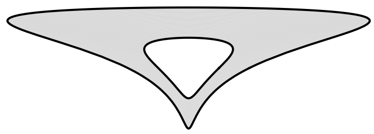
(a) An annular cross-section



(b) A “diamond-shaped” cross-section



(c) A “square-shaped” cross-section



(d) A “cusp-shaped” cross-section

In our case, we shall assume that the outer boundary $\partial_R \Omega_{\mathbb{R}}$ is earthed (which is equivalent to the idea that electrostatic potential thereon is zero) and that the inner boundary $\partial_r \Omega_{\mathbb{R}}$ is so charged that the voltage in between the boundaries is equal to one. This mathematically corresponds to the following Dirichlet boundary value problem (an analogy to the problem in [4, 2.5]):

$$\begin{cases} -\Delta\psi = 0 & \mathbf{x} \in \Omega_{\mathbb{R}}, \\ \psi = 0 & \mathbf{x} \in \partial_R \Omega_{\mathbb{R}}, \\ \psi = 1 & \mathbf{x} \in \partial_r \Omega_{\mathbb{R}}, \end{cases} \tag{1.1}$$

where ψ is the electrostatic potential and Δ is the Laplacian operator which acts upon a twice differentiable function as a sum of its second derivatives with respect to all independent variables, that is

$$\forall \psi \in C^2(\Omega_{\mathbb{R}}) : \Delta\psi = \frac{\partial^2 \psi}{\partial x_1^2} + \frac{\partial^2 \psi}{\partial x_2^2} + \frac{\partial^2 \psi}{\partial x_3^2}.$$

The classical way of defining electrostatic capacitance is such that it is the maximum amount of charge that can be placed on $\partial_r \Omega_{\mathbb{R}}$ when the voltage between the electrodes (created by this charge) is a unit (*cf.* [4, 2.5]). In other words it is charge related to unit of voltage. In our case, however, we shall first adopt a more general notion of p-capacity which is known to be equivalent to classical electrostatic capacitance in case of $p = 2$ (*cf.* [16, sec. 1 (f)]).

Definition 1.2.1 (p-capacity)**.** Let Λ be a measurable set, $\Gamma \subset \partial\Lambda$. Then the p-capacity of Γ with respect to Λ shall be defined as

$$\operatorname{cap}_p^{\Gamma}(\Lambda) := \inf \left\{ \int_{\Lambda} |\nabla\phi|^p : \phi \in C_0^{\infty}(\Lambda) \wedge \phi\big|_{\Gamma} = 1 \right\}.$$

Remark 1.2.1.1. In view of the Dirichlet principle (see Theorem B.3.3), if Λ has a boundary of class C^1 and is bounded, the minimizing function $\hat{\phi}$ satisfies

$$\begin{cases} -\Delta\hat{\phi} = 0 & \mathbf{x} \in \Lambda, \\ \hat{\phi} = 0 & \mathbf{x} \in \partial\Lambda \setminus \overline{\Gamma}, \\ \hat{\phi} = 1 & \mathbf{x} \in \overline{\Gamma}. \end{cases}$$

In particular case of ψ, however, the Dirichlet principle cannot be used as the set $\Omega_{\mathbb{R}}$ is not bounded. Even if the Dirichlet principle were to be postulated we get using Fubini's theorem

$$\operatorname{cap}(\Omega_{\mathbb{R}}) = \int_{\Omega_{\mathbb{R}}} |\nabla\psi|^2 = \int_{\mathbb{R}} \mathrm{d}x_1 \left(\int_{\omega} \mathrm{d}x_2\, \mathrm{d}x_3 |\nabla\psi|^2 \right).$$

Due to the translational symmetry of $\Omega_{\mathbb{R}}$, we can expect that ψ is independent of x_1 (this will be discussed at greater length later on). The integral, however, would then be infinite, for one has to integrate a non-zero constant over the set $\mathbb{R}$. This was to be expected, because, of course, an infinitely long capacitor can hold an infinite amout of charge.

It is for this exact reason that we shall consider only the capacity of a section of the capacitor. In case of ψ from (1.1) we would have (L is a real positive constant)

$$\operatorname{cap}_L(\Omega_{\mathbb{R}}) := \int_{\Omega_L} |\nabla\psi|^2 = \int_{\omega} \mathrm{d}x_2\, \mathrm{d}x_3 |\nabla\psi|^2.$$

Mathematically, it is also possible to consider a finite capacitor from the beginning with periodic boundary conditions imposed on the extremes. The Dirichlet boundary value problem corresponding to such situation can be written as

$$\begin{cases} -\Delta\psi = 0 & \mathbf{x} \in \Omega, \\ \psi = 0 & \mathbf{x} \in \partial_R\Omega, \\ \psi = 1 & \mathbf{x} \in \partial_r\Omega, \\ \psi(-L,\mathbf{x}') = \psi(L,\mathbf{x}') & \mathbf{x}' \in \omega, \\ \psi_{,1}(-L,\mathbf{x}') = \psi_{,1}(L,\mathbf{x}') & \mathbf{x}' \in \omega, \end{cases}$$

where

$$\begin{aligned} &\Omega := [-L,L] \times \omega, \\ &\partial_R\omega := \Upsilon(\hat{\omega} \cap \{\mathbf{x}' \in \mathbb{R}^2 : |\mathbf{x}'| = R\}), \\ &\partial_r\omega := \Upsilon(\hat{\omega} \cap \{\mathbf{x}' \in \mathbb{R}^2 : |\mathbf{x}'| = r\}), \\ &\partial_R\Omega := [-L,L] \times \partial_R\omega, \\ &\partial_r\Omega := [-L,L] \times \partial_r\omega, \end{aligned}$$

and $\psi_{,1}$ is the derivative of ψ with respect to the x_1-axis. Note that we have ommited L in the names of the sets, as we shall only consider the problem for fixed L.

If one were to redefine p-capacity so that the infimum is only taken over functions satisfying boundary conditions in the problem above, the Modified Dirichlet principle B.3.6 could be utilized to tie the capacitance (2-capacity) to ψ. This shall be done later in order to avoid repetition, as a family of capacitor shapes will be considered instead of only Ω.

Lastly, we shall state a lemma about the geometry of $\partial_R\omega$ that will be used later. Essentialy, it states the intuitive fact that $\partial_R\omega$ cannot be a subset of a line.

Lemma 1.2.1. *Let $a, b, c \in \mathbb{R}, a \neq 0 \vee b \neq 0$. Then*

$$\partial_R\omega \not\subset \left\{ \begin{pmatrix} x_2 \\ x_3 \end{pmatrix} \in \mathbb{R}^2 : ax_2 + bx_3 + c = 0 \right\}.$$

We shall omit the proof of Lemma 1.2.1, as it is a simple exercise on continuous maps and the intermediate value theorem.

1.3 Perturbating Transformation

A class of transformations that will be applied to the straight capacitor from the previous section will be now presented. We consider two maps $V_2, V_3 : [-L,L] \to \mathbb{R}$, $V_2, V_3 \in C^3([-L,L])$ with the conditions

$$V_2(-L) = V_2(L) = V_3(-L) = V_3(L) = 0 \tag{1.2}$$

and

$$\dot{V}_2 \neq 0 \wedge \dot{V}_3 \neq 0$$

(where the dot represents derivative) and define the perturbating transformation $\mathcal{P}_\varepsilon$ as

$$\forall \varepsilon \in \mathbb{R} : \forall \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \in [-L,L] \times \mathbb{R}^2 : \mathcal{P}_\varepsilon \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \varepsilon \begin{pmatrix} 0 \\ V_2(x_1) \\ V_3(x_1) \end{pmatrix}.$$

It is apparent that $\mathcal{P}_\varepsilon$ becomes the identity map for $\varepsilon = 0$. It is also an identity (for any ε) when we fix $x_1 = -L, L$. One can observe that $\mathcal{P}_\varepsilon$ is for a fixed $x_1 \in [-L, L]$ a translation in the transverse plane by the vector $\varepsilon(V_2(x_1), V_3(x_1))$.

Let $\Omega_\varepsilon = \mathcal{P}_\varepsilon(\Omega)$ be the new (perturbed) shape for the capacitor. It follows from the reasoning above that the manner in which $\mathcal{P}_\varepsilon$ acts upon the straight capacitor is that it keeps the ends of the capacitor fixed (this is needed because of the periodic boundary condition that will be imposed) and then for each $x_1 \in [-L, L]$ translates the cross section ω—while keeping it in the same plane that it resided before the translation—in a way continuous with respect to x_1.

The Jacobian matrix (*cf.* [7, def 1.7.8]) of the transformation $\mathcal{P}_\varepsilon$ at $\mathbf{x} = (x_1, x_2, x_3) \in [-L, L] \times \mathbb{R}^2$ can be easily computed to be

$$J_\varepsilon(\mathbf{x}) := J^{\mathcal{P}_\varepsilon}(\mathbf{x}) = \left(\frac{\partial(\mathcal{P}_\varepsilon)_i}{\partial x_j}\Big|_{\mathbf{x}} \right)_{i,j=1}^{3} = \begin{pmatrix} 1 & 0 & 0 \\ \varepsilon \dot{V}_2(x_1) & 1 & 0 \\ \varepsilon \dot{V}_3(x_1) & 0 & 1 \end{pmatrix}.$$

By J_ε we shall denote the map $J_\varepsilon : [-L, L] \times \mathbb{R}^2 \to \mathbb{R}^{3,3} : \mathbf{x} \mapsto J_\varepsilon(\mathbf{x})$. As a shorthand we shall also write J_ε^T instead of $(J_\varepsilon)^T$.

As $J_\varepsilon(\mathbf{x})$ is a triangular matrix, its determinant can be acquired by simply taking the product of its diagonal elements to get

$$\forall \mathbf{x} \in [-L, L] \times \mathbb{R}^2 : \det J_\varepsilon(\mathbf{x}) = 1.$$

This means $\mathcal{P}_\varepsilon$ is a volume-preserving transformation, more specifically, for any measurable set $M \subset [-L, L] \times \mathbb{R}^2$ one can write

$$\int_M 1 \, \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 = \int_{\mathcal{P}_\varepsilon(M)} 1 \, \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3$$

as a consequence of the integral substitution theorem.

The Jacobian matrix of the inverse transformation can be easily obtained after a trivial observation that $\mathcal{P}_\varepsilon$ can be inverted simply by changing the sign of ε, in other words $(\mathcal{P}_\varepsilon)^{-1} = \mathcal{P}_{-\varepsilon}$. We can thus write

$$J^{(\mathcal{P}_\varepsilon)^{-1}}(\mathbf{x}) = J^{\mathcal{P}_{-\varepsilon}}(\mathbf{x}) = J_{-\varepsilon}(\mathbf{x}).$$

Because the Jacobian matrix is dependent only on the first coordinate x_1, and the first component of $\mathcal{P}_\varepsilon$ is an identity, we can write

$$J_{-\varepsilon}(\mathbf{x}) = J_{-\varepsilon}(\mathcal{P}_\varepsilon(\mathbf{x})). \tag{1.3}$$

Later in this chapter, we shall adopt the same geometric approach as in [10] and treat the problem in curvilinear coordinates. In [10, 2.4], a metric tensor is defined and its use proves later convenient. It will soon become apparent, that the metric tensor can be a useful tool even in our case. The metric tensor of $\mathcal{P}_\varepsilon$ is defined as

$$g_\varepsilon(\mathbf{x}) := g^{\mathcal{P}_\varepsilon}(\mathbf{x}) = J_\varepsilon^T(\mathbf{x}) J_\varepsilon(\mathbf{x}),$$

Using the identity (1.3), the definition of the metric tensor and the inverse map theorem (*cf.* [7, thm 2.9.4]) we can derive a formula for the inverse metric tensor

$$g_\varepsilon^{-1}(\mathbf{x}) = J_{-\varepsilon}(\mathbf{x}) J_{-\varepsilon}^T(\mathbf{x}), \tag{1.4}$$

thusly

$$g_\varepsilon^{-1}(\mathbf{x}) := (g_\varepsilon(\mathbf{x}))^{-1} = (J_\varepsilon^T(\mathbf{x}) J_\varepsilon(\mathbf{x}))^{-1} = (J_\varepsilon(\mathbf{x}))^{-1} (J_\varepsilon^T(\mathbf{x}))^{-1} = J_{-\varepsilon}(\mathcal{P}_\varepsilon(\mathbf{x})) J_{-\varepsilon}^T(\mathcal{P}_\varepsilon(\mathbf{x})) = J_{-\varepsilon}(\mathbf{x}) J_{-\varepsilon}^T(\mathbf{x}).$$

(The fact that matrix transposition and inversion commute was employed)

After performing the matrix multiplication we get the explicit matrices

$$g_\varepsilon(\mathbf{x}) = \begin{pmatrix} \varepsilon^2\dot{V}_2(x_1)^2 + \varepsilon^2\dot{V}_3(x_1)^2 + 1 & \varepsilon\dot{V}_2(x_1) & \varepsilon\dot{V}_3(x_1) \\ \varepsilon\dot{V}_2(x_1) & 1 & 0 \\ \varepsilon\dot{V}_3(x_1) & 0 & 1 \end{pmatrix},$$

$$g_\varepsilon^{-1}(\mathbf{x}) = \begin{pmatrix} 1 & -\varepsilon\dot{V}_2(x_1) & -\varepsilon\dot{V}_3(x_1) \\ -\varepsilon\dot{V}_2(x_1) & \varepsilon^2\dot{V}_2(x_1)^2 + 1 & \varepsilon^2\dot{V}_2(x_1)\dot{V}_3(x_1) \\ -\varepsilon\dot{V}_3(x_1) & \varepsilon^2\dot{V}_2(x_1)\dot{V}_3(x_1) & \varepsilon^2\dot{V}_3(x_1)^2 + 1 \end{pmatrix}.$$

By g_ε^{-1} the map $g_\varepsilon^{-1} : [-L, L] \times \mathbb{R}^2 \to \mathbb{R}^{3,3} : \mathbf{x} \mapsto g_\varepsilon^{-1}(\mathbf{x})$ will be meant.

Lastly, we shall proceed to derive two formulas using the derivative of a composite function theorem. These formulas will prove convenient in future.

Proposition 1.3.1. *Let $\tilde{M} \subset [-L, L] \times \mathbb{R}^2$, $\tilde{\phi} \in W^{1,2}(\tilde{M})$. Denote $\phi := \tilde{\phi} \circ \mathcal{P}_\varepsilon \in W^{1,2}(M)$, where $M := (\mathcal{P}_\varepsilon)^{-1}(\tilde{M})$. We can write*

$$||\nabla\tilde{\phi}||^2 = ||J_{-\varepsilon}^T \nabla\phi||^2,$$

where the norms on the left and right are those of the $L^2(\tilde{M})$ and $L^2(M)$ spaces, respectively, and the gradients are to be understood in a weak sense (see Appendix C for details).

Proof. Firstly we can write (recall $(\mathcal{P}_\varepsilon)^{-1} = \mathcal{P}_{-\varepsilon}$)

$$||\nabla\tilde{\phi}||^2 = \int_{\tilde{M}} |\nabla\tilde{\phi}|^2 = \int_{\tilde{M}} |\nabla(\phi \circ \mathcal{P}_{-\varepsilon})|^2.$$

Now the derivative of a composite function theorem (chain rule) will be used on the integrand.

Note that we can rewrite the chain rule (for $\tilde{\mathbf{x}} \in \tilde{M}$, $\mathbf{x} := \mathcal{P}_{-\varepsilon}(\tilde{\mathbf{x}}) \in M$)

$$\forall i \in \{1, 2, 3\} : \frac{\partial\tilde{\phi}}{\partial x_i}\Big|_{\tilde{\mathbf{x}}} = \sum_{j=1}^{3} \frac{\partial(\mathcal{P}_{-\varepsilon})_j}{\partial x_i}\Big|_{\tilde{\mathbf{x}}} \frac{\partial\phi}{\partial x_j}\Big|_{\mathbf{x}}$$

into a more compact and convenient tensor form, thusly

$$(\nabla\tilde{\phi})\Big|_{\tilde{\mathbf{x}}} = (\nabla\mathcal{P}_{-\varepsilon})\Big|_{\tilde{\mathbf{x}}}(\nabla\phi)\Big|_{\mathbf{x}} = (J_{-\varepsilon}^T)\Big|_{\tilde{\mathbf{x}}}(\nabla\phi)\Big|_{\mathbf{x}} = (J_{-\varepsilon}^T)\Big|_{\mathbf{x}}(\nabla\phi)\Big|_{\mathbf{x}},$$

where definition of Jacobian matrix and (1.3) were used in the second-to-last and last equality, respectively. This justifies the following use of the integral substitution theorem (we remind that $\det J_{-\varepsilon} = 1$)

$$||\nabla\tilde{\phi}||^2 = \int_{\tilde{M}} \left(|J_{-\varepsilon}^T \nabla\phi|^2\right)\Big|_{\mathcal{P}_{-\varepsilon}(\tilde{\mathbf{x}})} \mathrm{d}\tilde{\mathbf{x}} = \int_M |J_{-\varepsilon}^T \nabla\phi|^2.$$

To finish the proof apply the definition of the $L^2(M)$ norm. □

Corollary 1.3.1.1. *With the same assumptions as in the proposition above, we can write*

$$||\nabla\tilde{\phi}||^2 = \langle\nabla\phi\,|\,g_\varepsilon^{-1}\,|\,\nabla\phi\rangle,$$

where $\langle\nabla\phi\,|\,g_\varepsilon^{-1}\,|\,\nabla\phi\rangle := \langle\nabla\phi\,|\,g_\varepsilon^{-1}\nabla\phi\rangle$ (see Section A.4).

Proof. One need only use the definitions of $|\cdot|^2$ and $||\cdot||^2$ and (1.4) to arrive at the statement, thusly

$$||\nabla\tilde{\phi}||^2 = \int_M |J_{-\varepsilon}^T \nabla\psi_\varepsilon|^2 = \int_\Omega (\nabla\overline{\phi})^T J_{-\varepsilon} J_{-\varepsilon}^T \nabla\phi = \int_\Omega (\nabla\overline{\phi})^T g_\varepsilon^{-1} \nabla\phi.$$

□

Proposition 1.3.2. *Let $\tilde{M} \subset [-L, L] \times \mathbb{R}^2$, $\tilde{\phi} \in C^2(\tilde{M})$.*
Denote $\phi := \tilde{\phi} \circ \mathcal{P}_\varepsilon \in C^2(M)$, where $M := (\mathcal{P}_\varepsilon)^{-1}(\tilde{M})$. We can write

$$\forall \tilde{\mathbf{x}} \in \tilde{M}, \mathbf{x} := (\mathcal{P}_\varepsilon)^{-1}(\tilde{\mathbf{x}}) : \left(\Delta\tilde{\phi}\right)\Big|_{\tilde{\mathbf{x}}} = \left((\nabla \cdot J_{-\varepsilon}^T)\nabla\phi + g_\varepsilon^{-1} \odot (\nabla(\nabla\phi))\right)\Big|_{\mathbf{x}},$$

where $\odot$ signifies the matrix element-wise product, that is,

$$\forall A, B \in \mathbb{R}^{3,3} : A \odot B := (A_{ij}B_{ij})_{i,j=1}^3 \in \mathbb{R}^{3,3}.$$

Proof. Let $\tilde{\mathbf{x}} \in \tilde{M}, \mathbf{x} := (\mathcal{P}_\varepsilon)^{-1}(\tilde{\mathbf{x}})$. By rewriting the the matrix and vector multiplications (only formally for ∇), we see one has to prove

$$\left(\sum_{i=1}^3 \frac{\partial^2\tilde{\phi}}{\partial x_i^2}\right)\Big|_{\tilde{\mathbf{x}}} = \left(\sum_{i,j=1}^3 \frac{\partial A_{ji}}{\partial x_i}\frac{\partial\phi}{\partial x_j} + \sum_{i,j,k=1}^3 A_{ki}A_{ji}\frac{\partial^2\phi}{\partial x_k\,\partial x_j}\right)\Big|_{\mathbf{x}},$$

where $\forall i, j \in \{1, 2, 3\} : A_{ij} := (J_{-\varepsilon})_{ij}$.

Since we have $A_{ij}(\mathbf{x}) = A_{ij}(\tilde{\mathbf{x}})$ and because the derivative of a composite function theorem was used in extensive detail in the proof of the previous proposition, we shall omit writing $\mathbf{x}$ and $\tilde{\mathbf{x}}$ thereon and instead refer to the variables of $\tilde{\phi}$ as $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3$.

Rest assured we can write without ambiguity

$$\forall i, m, n \in \{1, 2, 3\} : \frac{\partial\tilde{\phi}}{\partial\tilde{x}_i} = \sum_{j=1}^3 A_{ji}\frac{\partial\phi}{\partial x_j}, \quad \frac{\partial A_{mn}}{\partial\tilde{x}_i} = \frac{\partial A_{mn}}{\partial x_i}.$$

We begin on the left side and apply the derivative of a composite function theorem twice, as following

$$\Delta\tilde{\phi} = \sum_{i=1}^3 \frac{\partial}{\partial\tilde{x}_i}\frac{\partial\tilde{\phi}}{\partial\tilde{x}_i} = \sum_{i=1}^3 \frac{\partial}{\partial\tilde{x}_i}\left(A_{ji}\frac{\partial\phi}{\partial x_j}\right) = \sum_{i,j=1}^3 \left(\frac{\partial A_{ji}}{\partial x_i}\frac{\partial\phi}{\partial x_j} + A_{ji}\frac{\partial}{\partial\tilde{x}_i}\frac{\partial\phi}{\partial x_j}\right).$$

To finish the proof one only need write ($i, j \in \{1, 2, 3\}$)

$$\frac{\partial}{\partial\tilde{x}_i}\frac{\partial\phi}{\partial x_j} = \sum_{k=1}^3 A_{ki}\frac{\partial}{\partial x_k}\frac{\partial\phi}{\partial x_j}.$$

□

1.4 Perturbed Capacitor

Let us now consider the capacitor of perturbed shape $\Omega_\varepsilon = \mathcal{P}_\varepsilon(\Omega)$ and denote $\tilde{\psi}_\varepsilon \in W^{2,2}(\Omega_\varepsilon)$ its electrostatic potential. As in the case of the straight capacitor we shall assume the outer electrode to be earthed and the voltage between the electrodes to be a unit.

Figure 1.2 shows two concrete examples of capacitors perturbed by $\mathcal{P}_\varepsilon$. The outer electrode is cropped and transparent so that the inner electrode is visible. We remark that here the terms *bent* and

Figure 1.2: Examples of perturbed capacitors

(a) A bent capacitor with a "diamond-shaped" cross-section

(b) A twisted and slightly bent capacitor with an annular cross-section

twisted are used in an intuitive and loose fashion. For a mathematically rigorous treatment of these terms, consult [10, def 2.2, 2.3] and note that our vague notion of "bending" differs therefrom (1.2a and 1.2b could not be considered bent in terms of [10]).

For 1.2a we have chosen

$$(V_2, V_3) : x \mapsto (0, x^2 - L^2)$$

and in the case of 1.2b we have

$$(V_2, V_3) : x \mapsto (\cos(3\pi L^{-1}x) + 1, \sin(3\pi L^{-1}x) + \frac{1}{2}(x^2 - L^2))$$

.

For the same reasons as before, we impose periodic boundary conditions on the extremes of the capacitor. The Dirichlet boundary value problem for the electrostatic potential $\tilde{\psi}_\varepsilon$ can now be written as

$$\begin{cases} -\Delta\tilde{\psi}_\varepsilon = 0 & \mathbf{x} \in \Omega_\varepsilon, \\ \tilde{\psi}_\varepsilon \in \mathsf{BC}^1_\varepsilon, \end{cases} \tag{1.5}$$

where

$$\forall C \in \mathbb{R} : \mathsf{BC}^C_\varepsilon := \left\{ \phi \in W^{2,2}(\Omega_\varepsilon) : \begin{array}{ll} \phi = 0 & \mathbf{x} \in \partial_R\Omega_\varepsilon, \\ \phi = C & \mathbf{x} \in \partial_r\Omega_\varepsilon, \\ \phi(-L, \mathbf{x}') = \phi(L, \mathbf{x}') & \mathbf{x}' \in \omega, \\ \phi_{,1}(-L, \mathbf{x}') = \phi_{,1}(L, \mathbf{x}') & \mathbf{x}' \in \omega. \end{array} \right\},$$

$$\partial_R\Omega_\varepsilon := \mathcal{P}_\varepsilon(\partial_R\Omega), \quad \partial_r\Omega_\varepsilon := \mathcal{P}_\varepsilon(\partial_r\Omega).$$

A possible approach to a construction of a solution to (1.5) is that in first step one finds a function $\tilde{\eta}_\varepsilon \in \mathsf{BC}^1_\varepsilon$, that need not necessarily solve (1.5). The second step then involves solving a different system than (1.5), more precisely, a Poisson equation wherein the right side is $\Delta\tilde{\eta}_\varepsilon$ and the boundary condition is $\tilde{\varphi}_\varepsilon \in \mathsf{BC}^0_\varepsilon$. Mathematically this means finding a solution $\tilde{\varphi}_\varepsilon$ to

$$\begin{cases} -\Delta\tilde{\varphi}_\varepsilon = \Delta\tilde{\eta}_\varepsilon & \mathbf{x} \in \Omega_\varepsilon, \\ \tilde{\varphi}_\varepsilon \in \mathsf{BC}^0_\varepsilon, \end{cases} \tag{1.6}$$

which might in practice pose a simpler problem. The solution to (1.5) is then obtained as $\tilde{\psi}_\varepsilon = \tilde{\varphi}_\varepsilon + \tilde{\eta}_\varepsilon$, as can be checked by plugging back to (1.5).

We shall not prove existence and uniqueness of a solution to (1.6) as a full proof would extend beyond the scope of this thesis. A simple sketch of a proof that refers to generally known existence and uniqueness for a elliptic Dirichlet boundary condition problem on a bounded set (*cf.* [3]) is as follows.

It is possible to consider a continuously differentiable transformation of Ω_ε into a "hollow torus". If the transformation is constructed such that it "glues" the ends of the capacitor to each other (without rotating them), and is injective otherwise, then the periodic boundary conditions transform into a simple requirement for continuous differentiability on the "glued" cross-section. Since the Dirichlet conditions will not change, the existence and uniqueness then follow, as the "hollow torus" is a bounded set.

Generally, only a weak solution is guaranteed to exist. If the "glueing" transformation and the functions V_1 and V_2 were smooth as well as the boundaries $\partial_r\Omega_\varepsilon$ and $\partial_R\Omega_\varepsilon$, an existence of a smooth solution is shown in [3, thm. 6.3.6].

It should also be noted that it is not possible to simply choose $\tilde{\varphi}_\varepsilon = \tilde{\eta}_\varepsilon$ in order to solve (1.6), as each one of the functions is required to satisfy a different condition on the boundary $\partial_r\Omega_\varepsilon$.

We shall write the weak formulation of (1.6). For that one need multiply the first equation in (1.6) by an arbitrary test function $\overline{\phi} \in \mathsf{D}(\tilde{h}_\varepsilon)$ and integrate over the domain (which is equivalent to taking the L^2 scalar product of ϕ and $-\Delta\tilde{\varphi}_\varepsilon$). By integration by parts and the Gauss theorem one has

$$-\int_{\Omega_\varepsilon} \overline{\phi}\, \Delta\tilde{\varphi}_\varepsilon = \int_{\Omega_\varepsilon} \nabla\overline{\phi}\, \nabla\tilde{\varphi}_\varepsilon - \underbrace{\left(\int_{\omega(L)} \overline{\phi}\, \varphi_{\varepsilon,n} + \int_{\omega(-L)} \overline{\phi}\, \varphi_{\varepsilon,n}\right)}_{=0} - \underbrace{\int_{\partial_R\Omega_\varepsilon} \overline{\phi}\, \varphi_{\varepsilon,n}}_{=0} - \underbrace{\int_{\partial_r\Omega_\varepsilon} \overline{\phi}\, \varphi_{\varepsilon,n}}_{=0} = \langle \nabla\phi \,|\, \nabla\tilde{\varphi}_\varepsilon \rangle$$

where $\omega(l) = \Omega_\varepsilon \cap \{x_1 = l\}$ is the transverse cross-section for $l = -L, L$ and the underbraced terms vanish as a consequence of the boundary conditions imposed on ϕ and $\varphi_{\varepsilon,n}$.

If we now define a quadratic form $\tilde{h}_\varepsilon : \mathsf{D}(\tilde{h}_\varepsilon) \to \mathbb{C}$ such that

$$\begin{cases} \mathsf{D}(\tilde{h}_\varepsilon) = \widehat{\mathsf{BC}^0_\varepsilon}, \\ \forall\phi \in \mathsf{D}(\tilde{h}_\varepsilon) : \tilde{h}_\varepsilon[\phi] = \|\nabla\phi\|^2, \end{cases}$$

where $\widehat{\mathsf{BC}^0_\varepsilon}$ is same as $\mathsf{BC}^0_\varepsilon$ except that the last boundary condition is ommited, then the weak formulation of (1.6) reads as

$$\begin{cases} \forall\phi \in \mathsf{D}(\tilde{h}_\varepsilon) : \tilde{h}_\varepsilon(\phi, \tilde{\varphi}_\varepsilon) = 0 \\ \tilde{\varphi}_\varepsilon \in \mathsf{BC}^0_\varepsilon \end{cases} \tag{1.7}$$

The reason we have ommited the last boundary condition from $\mathsf{BC}^0_\varepsilon$ is that normal derivative is known to vanish upon taking a closure of a quadratic form (*cf.* [2, thm. 7.2.1]). Hence, we can expect $\tilde{h}_\varepsilon$ to be closed.

Before the capacitance of the perturbed capacitor is examined, two convenient propositions shall be proven. Firstly it will be shown that for the case $\varepsilon = 0$ the function $\tilde{\psi}_0$ is not dependent on x_1. Secondly, we shall demonstrate that the set BC^0_0 is orthogonal to $\tilde{\psi}_0$ in a certain sense.

Proposition 1.4.1. *The solution of (1.5) for $\varepsilon = 0$ is not dependent on x_1, that is*

$$\tilde{\psi}_{0,1} = 0.$$

Proof. Given the uniqueness of a solution for (1.5) we need only find a function that satisfies the system and is also independent of x_1. Indeed such a function can be found simply by considering a problem on the transverse cross-section ω

$$\begin{cases} \Delta\xi = 0 & \mathbf{x}' \in \omega, \\ \xi = 0 & \mathbf{x}' \in \partial_R\omega, \\ \xi = 1 & \mathbf{x}' \in \partial_r\omega. \end{cases}$$

Then the extension $\tilde{\xi}$ of ξ on the whole capacitor defined by

$$\forall (x_1, \mathbf{x}') \in [-L, L] \times \mathbb{R}^2 : \tilde{\xi}(x_1, \mathbf{x}') = \xi(\mathbf{x}')$$

is a solution to (1.5) for $\varepsilon = 0$ as can be checked by plugging into the system. □

Proposition 1.4.2. *Let $\phi \in \mathsf{BC}_0^0$. Then we have*

$$\langle \nabla\phi \,|\, \nabla\tilde{\psi}_0 \rangle = 0.$$

Proof. Let $\phi \in \mathsf{BC}_0^0$. By setting $\varepsilon = 0$ in (1.5), multiplying the resulting equation by $\overline{\phi}$ and integrating by parts one has

$$0 = -\int_\Omega \overline{\phi}\Delta\tilde{\psi}_0 = \int_{\Omega_\varepsilon} \nabla\overline{\phi}\,\nabla\tilde{\psi}_0 = \langle \nabla\phi \,|\, \nabla\tilde{\psi}_{0,n} \rangle.$$

(The boundary terms vanish as a consequence of the boundary conditions.) □

1.5 Curvilinear Coordinates

We will rewrite the problem (1.5) into a form wherein the domain of the solution will not be dependent on ε. This is done so that one can take the derivative of the problem with respect to ε without much effort. The easiest way is to introduce a new function $\psi_\varepsilon : \Omega \to \mathbb{R}$ such that $\psi_\varepsilon = \tilde{\psi}_\varepsilon \circ \mathcal{P}_\varepsilon$. By utilizing Proposition 1.3.2 we can, after careful matrix multiplication, write

$$\begin{aligned} \forall \tilde{\mathbf{x}} \in \Omega_\varepsilon : (\Delta\tilde{\psi}_\varepsilon)(\tilde{\mathbf{x}}) = (-\varepsilon(\ddot{V}_2\psi_{\varepsilon,2} + \ddot{V}_3\psi_{\varepsilon,3}) + \Delta\psi_\varepsilon - 2\varepsilon(\dot{V}_2\psi_{\varepsilon,12} + \dot{V}_3\psi_{\varepsilon,13}) \\ + \varepsilon^2(\dot{V}_2^2\psi_{\varepsilon,22} + \dot{V}_3^2\psi_{\varepsilon,33} + 2\dot{V}_2\dot{V}_3\psi_{\varepsilon,23}))(\mathcal{P}_{-\varepsilon}(\tilde{\mathbf{x}})). \end{aligned}$$

This can be rewritten as

$$\forall \mathbf{x} \in \Omega : (\Delta\tilde{\psi}_\varepsilon)(\mathcal{P}_\varepsilon(\mathbf{x})) = (((\partial_1 - \varepsilon\dot{V}_2\partial_2 - \varepsilon\dot{V}_3\partial_3)^2 + \partial_2^2 + \partial_3^2)\psi_\varepsilon)(\mathbf{x}).$$

The Dirichlet conditions are easy to transform, because we can write

$$\Big(\forall \tilde{\mathbf{x}} \in \partial_R\Omega_\varepsilon : \tilde{\psi}_\varepsilon(\tilde{\mathbf{x}}) = 0\Big) \Leftrightarrow \Big(\forall \tilde{\mathbf{x}} \in \partial_R\Omega_\varepsilon : \psi_\varepsilon((\mathcal{P}_\varepsilon)^{-1}(\tilde{\mathbf{x}})) = 0\Big) \Leftrightarrow \Big(\forall \mathbf{x} \in \partial_R\Omega : \psi_\varepsilon(\mathbf{x}) = 0\Big),$$

since $(\mathcal{P}_\varepsilon)^{-1}(\partial_r\Omega_\varepsilon) = \partial_r\Omega$. One can show similarly the transformation of the Dirichlet condition on $\partial_r\Omega$ and the periodic boundary condition for $\tilde{\psi}_\varepsilon$.

The periodic boundary condition for the normal derivative of $\tilde{\psi}_\varepsilon$, however, has to be rewritten using the derivative of a composite function theorem. Since we have already applied the theorem in previous sections, and shown its explicit use in detail, we only show the result, that is

$$\Big(\forall \mathbf{x}' \in \omega : \tilde{\psi}_{\varepsilon,n}(-L, \mathbf{x}') = -\tilde{\psi}_{\varepsilon,n}(L, \mathbf{x}')\Big) \Leftrightarrow \Big(\forall \mathbf{x}' \in \omega : \psi_{\varepsilon,\tilde{n}(\varepsilon)}(-L, \mathbf{x}') = -\psi_{\varepsilon,\tilde{n}(\varepsilon)}(L, \mathbf{x}')\Big),$$

where

$$\forall \phi \in C^1(\Omega) : \phi_{,\tilde{n}(\varepsilon)} := \phi_{,1} - \varepsilon\dot{V}_2\phi_{,2} - \varepsilon\dot{V}_3\phi_{,3}$$

If we now define a differential operator $H_\varepsilon : W^{2,2}(\Omega) \to L^2(\Omega)$ as

$$\forall \phi \in W^{2,2}(\Omega) : H_\varepsilon \phi = -((\partial_1 - \varepsilon \dot{V}_2 \partial_2 - \varepsilon \dot{V}_3 \partial_3)^2 + \partial_2^2 + \partial_3^2)\phi,$$

it is then apparent that one can transfer the problem (1.5) to the new form

$$\begin{cases} H_\varepsilon \psi_\varepsilon = 0 & \mathbf{x} \in \Omega, \\ \psi_\varepsilon = 0 & \mathbf{x} \in \partial_R \Omega, \\ \psi_\varepsilon = 1 & \mathbf{x} \in \partial_r \Omega, \\ \psi_\varepsilon(-L, \mathbf{x}') = \psi_\varepsilon(L, \mathbf{x}') & \mathbf{x}' \in \omega, \\ \psi_{\varepsilon, \tilde{n}(\varepsilon)}(-L, \mathbf{x}') = -\psi_{\varepsilon, \tilde{n}(\varepsilon)}(L, \mathbf{x}') & \mathbf{x}' \in \omega. \end{cases} \tag{1.8}$$

1.6 Capacitance under Perturbation

We shall now prove the main result of this chapter, that is, that a small deformation of the straight capacitor by the transformation $\mathcal{P}_\varepsilon$ results in an increase of the electrostatic capacity. Firstly we define the modified 2-capacity for the perturbed capacitor as

Definition 1.6.1 (Modified 2-capacity for the perturbed capacitor)**.**

$$\forall \varepsilon \in \mathbb{R} : \gamma(\varepsilon) := \inf \left\{ \int_{\Omega_\varepsilon} |\nabla \phi|^2 : \phi \in \mathsf{BC}_\varepsilon^1 \right\}. \tag{1.9}$$

As per the Modified Dirichlet principle B.3.6 we are allowed to write

$$\forall \varepsilon \in \mathbb{R} : \gamma(\varepsilon) = \int_{\Omega_\varepsilon} |\nabla \tilde{\psi}_\varepsilon|^2,$$

where $\tilde{\psi}_\varepsilon$ is the solution to (1.5)

Finally, we can inspect the first and second derivative of γ. The outcome of the inspection is summarized by the following theorem:

Theorem 1.6.2.

$$\gamma_0' := \frac{\mathrm{d}\gamma}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0} = 0, \quad \gamma_0'' := \frac{\mathrm{d}^2\gamma}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon=0} > 0.$$

Proof. Let $\varepsilon \in \mathbb{R}$. To prove the statement we first rewrite the integral in (1.9) so that the integration domain is no longer dependent on ε. For this purpose, we can use Corollary 1.3.1.1

$$\gamma(\varepsilon) = \int_{\Omega_\varepsilon} |\nabla \tilde{\psi}_\varepsilon|^2 = \|\nabla \tilde{\psi}_\varepsilon\|^2 = \langle \nabla \psi_\varepsilon \,|\, g_\varepsilon^{-1} \,|\, \nabla \psi_\varepsilon \rangle.$$

Secondly, we shall express g_ε^{-1} in powers of ε:

$$g_\varepsilon^{-1} = \mathbb{I} + \varepsilon(v^T + v) + \varepsilon^2 \, v^T v,$$

where

$$\mathbb{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad v = \begin{pmatrix} 0 & -\dot{V}_2 & -\dot{V}_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

For further purposes we also introduce the notation

$$\forall \phi \in W^{2,2}(\Omega) : \phi_{,v} := v\nabla\phi = -\dot{V}_2\phi_{,2} - \dot{V}_3\phi_{,3}.$$

It can be observed that

$$\forall \phi,\psi \in W^{2,2}(\Omega) : \langle \nabla\phi \,|\, v^T + v \,|\, \nabla\psi\rangle = \langle \phi_{,v} \,|\, \psi_{,1}\rangle + \langle \phi_{,1} \,|\, \psi_{,v}\rangle \wedge \langle \nabla\phi \,|\, v^T v \,|\, \nabla\psi\rangle = \langle \phi_{,v} \,|\, \psi_{,v}\rangle.$$

Thirdly, to continue the proof, we have to assume that $\tilde{\psi}_\varepsilon$ is analytic in ε at some neighbourhood of zero. Reasons as to why this claim should hold are stated in the remark below. If $\tilde{\psi}_\varepsilon$ were analytic, then ψ_ε would be as well, as $\mathcal{P}_\varepsilon$ is clearly analytic. This means one can use the Taylor's theorem on ψ_ε to obtain

$$\exists \varepsilon_0 \in \mathbb{R}, \varepsilon_0 > 0 : \forall \varepsilon \in (-\varepsilon_0, \varepsilon_0) : \exists \psi_0', \psi_0'' : \Omega \to \mathbb{R} : \psi_\varepsilon = \psi_0 + \varepsilon\psi_0' + \frac{\varepsilon^2}{2}\psi_0'' + O(\varepsilon^3). \tag{1.10}$$

By taking the derivative of the boundary value problem (1.8) with respect to ε at $\varepsilon = 0$ (H_ε is a polynomial in ε) we get

$$\begin{cases} -\Delta\psi_0' = -H_0'\psi_0 & \mathbf{x} \in \Omega, \\ \psi_0' = 0 & \mathbf{x} \in \partial_R\Omega, \\ \psi_0' = 0 & \mathbf{x} \in \partial_r\Omega, \\ \psi_0'(-L, \mathbf{x}') = \psi_0'(L, \mathbf{x}') & \mathbf{x}' \in \omega, \\ \psi_{0,n}'(-L, \mathbf{x}') = -\psi_{0,n}'(L, \mathbf{x}') & \mathbf{x}' \in \omega, \end{cases} \tag{1.11}$$

(we remind that the derivative with respect to $\tilde{n}$ is same as with respect to n for $\varepsilon = 0$) where $H_0' : W^{2,2}(\Omega) \to L^2(\Omega) : \phi \mapsto (\partial_1(\phi_{,v}) + \dot{V}_2\phi_{,21} + \dot{V}_3\phi_{,31})$, in particular

$$H_0'\psi_0 = \ddot{V}_2\psi_{0,2} + \ddot{V}_2\psi_{0,2}. \tag{1.12}$$

We can see that $\psi_0' \in \mathsf{BC}_0^0$. We can take the second derivative of (1.8) with respect to ε at $\varepsilon = 0$ and observe that $\psi_0'' \in \mathsf{BC}_0^0$. Thus, by proposition 1.4.2 we have

$$\langle \psi_0' \,|\, \psi_0\rangle = 0, \quad \langle \psi_0'' \,|\, \psi_0\rangle = 0.$$

because $\psi_0 = \tilde{\psi}_0$. The last equality also allows us to write

$$\psi_{0,1} = 0.$$

Bearing these identities in mind, continue by writing $\gamma(\varepsilon)$ in powers of ε (symmetry of the scalar product and realness of ψ_ε is also used)

$$\begin{aligned} \gamma(\varepsilon) = \langle \nabla\psi_\varepsilon \,|\, g_\varepsilon^{-1} \,|\, \nabla\psi_\varepsilon\rangle &= \langle \nabla(\psi_0 + \varepsilon\psi_0' + \tfrac{\varepsilon^2}{2}\psi_0'') \,|\, \mathbb{I} + \varepsilon(v^T + v) + \varepsilon^2 v^T v \,|\, \nabla(\psi_0 + \varepsilon\psi_0' + \tfrac{\varepsilon^2}{2}\psi_0'')\rangle + O(\varepsilon^3) \\ &= \|\psi_0\|^2 + \varepsilon\Big(\langle \nabla\psi_0 \,|\, v^T + v \,|\, \nabla\psi_0\rangle + 2\langle \nabla\psi_0' \,|\, \nabla\psi_0\rangle\Big) \\ &\quad + \varepsilon^2\Big(\langle \nabla\psi_0 \,|\, v^T v \,|\, \nabla\psi_0\rangle + \langle \nabla\psi_0'' \,|\, \nabla\psi_0\rangle + 2\langle \nabla\psi_0 \,|\, v^T + v \,|\, \nabla\psi_0'\rangle + \|\nabla\psi_0'\|^2\Big) + O(\varepsilon^3). \end{aligned}$$

This means that the first derivative of γ at $\varepsilon = 0$ is

$$\frac{1}{2}\frac{\mathrm{d}\gamma}{\mathrm{d}\varepsilon}\Big|_0 = \underbrace{\langle \psi_{0,1} \,|\, \psi_{0,v}\rangle}_{=0} + \underbrace{\langle \nabla\psi_0' \,|\, \nabla\psi_0\rangle}_{=0} = 0.$$

For the second derivative at $\varepsilon = 0$ we can write

$$\frac{1}{2}\frac{\mathrm{d}^2\gamma}{\mathrm{d}\varepsilon^2}\Big|_0 = \|\psi_{0,v}\|^2 + \underbrace{\langle\nabla\psi_0' \,|\, \nabla\psi_0\rangle}_{=0} + 2\langle\psi_{0,v} \,|\, \psi_{0,1}'\rangle + 2\underbrace{\langle\psi_{0,1} \,|\, \psi_{0,v}'\rangle}_{=0} + \|\nabla\psi_0'\|^2 =$$

$$\|\psi_{0,v}\|^2 + 2\langle\psi_{0,v} \,|\, \psi_{0,1}'\rangle + \|\psi_{0,1}'\|^2 + \|\nabla'\psi\|^2 = \|\psi_{0,v} + \psi_{0,1}'\|^2 + \|\nabla'\psi_0'\|^2 \geq 0,$$

where $\|\nabla'\psi_0'\|^2 := \|\psi_{0,2}'\|^2 + \|\psi_{0,3}'\|^2$. It remains to prove the strictness of the inequality. Following lemma guarantees that fact. □

Lemma 1.6.2.1. *Let ψ_0' be defined as in the proof above. Then*

$$\|\psi_{0,2}'\|^2 + \|\psi_{0,3}'\|^2 > 0 \vee \|\psi_{0,v} + \psi_{0,1}'\|^2 > 0$$

Proof. From the proof above (equation (1.11) and (1.12)) we know that

$$\Delta\psi_0' = \ddot{V}_2\psi_{0,2} + \ddot{V}_2\psi_{0,2}.$$

By taking the derivative of the above equation with respect to x_1, x_2, x_3, respectively, we get ($V_2^{(3)}$ and $V_3^{(3)}$ are the third derivatives of V_2 and V_3, respectively)

$$\Delta\psi_{0,1}' = V_2^{(3)}\psi_{0,2} + V_3^{(3)}\psi_{0,2},$$

$$\Delta\psi_{0,2}' = \ddot{V}_2\psi_{0,22} + \ddot{V}_3\psi_{0,32}, \tag{1.13}$$

$$\Delta\psi_{0,3}' = \ddot{V}_2\psi_{0,23} + \ddot{V}_3\psi_{0,33}. \tag{1.14}$$

(i) It is possible that $\ddot{V}_2 = \ddot{V}_3 = 0$. In such case, uniqueness of ψ_0' dictates that $\psi_0' = 0$ (recall $\psi_0' \in \mathsf{BC}_0^0$) and we have to show $\psi_{0,v} \neq 0$. Suppose (for future contradiction)

$$\psi_{0,v} = 0.$$

Now take the derivative of that equation with respect to x_2 and x_3, respectively. Those two equations along with the equation for ψ_0 yield a linear system for unknowns $\psi_{0,22}, \psi_{0,23}, \psi_{0,33}$:

$$\begin{pmatrix} 1 & 0 & 1 \\ \dot{V}_2 & \dot{V}_3 & 0 \\ 0 & \dot{V}_2 & \dot{V}_3 \end{pmatrix}\begin{pmatrix} \psi_{0,22} \\ \psi_{0,23} \\ \psi_{0,33} \end{pmatrix} = 0.$$

Its determinant is $\dot{V}_2^2 + \dot{V}_3^2$. We have

$$\exists x \in [-L, L] : \dot{V}_2^2(x) + \dot{V}_3^2(x) > 0.$$

That implies

$$\exists x \in [-L, L] : \forall \mathbf{x}' \in \omega : \psi_{0,22}(x, \mathbf{x}') = \psi_{0,23}(x, \mathbf{x}') = \psi_{0,33}(x, \mathbf{x}') = 0.$$

But ψ_0 is independent of its first argument, hence $\psi_{0,22} = \psi_{0,23} = \psi_{0,33} = 0$

(ii) We shall now step back and assume that either $\ddot{V}_2$ or $\ddot{V}_3$ is non-zero. In order for both $\psi_{0,2}'$ and $\psi_{0,3}'$ to be zero, right sides of equations (1.13) and (1.14) must be identically zero.

Assume (again, for future contradiction) that $\psi_{0,2}' = \psi_{0,3}' = 0$. This, along with the equation for ψ_0 yields

$$\begin{pmatrix} 1 & 0 & 1 \\ \ddot{V}_2 & \ddot{V}_3 & 0 \\ 0 & \ddot{V}_2 & \ddot{V}_3 \end{pmatrix}\begin{pmatrix} \psi_{0,22} \\ \psi_{0,23} \\ \psi_{0,33} \end{pmatrix} = 0$$

But the determinant of such system is $\ddot{V}_2^2 + \ddot{V}_3^2$ and thus we get by the same argument as before, that

$$\psi_{0,22} = \psi_{0,23} = \psi_{0,33} = 0.$$

In both cases (i) and (ii) we have made an assumption and arrived at a system of differential equations for the function ψ_0:

$$\psi_{0,22} = 0, \quad \psi_{0,23} = 0, \quad \psi_{0,33} = 0.$$

By directly integrating the first equation, then substituting the obtained solution into the second and third equation we get that (after solving for some uknown functions of x_3)

$$\exists a, b, c \in \mathbb{R} : \forall x_1, x_2, x_3 \in \Omega : \psi_0(x_1, x_2, x_3) = ax_2 + bx_3 + c$$

Given the boundary conditions on ψ_0, we know that either a or b must be non-zero, as ψ_0 cannot be a constant function. The set of all points where ψ_0 is 0 is therefore for a fixed $x_1 \in [-L, L]$ subset of

$$B := \left\{ \begin{pmatrix} x_2 \\ x_3 \end{pmatrix} \in \mathbb{R}^2 : ax_2 + bx_3 + c = 0 \right\}$$

By the boundary condition imposed on $\partial_R \Omega$ (at any fixed $x_1 \in [-L, L]$) we have the following

$$\partial_R \omega \subset B.$$

This is a contradiction with Lemma 1.2.1. □

Corollary 1.6.2.1. *We can write*

$$\exists \varepsilon_0 \in \mathbb{R}, \varepsilon_0 > 0 : \forall \varepsilon \in (-\varepsilon_0, \varepsilon_0), \varepsilon \neq 0 : \gamma(\varepsilon) > \gamma(0)$$

Proof. We can use the analycity (recall ψ_ε is analytical in ε) of γ to write (we have $\gamma_0' = 0$).

$$\exists \delta \in \mathbb{R}, \delta > 0 : \forall \varepsilon \in (-\delta, \delta) : \gamma(\varepsilon) = \gamma(0) + \frac{\varepsilon^2}{2}\gamma_0'' + \varepsilon^2 \alpha(\varepsilon), \ \lim_{\varepsilon \to 0} \alpha(\varepsilon) = 0$$

Limit of α at zero is zero, so we can write (γ_0'' is positive)

$$\exists \tilde{\delta} \in \mathbb{R}, \tilde{\delta} > 0 : \forall \varepsilon \in (-\tilde{\delta}, \tilde{\delta}) : |\alpha(\varepsilon)| < \frac{1}{2}\gamma_0''.$$

Finally, we set $\varepsilon_0 := \min\{\delta, \tilde{\delta}\}$ and obtain

$$\exists \varepsilon_0 \in \mathbb{R}, \varepsilon_0 > 0 : \forall \varepsilon \in (-\varepsilon_0, \varepsilon_0), \varepsilon \neq 0 : \gamma(\varepsilon) - \gamma(0) = \varepsilon^2 \underbrace{\left(\frac{1}{2}\gamma_0'' + \alpha(\varepsilon)\right)}_{>0} > 0,$$

which proves the corollary. □

Remark 1.6.2.1. To prove the theorem, analycity of $\tilde{\psi}_\varepsilon$ in ε is needed in order to use the Taylor expansion. This, however, is a mathematical claim that shall not be shown to hold in complete detail.

Instead, we refer mainly to [9] and only outline the reasoning behind the claim.

[9, sec. VII 4.2] defines a *Holomorphic family of sesquilinear forms* as a family of forms dependent on some parameter (in our case) ε in a holomorphic way. Such forms are also required to be closed and share the same domain.

Thus in our case, the family of forms $\tilde{h}_\varepsilon$ would not suffice, as the domains of functions that they admit are Ω_ε. A workaround to this inconvenience is to define a unitary operator $U_\varepsilon : \mathbf{L}^2(\Omega_\varepsilon, \mathrm{d}\mathbf{x}) \to \mathbf{L}^2(\Omega, \mathrm{d}\mathbf{x})$:

$$\forall \phi \in \mathbf{L}^2(\Omega_\varepsilon, \mathrm{d}\mathbf{x}) : U_\varepsilon \phi = \phi \circ \mathcal{P}_\varepsilon$$

and then a quadratic form $h_\varepsilon : \mathsf{D}(h_\varepsilon) := U_\varepsilon(\mathsf{D}(\tilde{h}_\varepsilon)) \to \mathbb{C}$ such that

$$\forall \phi \in \mathsf{D}(h_\varepsilon) : h_\varepsilon[\phi] = \|\nabla (U_\varepsilon)^{-1} \phi\|^2.$$

Because it can be shown that h_ε is for fixed arguments $\psi, \phi \in \mathsf{D}(h_\varepsilon)$ a polynomial in ε, such family of forms would by definition be a Holomorphic family of forms. Therefore, as Kato shows (if one adds several steps to his reasoning), the family of solutions to (1.5) should be analytic in ε.

Chapter 2

Twisting of a Quantum Waveguide

2.1 Introduction

The purpose of this chapter is to investigate the behavior of a twisted quantum waveguide. In particular, we start with a cylindrical one and transform it in a helical manner into a shape not dissimilar to that of a screw.

The main concern of analysis is the energy corresponding to the first eigenstate, more precisely, its first and second variation under the twisting transformation from a cylinder.

It should also be noted that the notation in this chapter greatly resembles that of the previous one. We emphasize that although same symbols are used as previously, in regard to certain analogy, they by no means refer to ones in the previous chapter. If the previous chapter is referred to, it is always explicitly stated so.

2.2 Unperturbed Case

Let $\Omega = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_1 \in (-L, L) \wedge x_2^2 + x_3^2 < R^2\}$ denote a cylinder in $\mathbb{R}^3$ for L, $R \in \mathbb{R}$, $R > 0$. Let us also define the inlet, outlet and lateral surface of the cylinder $E = \overline{\Omega} \cap \{x_1 = -L\}$, $S = \overline{\Omega} \cap \{x_1 = L\}$, $\Gamma = \partial\Omega \setminus (E \cup S)$, respectively. A quantum particle confined to Ω for R relatively small in comparison to L and with Dirichlet condition imposed on Γ and Neumann condition on E and S can be interpreted as a model of a quantum waveguide. Stationary states of such particle are described by wave function $\psi : \Omega \to \mathbb{C}$ given by the time-independent Schrödinger equation:

$$\begin{cases} -\Delta\psi = \lambda\psi & \mathbf{x} \in \Omega, \\ \psi = 0 & \mathbf{x} \in \Gamma, \\ \dfrac{\partial\psi}{\partial n} = 0 & \mathbf{x} \in E \cup S, \end{cases} \tag{2.1}$$

where n represents the outer normal. Note that since both E and S lie on planes perpendicular to the x_1-axis, the last boundary condition in (2.1) simplifies to

$$\frac{\partial\psi}{\partial x_1} = 0 \quad \mathbf{x} \in E \cup S$$

By transforming to cylindrical coordinates and utilizing the method of separation of variables, the lowest energy state of (2.1) can be found to be

$$\psi_0(x_1, x_2, x_3) = CJ_0(\frac{j_{0,1}}{R}\sqrt{x_2^2 + x_3^2}),\ \lambda_0 = \frac{j_{0,1}^2}{R^2},$$

where $C \in \mathbb{C}$, J_0 is the zero-th Bessel function of the first kind, $j_{0,1}$ is the first zero thereof and λ_0 is the corresponding eigenvalue. Note that the solution is independend of x_1.

Let us define the set of all admissible functions:

$$\mathsf{BC}_0 := \{\phi \in W^{2,2}(\Omega) : \phi\restriction_\Gamma = 0 \wedge \phi_{,1}\restriction_{E\cup S} = 0\}.$$

If $\phi \in \mathsf{BC}_0$ then we say that ϕ satistfies the Dirichlet boundary condition on Γ and the Neumann boundary condition on $E \cup S$.

By multiplying (2.1) by the complex conjugate of an arbitrary test function $\phi \in \mathsf{BC}_0$ and integrating over the domain, (2.1) can be rewritten into its weak form

$$\begin{cases} \forall\phi \in \mathsf{BC}_0 : \langle\nabla\phi\,|\,\nabla\psi\rangle = -\langle\phi\,|\,\Delta\psi\rangle = \lambda\langle\phi\,|\,\psi\rangle, \\ \psi \in \mathsf{BC}_0 \quad \wedge \quad \|\psi\|^2 = 1, \end{cases} \tag{2.2}$$

(The first equality in (2.2) follows from integration by parts and a normalization condition has been added to the system)

2.3 Twisting Transformation

At this point we define the twisting transformation $\tilde{\mathcal{T}}_\varepsilon : [-L, L] \times \mathbb{R}^2 \to [-L, L] \times \mathbb{R}^2$ as

$$\tilde{\mathcal{T}}_\varepsilon = \mathcal{R}_\theta \circ \mathcal{L}_\varepsilon,$$

where

$$\forall \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \in [-L, L] \times \mathbb{R}^2 : \mathcal{R}_\theta \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta(x_1) & \sin\theta(x_1) \\ 0 & -\sin\theta(x_1) & \cos\theta(x_1) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

is for each $x_1 \in [-L, L]$ a rotation with respect to the x_1-axis by the angle $\theta(x_1)$ for an arbitrary $\theta \in C^1([-L, L])$, $\frac{d\theta}{dx_1} := \dot{\theta} \neq 0$ and

$$\forall \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \in [-L, L] \times \mathbb{R}^2 : \mathcal{L}_\varepsilon \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 + \varepsilon \\ x_3 \end{pmatrix}$$

is a translation on the x_2-axis by ε. A more convenient twisting transformation would be such that it becomes identity for $\varepsilon = 0$. For this purpose we introduce $\mathcal{T}_\varepsilon : [-L, L] \times \mathbb{R}^2 \to \mathbb{R}^3$ by adding a technical untwisting:

$$\mathcal{T}_\varepsilon = \tilde{\mathcal{T}}_\varepsilon \circ \mathcal{R}_{-\theta} = \mathcal{R}_\theta \circ \mathcal{L}_\varepsilon \circ \mathcal{R}_{-\theta}.$$

Before explicit formulas are shown, we introduce a more compact notation

$$\cos\theta(x_1) := \mathrm{c}_\theta, \quad \sin\theta(x_1) := \mathrm{s}_\theta.$$

We shall also sometimes write θ instead of $\theta(x_1)$ and the same will be done with the derivative $\dot{\theta}$. The untwisting $\mathcal{R}_{-\theta}$ also simplifies the form of transformation which is

$$\mathcal{T}_\varepsilon \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} x \\ \mathrm{c}_\theta(\mathrm{c}_\theta x_2 - \mathrm{s}_\theta x_3 + \varepsilon) + \mathrm{s}_\theta(\mathrm{c}_\theta x_3 + \mathrm{s}_\theta x_2) \\ \mathrm{c}_\theta(\mathrm{c}_\theta x_3 + \mathrm{s}_\theta x_2) - \mathrm{s}_\theta(\mathrm{c}_\theta x_2 - \mathrm{s}_\theta x_3 + \varepsilon) \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 + \varepsilon \mathrm{c}_\theta \\ x_3 - \varepsilon \mathrm{s}_\theta \end{pmatrix}.$$

We can see that the transformation $\mathcal{T}_\varepsilon$ is, in fact, almost a special case of the transformation $\mathcal{P}_\varepsilon$ presented in the previous chapter concerning the perturbation of a shape of a coaxial capacitor. The only difference is that condition (1.2) does not apply. In this case, however, the fact that we have

$$\forall \mathbf{x}' \in \mathbb{R}^2 : \mathcal{T}_\varepsilon(-L, \mathbf{x}') = \mathcal{T}_\varepsilon(L, \mathbf{x})$$

will suffice.

Using the previous chapter, we can immediately write the Jacobian matrix of the transformation $\mathcal{T}_\varepsilon$ at $\mathbf{x} := (x_1, x_2, x_3) \in \mathbb{R}^3$

$$J_\varepsilon(\mathbf{x}) := J^{\mathcal{T}_\varepsilon}(\mathbf{x}) = \begin{pmatrix} 1 & 0 & 0 \\ -\varepsilon\dot{\theta}\mathrm{s}_\theta & 1 & 0 \\ -\varepsilon\dot{\theta}\mathrm{c}_\theta & 0 & 1 \end{pmatrix}. \tag{2.3}$$

Again, as in the previous chapter, by J_ε we shall denote the map $J_\varepsilon : [-L, L] \times \mathbb{R}^2 \to \mathbb{R}^{3,3} : \mathbf{x} \mapsto J_\varepsilon(\mathbf{x})$. As a shorthand we shall also write J_ε^T instead of $(J_\varepsilon)^T$. We also know from the previous chapter that

$$(\mathcal{T}_\varepsilon)^{-1} = \mathcal{T}_{-\varepsilon},$$

$$\forall \mathbf{x} \in [-L, L] \times \mathbb{R}^2 : J_\varepsilon(\mathbf{x}) = J_\varepsilon(\mathcal{P}_\varepsilon(\mathbf{x})), \tag{2.4}$$

$$\forall \mathbf{x} \in [-L, L] \times \mathbb{R}^2 : \det J_\varepsilon(\mathbf{x}) = 1,$$

$$\forall \mathbf{x} \in [-L, L] \times \mathbb{R}^2 : (J_\varepsilon(\mathbf{x}))^{-1} = J_{-\varepsilon}(\mathbf{x}).$$

2.4 Curvilinear Coordinates

Let $\Omega_\varepsilon = \mathcal{T}_\varepsilon(\Omega)$ be the new shape for the waveguide. A quantum particle confined in such space will be described by a wavefunction $\tilde{\psi}_\varepsilon : \Omega_\varepsilon \to \mathbb{C}$ that is a solution to a problem analogous to (2.2), in particular,

$$\begin{cases} \forall \phi \in \mathsf{D}(\tilde{h}_\varepsilon) : \tilde{h}_\varepsilon(\phi, \tilde{\psi}_\varepsilon) = \lambda_\varepsilon \langle \phi \,|\, \tilde{\psi}_\varepsilon \rangle, \\ \tilde{\psi}_\varepsilon \in \widetilde{\mathsf{BC}}_\varepsilon \quad \wedge \quad \|\tilde{\psi}_\varepsilon\|^2 = 1, \end{cases} \tag{2.5}$$

where

$$\widetilde{\mathsf{BC}}_\varepsilon := \{\phi \in W^{2,2}(\Omega_\varepsilon) : \phi \restriction_{\Gamma_\varepsilon} = 0 \wedge \phi_{,1} \restriction_{E_\varepsilon \cup S_\varepsilon} = 0\},$$

and $\tilde{h}_\varepsilon$ is the closure of the sesquilinear form corresponding to a negative laplacian operator that operates on $\widetilde{\mathsf{BC}}_\varepsilon$, more precisely

$$\begin{cases} \mathsf{D}(\tilde{h}_\varepsilon) = \{\phi \in W^{1,2}(\Omega_\varepsilon) : \phi \restriction_{\Gamma_\varepsilon} = 0\}, \\ \forall \phi \in \mathsf{D}(\tilde{h}_\varepsilon) : \tilde{h}_\varepsilon[\phi] = \|\nabla \phi\|^2, \end{cases}$$

and $\Gamma_\varepsilon = \mathcal{T}_\varepsilon(\Gamma)$, $S_\varepsilon = \mathcal{T}_\varepsilon(S)$ and $E_\varepsilon = \mathcal{T}_\varepsilon(E)$ are the images of the corresponding sets by $\mathcal{T}_\varepsilon$.

Figure 2.1: Examples of twisted waveguides

(a) A somewhat slightly twisted waveguide

(b) A very twisted waveguide

Note that since we are only interested in the properties of the first eigenfunction, that is, the one corresponding to the lowest eigenvalue, we can write (in accordance with the minimax theorem)

$$\lambda_\varepsilon = \inf_{\substack{\phi \in \mathsf{D}(\tilde{h}_\varepsilon) \\ \phi \neq 0}} \frac{\|\nabla \phi\|^2}{\|\phi\|^2} \tag{2.6}$$

so λ_ε is now a well defined map $\mathbb{R} \to \mathbb{R} : \varepsilon \mapsto \lambda_\varepsilon$.

In Figure 2.1, we show two twisted waveguides, 2.1a being less twisted than 2.1b (in terms of the transformation factor ε), with the choice $\theta : x \mapsto 6\pi L^{-1} x$.

We will, for convenience, reformulate the problem (2.5) into such form that the integration domain is no longer dependent on ε. This can be achieved by integral substitution, more precisely, by introduction of an operator $U_\varepsilon : \mathbf{L}^2(\Omega_\varepsilon, \mathrm{d}\mathbf{x}) \to \mathbf{L}^2(\Omega, \mathrm{d}\mathbf{x})$ defined as

$$\forall \phi \in \mathbf{L}^2(\Omega_\varepsilon, \mathrm{d}\mathbf{x}) : U_\varepsilon \phi = \phi \circ \mathcal{T}_\varepsilon.$$

U_ε is clearly a bijection, since one can easily check that the inverse operator $(U_\varepsilon)^{-1}$ can be defined as

$$\forall \phi \in \mathbf{L}^2(\Omega, \mathrm{d}\mathbf{x}) : (U_\varepsilon)^{-1} \phi = \phi \circ (\mathcal{T}_\varepsilon)^{-1}.$$

It can be trivially observed that

$$\mathsf{D}(\tilde{h}_\varepsilon) \subset \mathsf{D}(U_\varepsilon) \wedge U_\varepsilon(\mathsf{D}(\tilde{h}_\varepsilon)) \subset \mathsf{D}((U_\varepsilon)^{-1}).$$

This justifies the definition of the quadratic form $h_\varepsilon : \mathsf{D}(h_\varepsilon) := U_\varepsilon(\mathsf{D}(\tilde{h}_\varepsilon)) \to \mathbb{C}$ such that

$$\forall \phi \in \mathsf{D}(h_\varepsilon) : h_\varepsilon[\phi] = \|\nabla (U_\varepsilon)^{-1} \phi\|^2.$$

We can observe that the quadratic form h_ε is symmetric, as per the alternative definition of a symmetric form C.2.4, since its diagonal is real.

We shall also define

$$\mathsf{BC}_\varepsilon := U_\varepsilon(\widetilde{\mathsf{BC}_\varepsilon})$$

The definition of h_ε admits the following:

Theorem 2.4.1. *(i) The boundary condition problem (2.5) together with the condition (2.6) has a unique positive solution.*

(ii) *Moreover, if we denote the aforementioned solution $\tilde{\psi}_\varepsilon$, then the function $\psi_\varepsilon := U_\varepsilon\tilde{\psi}_\varepsilon$ is the unique positive solution of the problem*

$$\begin{cases} \forall\phi \in \mathsf{D}(h_\varepsilon) : h_\varepsilon(\phi, \psi_\varepsilon) = \lambda_\varepsilon\langle\phi\,|\,\psi_\varepsilon\rangle, \\ \psi_\varepsilon \in \mathsf{BC}_\varepsilon \quad\wedge\quad \|\psi_\varepsilon\|^2 = 1 \quad\wedge\quad \lambda_\varepsilon = \inf\limits_{\substack{\phi\in\mathsf{D}(h_\varepsilon)\\ \phi\neq 0}} \dfrac{h_\varepsilon[\phi]}{\|\phi\|^2}, \end{cases} \tag{2.7}$$

also conversely, if ψ_ε denotes the solution of (2.7) then $(U_\varepsilon)^{-1}\psi_\varepsilon$ is a solution of (2.5) with the condition (2.6).

(iii) *Furthermore, one can write*

$$\mathsf{BC}_\varepsilon = \{\phi \in W^{2,2}(\Omega) : \phi\restriction_\Gamma = 0 \wedge (\phi_{,1} + \varepsilon\dot{\theta}\phi_{,\tau})\restriction_{E\cup S} = 0\},$$

$$\mathsf{D}(h_\varepsilon) = \{\phi \in W^{2,2}(\Omega) : \phi\restriction_\Gamma = 0\},$$

$$\forall\phi \in \mathsf{D}(h_\varepsilon) : h_\varepsilon[\phi] = \|\phi_{,1} + \varepsilon\dot{\theta}\phi_{,\tau}\|^2 + \|\nabla'\phi\|^2,$$

where

$$\nabla'\phi := \begin{pmatrix}\phi_{,2}\\ \phi_{,3}\end{pmatrix}, \quad \phi_{,\tau} := \mathrm{s}_\theta\phi_{,2} + \mathrm{c}_\theta\phi_{,3}.$$

Proof. (i) follows from Theorem C.5.1.

To prove (ii) we shall first show that U_ε is unitary. This will be a simple consequence of the integral substitution theorem. Let $\tilde{\psi}, \tilde{\varphi} \in \mathbf{L}^2(\Omega_\varepsilon, \mathrm{d}\mathbf{x})$. Then

$$\langle U_\varepsilon\tilde{\varphi}\,|\,U_\varepsilon\tilde{\psi}\rangle = \int_\Omega \overline{U_\varepsilon\tilde{\varphi}}\,U_\varepsilon\tilde{\psi} = \int_\Omega \overline{\tilde{\varphi}\circ\mathcal{T}_\varepsilon}\,\tilde{\psi}\circ\mathcal{T}_\varepsilon = \int_{\mathcal{T}_\varepsilon^{-1}(\Omega)} \overline{\tilde{\varphi}(\mathbf{x})}\,\tilde{\psi}(\mathbf{x})\det J^{(\mathcal{T}_\varepsilon)^{-1}}(\mathbf{x})\mathrm{d}\mathbf{x} = \int_{\Omega_\varepsilon} \overline{\tilde{\varphi}}\,\tilde{\psi} = \langle\tilde{\varphi}\,|\,\tilde{\psi}\rangle$$

Let $\tilde{\psi}_\varepsilon$ be the unique positive solution from (i), $\psi_\varepsilon := U_\varepsilon\tilde{\psi}_\varepsilon$ and let $\phi \in \mathsf{D}(h_\varepsilon)$, $\phi = U_\varepsilon\tilde{\phi}$, $\tilde{\phi} \in \mathsf{D}(\tilde{h}_\varepsilon)$. We can now write

$$\begin{aligned} h_\varepsilon(\phi, \psi_\varepsilon) &= \langle\nabla(U_\varepsilon)^{-1}\phi\,|\,\nabla(U_\varepsilon)^{-1}\psi_\varepsilon\rangle = \langle\nabla(U_\varepsilon)^{-1}U_\varepsilon\tilde{\phi}\,|\,\nabla(U_\varepsilon)^{-1}U_\varepsilon\tilde{\psi}_\varepsilon\rangle \\ &= \langle\nabla\tilde{\phi}\,|\,\nabla\tilde{\psi}_\varepsilon\rangle = \lambda_\varepsilon\langle\tilde{\phi}\,|\,\tilde{\psi}_\varepsilon\rangle = \lambda_\varepsilon\langle U_\varepsilon\tilde{\phi}\,|\,U_\varepsilon\tilde{\psi}_\varepsilon\rangle = \lambda_\varepsilon\langle\phi\,|\,\psi_\varepsilon\rangle \end{aligned}$$

So it only remains to show that the infimum condition is satisfied to prove the first part of (ii). In fact, it will again follow directly from the definition of h_ε and unitarity of U_ε, one need only substitute $\tilde{\phi} \in \mathsf{D}(\tilde{h}_\varepsilon)$ for $\phi := U_\varepsilon\tilde{\phi} \in \mathsf{D}(h_\varepsilon)$:

$$\lambda_\varepsilon = \inf_{\substack{\tilde{\phi}\in\mathsf{D}(\tilde{h}_\varepsilon)\\ \tilde{\phi}\neq 0}} \frac{\|\nabla\tilde{\phi}\|^2}{\|\tilde{\phi}\|^2} = \inf_{\substack{U_\varepsilon\tilde{\phi}\in\mathsf{D}(h_\varepsilon)\\ U_\varepsilon\tilde{\phi}\neq 0}} \frac{\|\nabla(U_\varepsilon)^{-1}U_\varepsilon\tilde{\phi}\|^2}{\|U_\varepsilon\tilde{\phi}\|^2} = \inf_{\substack{\phi\in\mathsf{D}(h_\varepsilon)\\ \phi\neq 0}} \frac{h_\varepsilon[\phi]}{\|\phi\|^2}$$

Proof of the converse statement is analogous, we start with solution from $\mathsf{D}(h_\varepsilon)$, define its counterpart belonging to $\mathsf{D}(\tilde{h}_\varepsilon)$, take arbitrary function from $\mathsf{D}(\tilde{h}_\varepsilon)$, again define the counterpart (this time from $\mathsf{D}(h_\varepsilon)$) and proceed in fashion almost same as before, only in reverse.

Statement (iii) can be proven using using the chain rule for derivatives and by performing trivial algebraic manipulation. And so let $\phi \in \mathsf{D}(h_\varepsilon)$, $\phi = U_\varepsilon\tilde{\phi}$, $\tilde{\phi} \in \mathsf{D}(\tilde{h}_\varepsilon)$. The implication

$$\tilde{\phi}\restriction_{\Gamma_\varepsilon} = 0 \Rightarrow \phi\restriction_\Gamma = 0$$

is intuitive, but we shall prove it nonetheless by a series of equivalences (it actually applies both ways as could be expected).

$$\tilde{\phi}\restriction_{\Gamma_\varepsilon}=0 \Leftrightarrow \left(\forall \tilde{\mathbf{x}} \overset{a.e.}{\in} \Gamma_\varepsilon : 0 = \tilde{\phi}(\tilde{\mathbf{x}}) = \phi((\mathcal{T}_\varepsilon)^{-1}(\tilde{\mathbf{x}}))\right)$$
$$\Leftrightarrow \left(\forall (\mathcal{T}_\varepsilon)^{-1}(\tilde{\mathbf{x}}) \overset{a.e.}{\in} (\mathcal{T}_\varepsilon)^{-1}(\Gamma_\varepsilon) = \Gamma : 0 = \phi((\mathcal{T}_\varepsilon)^{-1}(\tilde{\mathbf{x}}))\right) \Leftrightarrow \left(\forall \mathbf{x} \overset{a.e.}{\in} \Gamma : \phi(\mathbf{x}) = 0\right) \Leftrightarrow \phi\restriction_\Gamma = 0.$$

Now suppose $\phi \in \mathsf{BC}_\varepsilon$, hence $\tilde{\phi} \in \widetilde{\mathsf{BC}_\varepsilon}$, and let $\tilde{\mathbf{x}} \in \Omega_\varepsilon$, and $\mathbf{x} := (\mathcal{T}_\varepsilon)^{-1}(\tilde{\mathbf{x}})$. If we make use of the previously derived identity $(\mathcal{T}_\varepsilon)^{-1} = \mathcal{T}_{-\varepsilon}$, the derivative $\tilde{\phi}_{,1}$ at $\mathbf{x}$ can be written as (in accordance with the chain rule)

$$\frac{\partial\tilde{\phi}}{\partial x_1}\Big|_{\tilde{\mathbf{x}}} = \frac{\partial(\phi\circ\mathcal{T}_{-\varepsilon})}{\partial x_1}\Big|_{\tilde{\mathbf{x}}} = \sum_{\mu=1}^{3}\frac{\partial(\mathcal{T}_{-\varepsilon})_\mu}{\partial x_1}\Big|_{\tilde{\mathbf{x}}}\frac{\partial\phi}{\partial x_\mu}\Big|_{\mathbf{x}}.$$

Now using the definition of $\mathcal{T}_\varepsilon$ we get the following:

$$\frac{\partial\tilde{\phi}}{\partial x_1}\Big|_{\tilde{\mathbf{x}}} = \frac{\partial\phi}{\partial x_1}\Big|_{\mathbf{x}} + \varepsilon\dot{\theta}\mathrm{s}_\theta\frac{\partial\phi}{\partial x_2}\Big|_{\mathbf{x}} + \varepsilon\dot{\theta}\mathrm{c}_\theta\frac{\partial\phi}{\partial x_3}\Big|_{\mathbf{x}} := \phi_{,1}(\mathbf{x}) + \varepsilon\dot{\theta}\phi_{,\tau}(\mathbf{x}),$$

which can be used to write

$$\tilde{\phi}_{,1}\restriction_{E_\varepsilon\cup S_\varepsilon}=0 \Leftrightarrow \left(\forall\tilde{\mathbf{x}} \overset{a.e.}{\in} E_\varepsilon\cup S_\varepsilon : 0 = \tilde{\phi}_{,1}(\tilde{\mathbf{x}}) = \phi_{,1}(\mathbf{x}) + \varepsilon\dot{\theta}\phi_{,\tau}(\mathbf{x})\right) \Leftrightarrow (\phi_{,1}+\varepsilon\dot{\theta}\phi_{,\tau})\restriction_{E\cup S}=0,$$

where some steps were skipped over as they are completely analogous to the ones used to show the transform of the Dirichlet condition above.

Lastly, the stated form of h_ε has to be shown. Let $\phi \in \mathsf{D}(h_\varepsilon)$, $\tilde{\phi} := \phi\circ\mathcal{T}_{-\varepsilon}$, then, by Proposition 1.3.1 from the previous chapter we get

$$h_\varepsilon[\phi] = \|\nabla(U_\varepsilon)^{-1}\phi\|^2 = \|\nabla(\phi\circ\mathcal{T}_{-\varepsilon})\|^2 = \|J_{-\varepsilon}^T\nabla\phi\|^2.$$

To get the final structure of $h_\varepsilon[\phi]$ one only need use the explicit form of the Jacobian matrix (2.3). □

Remark 2.4.1.1. We shall now only consider positive ψ_ε. The uniqueness of a positive solution to (2.7) then gives us a well defined map $\psi_\varepsilon : \mathbb{R} \to \mathsf{D}(h_\varepsilon) : \varepsilon \mapsto \psi_\varepsilon$.

Remark 2.4.1.2. The sesquilinear form associated to h_ε can be written as

$$\forall\phi,\psi\in\mathsf{D}(h_\varepsilon) : h_\varepsilon(\phi,\psi) = \langle\phi_{,1}+\varepsilon\dot{\theta}\phi_{,\tau}\,|\,\psi_{,1}+\varepsilon\dot{\theta}\psi_{,\tau}\rangle + \langle\nabla^{|}\phi\,|\,\nabla^{|}\psi\rangle,$$

due to the polarization identity.

2.5 The Principal Eigenvalue

2.5.1 Upper Bound

In this subsection we shall present a simple proof that shows that the graph of the function λ_ε lies under that of a parabola, with there being a single point at which they intersect - zero on the ε-axis.

Theorem 2.5.1.

$$\exists C\in\mathbb{R}, C>0 : \forall\varepsilon\in\mathbb{R}, \varepsilon\neq 0 : \lambda_\varepsilon < \lambda_0 + C\varepsilon^2.$$

Proof. Let $\varepsilon \in \mathbb{R}, \varepsilon \neq 0$. We begin by reformulating $h_\varepsilon[\psi_0]$ (recall $\psi_{0,1} = 0$):

$$h_\varepsilon[\psi_0] = \|\psi_{0,1} + \varepsilon\dot{\theta}\psi_{0,\tau}\|^2 + \|\nabla'\psi_0\|^2 = \|\varepsilon\dot{\theta}\psi_{0,\tau}\|^2 + \|\psi_{0,1}\|^2 + \|\nabla'\psi_0\|^2$$
$$= \|\varepsilon\dot{\theta}\psi_{0,\tau}\|^2 + \|\nabla\psi_0\|^2 = \|\varepsilon\dot{\theta}\psi_{0,\tau}\|^2 + \lambda_0\|\psi_0\|^2.$$

Now we use the minimax definition of λ_ε as applied to ψ_0 to obtain

$$\lambda_\varepsilon \leq \frac{h_\varepsilon[\psi_0]}{\|\psi_0\|^2} = \lambda_0 + \frac{\|\dot{\theta}\psi_{0,\tau}\|^2}{\|\psi_0\|^2}\varepsilon^2 < \lambda_0 + \left(\frac{\|\dot{\theta}\psi_{0,\tau}\|^2}{\|\psi_0\|^2} + 1\right)\varepsilon^2.$$

To finish the proof one only need set C to be the bracketed expression.

□

2.5.2 Lower Bound

Here we present the main result of this chapter. It will be shown that the first eigenvalue λ_ε of a twisted waveguide is always higher than that of an untwisted waveguide. Since the operator considered is, in fact, a Hamiltonian, the first eigenvalue corresponds to the energy of the ground state.

This theorem and its proof is an adaptation of [10, lemma 6.1].

Theorem 2.5.2 (Waveguide Lower Bound Theorem)**.**

$$\forall\varepsilon \in \mathbb{R}, \varepsilon \neq 0 : \lambda_\varepsilon > \lambda_0.$$

We shall first prove a weaker proposition that states only a non-strict inequality. This proposition will be preceeded by a lemma, a problem on the transverse cross-section of the waveguide.

Lemma 2.5.2.1. *Let ω be a closed disc of radius R in $\mathbb{R}^2$. Denote $\lambda_1^D(\omega)$ the principal eigenvalue of the operator $-\Delta_\omega^D$, defined by*

$$\begin{cases} -\Delta_\omega^D \overset{1:1}{\longleftrightarrow} h_\omega^D, \\ \mathsf{D}(h_\omega^D) = W_0^{1,2}(\omega), \\ \forall\phi \in \mathsf{D}(h_\omega^D) : h_\omega^D[\phi] = \|\nabla\phi\|^2. \end{cases}$$

Then $-\Delta_\omega^D$ has a principle eigenvalue which we denote $\lambda_1^D(\omega)$ and we can write

$$\lambda_0 = \lambda_1^D(\omega).$$

Proof. Firstly, consider the following problem:

$$\begin{cases} \forall\phi \in \mathsf{D}(h_\omega^D) : h_\omega^D(\phi, \phi_1) = \lambda_1^D(\omega)\langle\phi\,|\,\phi_1\rangle, \\ \phi_1 \in \mathsf{D}(h_\omega^D) \quad\wedge\quad \|\phi_1\|^2 = 1 \quad\wedge\quad \lambda_1^D(\omega) = \inf\limits_{\substack{\phi\in\mathsf{D}(h_\omega^D)\\ \phi\neq 0}} \dfrac{h_\omega^D[\phi]}{\|\phi\|^2}, \end{cases} \tag{2.8}$$

then, by virtue of Theorem C.5.1, we have that a unique positive solution ϕ_1 exists and $\lambda_1^D(\omega)$ is a principal eigenvalue. The solution ϕ_1 can be plugged into the minimax property of λ_0 to obtain

$$\lambda_0 \leq \frac{\|\nabla\phi_1\|^2}{\|\phi_1\|^2} = \lambda_1^D(\omega),$$

where the last equality follows from (2.8) if one sets $\phi := \phi_1$.

Secondly, it follows from the minimax theorem that

$$\lambda_1^D(\omega) = \inf_{\substack{\phi \in W_0^{1,2}(\omega) \\ \phi \neq 0}} \frac{\|\nabla\phi\|^2}{\|\phi\|^2}. \tag{2.9}$$

We know that ψ_0 does not depend on x_1, therefore it can be identified with a function on ω. We can write $\psi_0 \in W_0^{1,2}(\omega)$, as per the boundary conditions imposed on ψ_0. Thus (2.9) yields

$$\lambda_1^D(\omega) \leq \frac{\|\nabla\psi_0\|^2}{\|\psi_0\|^2} = \lambda_0,$$

where the last equality follows from (2.7) if one sets $\varepsilon := 0$ and $\phi := \psi_0$. This concludes the proof. □

Remark 2.5.2.1. We can combine (2.9) with the statement in the theorem to obtain

$$\forall\phi \in W_0^{1,2}(\omega) : \int_\omega |\nabla\phi|^2 \geq \lambda_0 \int_\omega |\phi|^2.$$

Proposition 2.5.3.

$$\forall\varepsilon \in \mathbb{R} : \lambda_\varepsilon \geq \lambda_0.$$

Proof. Let $\psi \in \mathsf{D}(h_\varepsilon)$. Then one can write

$$h_\varepsilon[\psi] = \|\psi_{,1} + \varepsilon\dot{\theta}\psi_{,\tau}\|^2 + \|\nabla^{\mathsf{l}}\psi\|^2.$$

Since the first term is non-negative, we can neglect it to get a lower bound. One can then use the definition of $\|\cdot\|^2$ and then apply the Fubini theorem (we have $\Omega = (-L, L) \times \omega$, ω being closed disc of radius R, centered at the origin) to separate the transverse and lateral part of the integral and proceed thusly:

$$h_\varepsilon[\psi] \geq \|\nabla^{\mathsf{l}}\psi\|^2 = \int_{(-L,L)} \mathrm{d}x_1 \int_\omega \mathrm{d}x_2\mathrm{d}x_3|\nabla^{\mathsf{l}}\psi|^2 \geq \lambda_0 \int_{(-L,L)} \mathrm{d}x_1 \int_\omega \mathrm{d}x_2\mathrm{d}x_3|\psi|^2 = \lambda_0\|\psi\|^2,$$

where the last inequality follows from the remark above, since for a fixed $x_1 \in (-L, L)$ the function ψ can be considered an element of $W_0^{1,2}(\omega)$.

Now one need only use the minimax definition of λ_ε

$$\lambda_\varepsilon = \inf_{\substack{\psi \in \mathsf{D}(h_\varepsilon) \\ \psi \neq 0}} \frac{h_\varepsilon[\psi]}{\|\psi\|^2} \geq \lambda_0.$$

□

Proof of theorem 2.5.2. We shall prove the theorem by contradiction. Bearing in mind the previous proposition, we assume

$$\exists\varepsilon \in R, \varepsilon \neq 0 : \lambda_\varepsilon = \lambda_0.$$

It has been shown in 2.4.1 that the problem (2.7) has a solution, thus

$$\exists\psi \in \mathsf{BC}_\varepsilon, \|\psi\|^2 = 1 : \|\psi_{,1} + \varepsilon\dot{\theta}\psi_{,\tau}\|^2 + \|\nabla'\psi\|^2 = h_\varepsilon[\psi] = \lambda_\varepsilon\|\psi\|^2 = \lambda_0\|\psi\|^2.$$

Subtracting $\lambda_0\|\psi\|^2$ from both sides we get

$$\underbrace{\|\psi_{,1} + \varepsilon\dot{\theta}\psi_{,\tau}\|^2}_{\geq 0} + \underbrace{\|\nabla'\psi\|^2 - \lambda_0\|\psi\|^2}_{\geq 0} = 0,$$

where the second inequality follows from Remark 2.5.2.1 as one can apply it to ψ for a fixed x_1 and then integrate the inequality in remark over $(-L, L)$. Since both underbraced expressions are non-negative and their sum has to be zero, they both have to be zero. Therefore we have

(I) $\|\nabla'\psi\|^2 - \lambda_0\|\psi\|^2 = 0$,

(II) $\|\psi_{,1} + \varepsilon\dot{\theta}\psi_{,\tau}\|^2 = 0$.

Let ω be a closed disk of radius R centered at $(0, 0)$. At this point we take into consideration operator $-\Delta_\omega^D$ defined (in the same manner as in the lemma above) as

$$\begin{cases} -\Delta_\omega^D \overset{1:1}{\longleftrightarrow} h_\omega^D, \\ \mathsf{D}(h_\omega^D) = W_0^{1,2}(\omega), \\ \forall\phi \in \mathsf{D}(h_\omega^D) : h_\omega^D[\phi] = \|\nabla\phi\|^2. \end{cases}$$

Let λ be the first eigenvalue of $-\Delta_\omega^D$ and $\phi_1 \in W_0^{1,2}(\omega)$ the corresponding normed eigenfunction. In other words, let ϕ_1 be solution of the problem

$$\begin{cases} \forall\phi \in \mathsf{D}(h_\omega^D) : h_\omega^D(\phi, \phi_1) = \lambda\langle\phi\,|\,\phi_1\rangle, \\ \phi_1 \in \mathsf{D}(h_\omega^D) \quad \wedge \quad \|\phi_1\|^2 = 1 \quad \wedge \quad \lambda = \inf\limits_{\substack{\phi\in\mathsf{D}(h_\omega^D) \\ \phi\neq 0}} \dfrac{h_\omega^D[\phi]}{\|\phi\|^2}, \end{cases}$$

Next, we will show that

$$\exists\eta \in W^{1,2}((-L, L)) : \forall(x_1, x_2, x_3) \in \mathsf{D}(\psi) : \psi(x_1, x_2, x_3) = \eta(x_1)\phi_1(x_2, x_3).$$

Let $x_1 \in (-L, L)$ and denote $\psi_{(x_1)} : (x_2, x_3) \mapsto \psi(x_1, x_2, x_3)$ the function ψ for a fixed x_1. We can write $\psi_{(x_1)} \in W_0^{1,2}(\omega)$. Using the fact that the normed eigenfunctions of $-\Delta_\omega^D$ form an orthonormal base (let us call it $\mathcal{B}$) in $L^2(\omega)$, we can write

$$\forall\mathbf{x}' \in \omega : \psi(x_1, \mathbf{x}') = \psi_{(x_1)}(\mathbf{x}') = \eta(x_1)\phi_1(\mathbf{x}') + \Phi(x_1, \mathbf{x}'),$$

$$\eta(x_1) := \langle\phi_1\,|\,\psi_{(x_1)}\rangle,\ \Phi(x_1, \mathbf{x}') := \sum_{\substack{\phi\in\mathcal{B} \\ \phi\neq\phi_1}} a_{x_1,\phi}\phi(\mathbf{x}'),\ a_{x_1,\phi} := \langle\phi\,|\,\psi_{(x_1)}\rangle.$$

Since $\mathcal{B}$ is orthonormal and ϕ_1 is an eigenfunction of $-\Delta_\omega^D$, one can write (with the use of Fubini theorem)

$$\langle\nabla'(\eta\phi_1)\,|\,\nabla'\Phi\rangle_\Omega = \int_{-L}^{L} \mathrm{d}x_1\ \langle\nabla'(\eta\phi_1)\,|\,\nabla' \sum_{\substack{\phi\in\mathcal{B} \\ \phi\neq\phi_1}} a_{x_1,\phi}\phi\rangle_\omega = \int_{-L}^{L} \mathrm{d}x_1\ \overline{\eta} \sum_{\substack{\phi\in\mathcal{B} \\ \phi\neq\phi_1}} a_{x_1,\phi}\langle\nabla\phi_1\,|\,\nabla\phi\rangle_\omega = 0,$$

where the last equality follows from

$$\forall\phi \in \mathcal{B}, \phi \neq \phi_1 : \langle\nabla\phi_1\,|\,\nabla\phi\rangle_\omega = -\langle\Delta\phi_1\,|\,\phi\rangle_\omega = \lambda\langle\phi_1\,|\,\phi\rangle_\omega = 0.$$

($\langle\cdot\,|\,\cdot\rangle_\Omega$ and $\langle\cdot\,|\,\cdot\rangle_\omega$ denote the scalar products on $L^2(\Omega_\varepsilon)$ and $L^2(\omega)$, respectively)

The minimax principle for $-\Delta_\omega^D$ applied to the function $\Phi_{(x_1)} \in W_0^{1,2}(\omega)$, $\Phi_{(x_1)} : (x_2, x_3) \mapsto \Phi(x_1, x_2, x_3)$ yields

$$\|\nabla'\Phi_{(x_1)}\|_\omega^2 \geq \tilde{\lambda}\|\Phi_{(x_1)}\|_\omega^2 > \lambda\|\Phi_{(x_1)}\|_\omega^2,$$

where $\tilde{\lambda}$ is the second eigenvalue of $-\Delta_\omega^D$, as $\Phi_{(x_1)}$ lies in a subspace of $W_0^{1,2}(\omega)$ orthogonal to the one-dimensional subspace generated by ϕ_1. We can integrate (2.10) (as it contains functions of x_1) over $(-L, L)$ and get the same expression, but this time for $\|\cdot\|_\Omega^2$ and without fixed x_1:

$$\|\nabla'\Phi\|_\Omega^2 \geq \tilde{\lambda}\|\Phi\|_\Omega^2 > \lambda\|\Phi\|_\Omega^2. \tag{2.10}$$

It has been already shown in proof of lemma 2.5.2.1 that the eigenvalue corresponding to ϕ_1 is λ_0 so we have $\lambda = \lambda_0$. To show that Φ is zero one only need rewrite $\|\nabla'\psi\|_\Omega^2$ and use (I) with (2.10), thusly:

$$\|\nabla'\psi\|_\Omega^2 = \|\eta\nabla'\phi_1\|_\Omega^2 + \|\nabla'\Phi\|_\Omega^2 + 2\Re\underbrace{\langle\nabla'(\eta\phi_1)\,|\,\nabla'\Phi\rangle_\Omega}_{=0} = \lambda_0\|\eta\phi_1\|_\Omega^2 + \|\nabla'\Phi\|_\Omega^2.$$

Now subtract $\lambda_0\|\psi\|_\Omega^2 = \lambda_0\|\eta\phi_1\|_\Omega^2 + \lambda_0\|\Phi\|_\Omega^2$ from the left-most and right-most side to get

$$0 \overset{(I)}{=} \|\nabla'\psi\|_\Omega^2 - \lambda_0\|\psi\|_\Omega^2 = \|\nabla'\Phi\|_\Omega^2 - \lambda_0\|\Phi\|_\Omega^2 \overset{(2.10)}{\geq} \underbrace{(\tilde{\lambda} - \lambda_0)}_{>0}\|\Phi\|_\Omega^2.$$

This implies $\Phi = 0$ and so

$$\exists\eta \in W^{1,2}((-L, L)) : \forall(x_1, x_2, x_3) \in \mathsf{D}(\psi) : \psi(x_1, x_2, x_3) = \eta(x_1)\phi_1(x_2, x_3).$$

To arrive at the contradiction one need only rewrite (II)

$$\begin{aligned} 0 = \|\psi_{,1} + \varepsilon\dot{\theta}\psi_{,\tau}\|_\Omega^2 &= \|\eta'\phi_1\|_\Omega^2 + \varepsilon^2\|\dot{\theta}\eta\phi_{1,\tau}\|_\Omega^2 + 2\varepsilon\Re\langle\eta'\phi_1\,|\,\dot{\theta}\eta\phi_{1,\tau}\rangle_\Omega = \\ &\geq \varepsilon^2\|\dot{\theta}\eta\phi_{1,\tau}\|_\Omega^2 + 2\varepsilon\Re\int_{-L}^{L}\mathrm{d}x_1\,\overline{\eta'}\eta\dot{\theta}\underbrace{\int_\omega \mathrm{d}\mathbf{x}'\,\frac{\partial}{\partial\tau}(\frac{1}{2}(\phi_1)^2)}_{=0} = \varepsilon^2\|\dot{\theta}\eta\phi_{1,\tau}\|_\Omega^2 > 0 \end{aligned} \tag{2.11}$$

because

$$\int_\omega \frac{\partial}{\partial\tau}(\frac{1}{2}(\phi_1)^2) = \int_\omega \Big(\mathrm{s}_\theta\frac{\partial}{\partial y}(\frac{1}{2}(\phi_1)^2) + \mathrm{c}_\theta\frac{\partial}{\partial z}(\frac{1}{2}(\phi_1)^2)\Big)$$

and if we use the Dirichlet boundary condition along with Fubini's theorem

$$\int_{-R}^{R}\mathrm{d}z\int_{-\sqrt{R^2-z^2}}^{\sqrt{R^2-z^2}}\mathrm{d}y\,\mathrm{s}_\theta\frac{\partial}{\partial y}(\frac{1}{2}(\phi_1)^2) = \frac{1}{2}\mathrm{s}_\theta\int_{-R}^{R}\mathrm{d}z\,\underbrace{\Big[(\phi_1)^2\Big]_{y=-\sqrt{R^2-z^2}}^{y=\sqrt{R^2-z^2}}}_{=0} = 0$$

and similarily for the other term.

The last inequality (2.11) is a consequence of the fact that $\dot{\theta}$, η and $\phi_{1,\tau}$ are all non-trivial functions.

□

2.5.3 Derivative with Respect to the Twisting Parameter

Formulas for the first and second derivative of the sesquilinear form h_ε at $\varepsilon = 0$ are first derived, then we proceed to infer expressions for the first and second derivative of the function λ_ε.

Lemma 2.5.1.

$$\begin{aligned}\forall \phi, \psi \in \mathsf{D}(h_\varepsilon) : h_0'(\phi, \psi) := \frac{\mathrm{d}h_\varepsilon(\phi, \psi)}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0} &= \langle \phi_{,1} \,|\, \dot\theta \psi_{,\tau} \rangle + \langle \dot\theta \phi_{,\tau} \,|\, \psi_{,1} \rangle, \\ h_0''(\phi, \psi) := \frac{\mathrm{d}^2 h_\varepsilon(\phi, \psi)}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon=0} &= 2\,\langle \dot\theta \phi_{,\tau} \,|\, \dot\theta \psi_{,\tau} \rangle.\end{aligned}$$

Proof. Bearing Remark 2.4.1.2 in mind, the sesquilinear form h_ε can for fixed functions $\phi, \psi \in \mathsf{D}(h_\varepsilon)$ be expressed as a polynomial in ε:

$$h_\varepsilon(\phi, \psi) = \langle \nabla\phi \,|\, \nabla\psi \rangle + \varepsilon\Big(\langle \phi_{,1} \,|\, \dot\theta \psi_{,\tau} \rangle + \langle \dot\theta \phi_{,\tau} \,|\, \psi_{,1} \rangle\Big) + \frac{\varepsilon^2}{2}\, 2\,\langle \dot\theta \phi_{,\tau} \,|\, \dot\theta \psi_{,\tau} \rangle.$$

The lemma follows simply by taking the derivative and setting $\varepsilon = 0$. □

Proposition 2.5.4. *We can write*

(i) $\lambda_0' := \frac{\mathrm{d}\lambda_\varepsilon}{\mathrm{d}\varepsilon}\Big|_{\varepsilon=0} = 0,$

(ii) $\lambda_0'' := \frac{\mathrm{d}^2\lambda_\varepsilon}{\mathrm{d}\varepsilon^2}\Big|_{\varepsilon=0} = 2\|\dot\theta \psi_{0,\tau}\|^2 + 2\langle \dot\theta \psi_{0,\tau} \,|\, \psi_{0,1}' \rangle,$

Proof. We shall admit the fact that ψ_ε is analytical in ε without proof. Justification for this is given in Remark 2.5.4.4. Taking the first derivative of equation (2.7) with respect to ε at $\varepsilon = 0$ yields

$$\forall \phi \in \mathsf{D}(h_0) : h_0'(\phi, \psi_0) + h_0(\phi, \psi_0') = \lambda_0' \langle \phi \,|\, \psi_0 \rangle + \lambda_0 \langle \phi \,|\, \psi_0' \rangle. \tag{2.12}$$

In accordance with the Taylor's theorem, we have existence of two functions ψ_0' and ψ_0'', such that for some ε-neighbourhood of zero we can write

$$\psi_\varepsilon = \psi_0 + \varepsilon\,\psi_0' + \frac{\varepsilon^2}{2}\psi_0'' + O(\varepsilon^2).$$

By taking the first and second derivative with respect to ε at $\varepsilon = 0$ of the boundary conditions in (2.7), one can observe that $\psi_0', \psi_0'' \in \mathsf{BC}_0$.

Hence, one can set $\varepsilon := 0$ and $\phi := \psi_0'$ in equation (2.7) to obtain the identity (also using expression for h_0 from Remark 2.4.1.2)

$$\langle \nabla\psi_0' \,|\, \nabla\psi_0 \rangle = \lambda_0 \langle \psi_0' \,|\, \psi_0 \rangle, \tag{2.13}$$

then set $\phi = \psi_0$ in equation (2.12) and rewrite it using the above lemma (and Remark 2.4.1.2) as follows (last term on the right hand side is moved to left):

$$\underbrace{\Big(\langle \psi_{0,1} \,|\, \dot\theta \psi_{0,\tau} \rangle + \langle \dot\theta \psi_{0,\tau} \,|\, \psi_{0,1} \rangle\Big)}_{=0} + \underbrace{\Big(\langle \nabla\psi_0 \,|\, \nabla\psi_0' \rangle - \lambda_0 \langle \psi_0 \,|\, \psi_0' \rangle\Big)}_{=0} = \lambda_0' \|\psi_0\|^2.$$

First underbraced expression is zero due to the fact that ψ_0 is not dependent on the first coordinate x_1. Second underbraced term vanishes as a consequence of (2.13) (one only need take the complex conjugate thereof). This proves statement (i).

To prove the second statement, we shall take the second derivative of equation (2.7) with respect to ε at $\varepsilon = 0$ to obtain (recall that $\lambda_0' = 0$)

$$\forall \phi \in \mathsf{D}(h_0) : h_0''(\phi, \psi_0) + 2h_0'(\phi, \psi_0') + h_0(\phi, \psi_0'') = \lambda_0'' \langle \phi \,|\, \psi_0 \rangle + \lambda_0 \langle \phi \,|\, \psi_0'' \rangle. \tag{2.14}$$

Similarily to the part above, we set $\varepsilon = 0$ and $\phi = \psi_0''$ in (2.7) to get

$$\langle \nabla \psi_0'' \,|\, \nabla \psi_0 \rangle = \lambda_0 \langle \psi_0'' \,|\, \psi_0 \rangle. \tag{2.15}$$

To finish the proof, we set $\phi := \psi_0$ in (2.14), use the same remark and lemma as before and subtract the complex conjugate of (2.15) from the obtained equation. After recalling that $\|\psi_0\|^2 = 1$ we get statement (ii). □

Remark 2.5.4.1. The statement (i) should be no cause for surprise, considering the symmetry of the problem. The meaning of this result is such that it matters not whether one twists the cylinder in one way or the other.

Remark 2.5.4.2. By plugging $\lambda_0' = 0$ back into (2.12), setting $\phi = \psi_0'$ and expressing the yielded equation using remark 2.4.1.2 and the above lemma, one can write after rearrangement

$$\langle \dot{\theta} \psi_{0,\tau} \,|\, \psi_{0,1}' \rangle = \lambda_0 \|\psi_0'\|^2 - \|\nabla \psi_0'\|^2 \leq 0$$

where the inequality stems directly from the minimax property of λ_0. So the second derivative of the eigennumber can be written alternatively as

$$\frac{\lambda_0''}{2} = \|\dot{\theta} \psi_{0,\tau}\|^2 + \lambda_0 \|\psi_0'\|^2 - \|\nabla \psi_0'\|^2$$

Remark 2.5.4.3. λ_ε is analytical, therefore we can write

$$\lambda_\varepsilon = \lambda_0 + \varepsilon \lambda_0' + \frac{\varepsilon^2}{2} \lambda_0'' + O(\varepsilon^3)$$

Using (i) and the result from Theorem 2.5.2, one obtains (for $\varepsilon \neq 0$)

$$\lambda_0 + \frac{\varepsilon^2}{2} \lambda_0'' + O(\varepsilon^3) = \lambda_\varepsilon > \lambda_0 \Rightarrow \frac{\varepsilon^2}{2} \lambda_0'' + O(\varepsilon^3) > 0$$

Since the inequality holds for all non-zero ε at some neighbourhood of zero it can be conluded by diving the last inequality by $\frac{\varepsilon^2}{2}$ and taking the limit $\varepsilon \to 0$ that

$$\lambda_0'' \geq 0$$

Remark 2.5.4.4. Again, as in the previous chapter that dealt with a perturbation of the shape of a coaxial capacitor, we need the analycity of ψ_ε and λ_ε at some neighbourhood of zero. As before, refer to [9] and the fact that h_ε is a polynomial in ε.

2.6 Hardy's Inequalities

In this section, we shall deal with a mathematical tool called the Hardy's inequality. We shall first somewhat informally introduce the overall idea of [10]. Then, we deal with some Hardy's inequalities derived in [10].

In [10], the effect of twisting and bending of quantum waveguides is explored. That approach is similar to that of ours in Chapter 2, however, an infinitely long waveguide is considered, and moreover, a more general perturbating transformation is employed.

Firstly, the geometry of the waveguide is laid out via a reference curve set in a modified Frenet frame and a cross-section (a bounded open connected subset of $\mathbb{R}^2$) that is extended along the reference curve. There are certain similarities to the method we have introduced in Chapter 1, in fact, the transformation $\mathcal{P}_\varepsilon$ from Chapter 1 is a special case of the transformation $\mathcal{L}$ in [10].

There is, nonetheless, one crucial aspect that $\mathcal{L}$ posseses and $\mathcal{P}_\varepsilon$ does not (at least not on the same level of generality). It is the fact that $\mathcal{L}$ can be set such that it rotates the cross-section in its own plane. Such an effect is (under other certain natural assumptions, such as that the cross-section is not rotationally invariant) is then considered to be *twisting* by [10].

Another, a more simple feature of $\mathcal{L}$ is that it can bend the waveguide. More precisely, a waveguide is considered *bent*, whenever the reference curve has non-zero curvature at some point.

Next, the Hamiltonian of the system is dealt with. No potential is considered, as is usual with waveguides, hence the Hamiltonian is a Laplacian operator and, of course, the Dirichlet boundary condition is imposed on the boundary. A strategy of transferring the problem into curvilinear coordinates is utilized, much like we have done in Chapter 2.

Later, a result concerning the essential spectrum of the Hamiltonian is proposed in [10, thm 4.1]. An assumption that the transformed waveguide becomes straight as it tends to infinities (both positive and negative) has to be taken. The theorem then states that the essential spectrum of a straight waveguide (i.e. $\mathbb{R} \times \omega$, where ω is the cross-section mentioned before) does not differ from that of the transformed waveguide (that is, $\mathcal{L}(\mathbb{R} \times \omega)$).

Then, the effect of bending of a untwisted waveguide is inspected. It is shown in [10, thm 5.1] that the infimum of the spectrum of the Hamiltonian is strictly lower than that of the straight waveguide. In view of the previous result about the stability of the essential spectrum, one has that the bent waveguide has a non-empty discrete spectrum, as opposed to the straight waveguide, the discrete spectrum of which is empty.

Afterward, the examination turns to the twisting effect and Hardy's inequalities on twisted tubes. We shall now take a more formal approach and define the appropriate tools.

Firstly, we define an ordering on the class of self-adjoint operators.

Definition 2.6.1. Let A, B be self-adjoint operators bounded from below, denote a and b their corresponding quadratic forms, respectively. We write

$$A \geq B$$

if, and only if both of the following apply:

(i) $\mathsf{D}(a) \subset \mathsf{D}(b)$,

(ii) $\forall \psi \in \mathsf{D}(a) : a[\psi] \geq b[\psi]$.

Remark 2.6.1.1. The definitions of $\leq$, $<$ and $>$ for operators can, of course, also be made in an analogous way, which is entirely obvious, hence we omit them here.

Definition 2.6.2. Let $\Omega \subset \mathbb{R}^d$ be an open set for some $d \in \mathbb{N}$ and let H be a self-adjoint operator bounded from below on $L^2(\Omega)$. We say that H *satisfies the Hardy inequality*, or equivalently

$$H \text{ satisfies HI}$$

precisely when

$$\exists \rho : \Omega \to [0,\infty), \rho \text{ is measurable}, \rho \neq 0 : H - \inf \sigma(H) \geq \hat{\rho},$$

where $\hat{\rho}$ denotes the $L^2(\Omega)$ operator of multiplication by ρ, more specifically:

$$\forall \psi \in L^2(\Omega) : \hat{\rho}\psi := \rho\psi.$$

We shall also say that the Hardy's inequality is *global*, whenever ρ can be chosen such that

$$\forall \mathbf{x} \overset{a.e.}{\in} \Omega : \rho(\mathbf{x}) > 0$$

Remark 2.6.2.1. Henceforth, we shall omit the symbol ˆ (hat) and thus identify a function with its multiplication operator.

At this point we return to [10] and quote the definition of the Hamiltonian of a bounded waveguide.

Retaining ω to be the aforementioned cross-section of the waveguide and lettinng I to be an open bounded interval, we define H_α^I, for a bounded function $\alpha : I \to \mathbb{R}$, to be the operator corresponding to the quadratic form Q_α^I defined by

$$\begin{cases} \mathsf{D}(Q_\alpha^I) := \{\psi\big|_{I\times\omega} : \psi \in W_0^{1,2}(\mathbb{R}\times\omega)\}, \\ \forall \psi \in \mathsf{D}(Q_\alpha^I) : Q_\alpha^I[\psi] := \|\psi_{,1} - \alpha\psi_{,u}\|^2 + \|\nabla'\psi\|^2, \end{cases}$$

where

$$\forall (s,t_2,t_3) \in I \times \omega : \psi_{,u}(s,t_2,t_3) := t_3\psi_{,2}(s,t_2,t_3) - t_2\psi_{,3}(s,t_2,t_3)$$

and

$$\nabla'\psi := \begin{pmatrix} \psi_{,2} \\ \psi_{,3} \end{pmatrix}$$

and the norm is that of the $L^2(I \times \Omega)$ space.

In [10, lemma 6.1] a result similar to that of in Chapter 2, Theorem 2.5.2 is shown. Here α plays a similar role as $\dot{\theta}$ did in Chapter 2. If one constricts the investigation to a connected bounded portion of the waveguide (i.e. $\mathcal{L}(I \times \omega)$), then the Hamiltonian H_α^I has only a discrete spectrum and its principal eigenvalue is strictly higher than that of a bounded straight waveguide (which is, in this case, $I \times \omega$). More precisely, if we define E_1 to be the principal eigenvalue of a negative Dirichlet Laplacian operator on ω, and then set

$$\lambda(\alpha, I) := \inf\{Q_\alpha^I[\psi] - E_1 : \psi \in \mathsf{D}(Q_\alpha^I) \wedge \|\psi\|^2 = 1\},$$

then we can quote the following result of [10]:

Lemma 2.6.2.1. *Let $I \subset \mathbb{R}$ be a bounded open interval. Let ω be not rotationally invariant with respect to the origin. Let $\alpha \in L^\infty(I)$ be a non-trivial (i.e., $\alpha \neq 0$ on a subset of I of positive measure) real-valued function. Then*

$$\lambda(\alpha, I) \geq \lambda_0,$$

where λ_0 is a positive constant depending on $\|\alpha\|$ and ω.

Remark 2.6.2.2. $\omega \subset \mathbb{R}^2$ is said to be rotationally invariant with respect to origin, if for any two-dimensional rotation R_θ with respect to $(0,0)$ by an angle θ, i.e., for any $\theta \in (0, 2\pi)$

$$R_\theta := \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix},$$

we have that the image of ω by R_θ is equal to ω (in a matrix-vector multiplication sense, of course).

Using the previous lemma, [10] proves the following Hardy's inequality for the operator H^I_α (*cf.* [10, thm 6.5] for details of the proof):

Theorem 2.6.3. *Let $\alpha \in L^\infty(I)$ be a real-valued function and $I \subset \mathbb{R}$ and open interval (not necessarily bounded). Let $K \subset \mathbb{N}$ and $\{I_j\}_{j\in K}$ be a set consisting of disjoint open subintervals of I. Then*

$$H^I_\alpha - E_1 \geq \sum_{j\in K} \lambda(\alpha, I_j)\chi_{I_j},$$

where $\forall i \in K$, χ_{I_j} is the characteristic function of I_j, i.e.,

$$\forall j \in K : \forall s \in I : \chi_{I_j}(s) = \begin{cases} 1 & \text{if } s \in I_j, \\ 0 & \text{otherwise}. \end{cases}$$

Remark 2.6.3.1. We remind that as per Remark 2.6.2.1, the right side of the inequality above is to be understood as a multiplication operator, rather than as a function.

[10, cor 6.6] also shows a consequence of theorem 2.6.3, which finally establishes the effect of twisting of a unbent waveguide, that does not become straight at the negative and positive infinities.

Corollary 2.6.3.1. *Let $\alpha \in L^\infty(I)$ be a real-valued function and $I \subset \mathbb{R}$ and open interval. Suppose that ω is rotationally invariant with respect to origin and that*

$$\exists \alpha_0 \in \mathbb{R}, \alpha_0 > 0 : \forall s \overset{a.e.}{\in} I : |\alpha| \geq \alpha_0.$$

Then we have

$$\inf \sigma(H^I_\alpha) > E_1.$$

Finally, [10, thm 6.7] provides a proof that there exists a Hardy's inequality for H^I_α which is, in fact, global, in the sense that the right side of the inequality is always non-zero.

Theorem 2.6.4. *Let $I \subset \mathbb{R}$ be an open interval. Let ω be not rotationally invariant with respect to the origin. Let $\alpha \in L^\infty(I)$ be a non-trivial real-valued function of compact support in I. Then*

$$H^I_\alpha - E_1 \geq \frac{c}{1+\delta^2}.$$

Here $\delta : I \times \omega \to \mathbb{R} : (s, t_2, t_3) \mapsto |s - s_0|$, where s_0 is the mid-point of the interval $(\inf \operatorname{supp} \alpha, \sup \operatorname{supp} \alpha)$, *and c is a positive constant depending on α and ω.*

Chapter 3

Optimality of a Cylindrical Pipe in Fluid Mechanics

3.1 Introduction

In this section, we shall interest ourselves in a shape optimization problem concerning fluid dynamics. In particular, two mathematical models (from two different articles) of steady viscous flow in a pipe will be presented.

Both articles endeavor to study the optimality of steady viscous flow in a cylidrical pipe, aiming to minimise energy dissipated by the viscosity of the fluid. The Navier-Stokes equations (and also, in [6], the Stokes equations) are utilized to model the behaviour of a non-compressible viscous fluid. The two articles, however, each differ in boundary conditions chosen for the equation system.

The first article, [6], aims to inquire whether there exists a minimiser for their proposed model, and furthermore, investigates whether a cylindrical pipe is the minimiser. They produce a peculiar and somewhat unintuitive result – that the cylindrical pipe does not minimise energy dissipation. Some numerical simulations and the conclusions thereof are also offered.

The second paper, [15], is a reaction to the first one and can be regarded as a rebuttal of the non-optimality claim in [6]. A different class of admissible functions and boundary conditions is proposed and the new outcome is that the cylindrical pipe is, in fact, optimal in terms of energy dissipation. Moreover, an argument is presented that the non-optimality claimed in [6] is a result of the choice of the boundary conditions.

We shall divide the overview of the articles into three parts as follows. Firstly, basic terms of fluid dynamics are defined. Secondly and thirdly, main results of [6] and [15], respectively, are quoted and explained. Since [15] reacts to [6], the third section also contains a comparison of the models.

3.2 Basic Elements of the Navier-Stokes System

First and foremost, we shall present the Navier-Stokes equation system. More specifically, we define the time independent (steady state) Navier-Stokes equations for incompressible viscous fluid without sources. Let $\Omega \subset \mathbb{R}^3$ be an open set, $\mu \in \mathbb{R}$, $\mu > 0$ and $\mathbf{u} = (u_1, u_2, u_3) \in (W^{2,2}(\Omega))^3$, $p \in W^{1,2}(\Omega)$. The Navier-Stokes equations (or rather, our case thereof) then read (the derivatives are to be understood in a weak sense)

$$\begin{cases} -\mu\Delta\mathbf{u} + \nabla p + (\nabla\mathbf{u})\mathbf{u} = 0 & \mathbf{x} \in \Omega, \\ \nabla \cdot \mathbf{u} = 0 & \mathbf{x} \in \Omega, \end{cases} \tag{3.1}$$

where Δ is the Laplacian operator, which upon $\mathbf{u}$ acts as

$$\Delta\mathbf{u} = \begin{pmatrix} \dfrac{\partial^2 u_1}{\partial x_1^2} + \dfrac{\partial^2 u_1}{\partial x_2^2} + \dfrac{\partial^2 u_1}{\partial x_3^2} \\ \dfrac{\partial^2 u_2}{\partial x_1^2} + \dfrac{\partial^2 u_2}{\partial x_2^2} + \dfrac{\partial^2 u_2}{\partial x_3^2} \\ \dfrac{\partial^2 u_3}{\partial x_1^2} + \dfrac{\partial^2 u_3}{\partial x_2^2} + \dfrac{\partial^2 u_3}{\partial x_3^2} \end{pmatrix} \in (L^2(\Omega))^3$$

and $\nabla \cdot \mathbf{u}$ is the divergence of $\mathbf{u}$, that is,

$$\nabla \cdot \mathbf{u} = \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}.$$

It should also be noted that since $\mathbf{u}$ is a three-component vector function then $\nabla\mathbf{u}$ has to be interpreted as a matrix:

$$\nabla\mathbf{u} = \begin{pmatrix} \dfrac{\partial u_1}{\partial x_1} & \dfrac{\partial u_1}{\partial x_2} & \dfrac{\partial u_1}{\partial x_3} \\ \dfrac{\partial u_2}{\partial x_1} & \dfrac{\partial u_2}{\partial x_2} & \dfrac{\partial u_2}{\partial x_3} \\ \dfrac{\partial u_3}{\partial x_1} & \dfrac{\partial u_3}{\partial x_2} & \dfrac{\partial u_3}{\partial x_3} \end{pmatrix},$$

so the $(\nabla\mathbf{u})\mathbf{u}$ is to be understood in a matrix-vector multiplication sense.

One can see that the problem (3.1) is a non-linear system of four second-order partial differential equations for four uknown scalar three-variable functions u_1, u_2, u_3, p.

For each (or at least almost everywhere) $\mathbf{x} \in \Omega$, $\mathbf{u}(\mathbf{x})$ is a vector in three dimensions. Thus, $\mathbf{u}$ can be interpreted as a vector field. Its role in the Navier-Stokes system is that it represents the velocity of the fluid at each point in Ω. The scalar function p is then intepreted as pressure and the positive constant μ is the viscosity of the fluid.

If we set the density of the fluid to be a unit, then the term $-\mu\Delta\mathbf{u}$ in (3.1) represents viscous forces, ∇p is the pressure force and $(\nabla\mathbf{u})\mathbf{u}$ is called the convective acceleration. The last equation $\nabla \cdot \mathbf{u} = 0$ is called the continuity equation and is essentialy a formulation of the law of conservation of mass (*cf.* [12, 3.5.1, 3.5.2]).

A simpler version of the Navier-Stokes system (3.1), called the Stokes system, can be obtained if one neglects the non-linear convective term $(\nabla\mathbf{u})\mathbf{u}$ (*cf.* [11, 17]). Then the equations become linear and we get

$$\begin{cases} -\mu\Delta\mathbf{u} + \nabla p = 0 & \mathbf{x} \in \Omega, \\ \nabla \cdot \mathbf{u} = 0 & \mathbf{x} \in \Omega. \end{cases} \tag{3.2}$$

Lastly, we shall define the criterion for minimisation – the energy dissipated by the fluid (viscosity energy):

$$J(\mathbf{u}, \Omega) := 2\mu \int_\Omega \varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u}), \tag{3.3}$$

where $\varepsilon(\mathbf{u})$ is a 3×3 matrix called the stretching tensor and is given by

$$\forall i, j \in \{1, 2, 3\} : (\varepsilon(\mathbf{u}))_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

and : stands for the inner product of matrices, i.e.,

$$\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u}) := \sum_{i,j=1}^{3} (\varepsilon(\mathbf{u}))_{ij} (\varepsilon(\mathbf{u}))_{ij}.$$

3.3 Non-optimality of a Cylindrical Pipe

Having the most important terms defined, we can now turn to the results presented by [6].

The set of admissible pipes (the domains for the function $\mathbf{u}$) that is chosen is as follows.

$$\mathcal{O}_V^\varepsilon := \{\Omega \subset \mathbb{R}^2 \times (0, L) : \Omega \text{ is bounded, simply connected and satisfies the } \varepsilon\text{-cone property}, |\Omega| = V \wedge \Pi_0 \cup \Omega = S \wedge \Pi_0 \cup \Omega = E\},$$

where ε, L and V are real positive constants, $|\Omega|$ is the Lebesgue measure of Ω, Π_0, Π_L are the planes $\{x_3 = 0\}$, $\{x_3 = L\}$, respectively. S and E are called the inlet and outlet, respectively, given by

$$S := \{(x_1, x_2, 0) \in \mathbb{R}^3 : x_1^2 + x_2^2 \leq R\},$$
$$E := \{(x_1, x_2, L) \in \mathbb{R}^3 : x_1^2 + x_2^2 \leq R\}.$$

Here R is some positive real constant.

The ε-cone property is a way of making $\Omega \in \mathcal{O}_V^\varepsilon$ regular in a certain sense. We shall not give the definition here, as it is not important to our cause. It only suffices to say that given this property, existence and uniqueness of the solution (to system that will be soon introduced) is guaranteed.

One can observe that $\mathcal{O}_V^\varepsilon$ consists of domains with fixed volume V that begin at the plane Π_0 with the shape of a disk, then extend in the x_3-dimension in a regular manner (as by the ε-cone property) and end at the plane Π_L, again, with the shape of a disc. Note that the sets S and E are fixed to be the same for all domains in $\mathcal{O}_V^\varepsilon$.

We also remark that as opposed to Chapters 1 and 2, the shape of Ω here is such that it "extends lengthwise" in the x_3 direction (in Chapters 1 and 2 it was the x_1 direction). This is done so that we are consistent with the notation of [6].

The problem for the velocity field $\mathbf{u}$ and pressure p in [6] reads

$$\begin{cases} -\mu\Delta\mathbf{u} + \nabla p + \nabla\mathbf{u} \cdot \mathbf{u} = 0 & \mathbf{x} \in \Omega, \\ \nabla \cdot \mathbf{u} = 0 & \mathbf{x} \in \Omega, \\ \mathbf{u} = \mathbf{u_0} := (0, 0, c(x_1^2 + x_2^2 - R^2)) & \mathbf{x} \in E, \\ \mathbf{u} = 0 & \mathbf{x} \in \Gamma, \\ -p\mathbf{n} + 2\mu\varepsilon(\mathbf{u}) \cdot \mathbf{n} = (2\mu c x_1, 2\mu c x_2, -p_1) & \mathbf{x} \in S. \end{cases} \tag{3.4}$$

Here $\Omega \in \mathcal{O}_V^\varepsilon$, $\Gamma := \partial\Omega \setminus (E \cup S)$, c is a real negative constant, p_1 is a prescribed pressure value on S (a real constant) and $\mathbf{n} := (0, 0, 1)$ is the outer normal vector at S.

We shall sometimes write $\mathbf{u}(\Omega)$ instead of $\mathbf{u}$ to emphasize the dependence on Ω.

The boundary condition on S in (3.4) is called the parabolic inflow, the condition on Γ is called the no-slip condition and is, in fact, a Dirichlet boundary condition.

If Ω_0 is chosen to be a cylinder of radius R and height L, such that

$$\Omega_0 := \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 \in (0, L) \wedge x_1^2 + x_2^2 < R^2\} \tag{3.5}$$

then $\Omega_0 \in \mathcal{O}_V^\varepsilon$ and the system (3.4) has an explicit solution, called the Poiseuille law, which is given by

$$\forall (x_1, x_2, x_3) \in \Omega_0 : \begin{cases} \mathbf{u}(x_1, x_2, x_3) = (0, 0, c(x_1^2 + x_2^2 - R^2)), \\ p(x_1, x_2, x_3) = 4\mu c(x_3 - L) + p_1. \end{cases} \tag{3.6}$$

It is claimed in [6] that the choice of the bounary condition on S in (3.4) is motivated by the fact that it ensures the parabolic profile in the Poiseuille law if $\Omega = \Omega_0$.

In [6, thm 1], the existence and uniqueness of a weak solution to (3.4) is proven. More specifically, we have a solution $(\mathbf{u}, p) \in W^{1,2}(\Omega) \times L^2(\Omega)$.

Next, it is shown in [6, thm 2] that the minimiser problem for Ω

$$\begin{cases} J(\mathbf{u}(\Omega), \Omega) \text{ has a minimiser}, \\ \Omega \in \mathcal{O}_V^\varepsilon, \end{cases} \tag{3.7}$$

(where $\mathbf{u}(\Omega)$ is the solution to (3.4) and J is given by (3.3)) has a solution.

Moreover, if one can consider the Stokes system (3.2) with the same boundary conditions as in (3.4), that is (with $\Omega \in \mathcal{O}_V^\varepsilon$ and c, p_1 as before)

$$\begin{cases} -\mu\Delta\mathbf{u} + \nabla p = 0 & \mathbf{x} \in \Omega, \\ \nabla \cdot \mathbf{u} = 0 & \mathbf{x} \in \Omega, \\ \mathbf{u} = \mathbf{u_0} := (0, 0, c(x_1^2 + x_2^2 - R^2)) & \mathbf{x} \in E, \\ \mathbf{u} = 0 & \mathbf{x} \in \Gamma, \\ -p\mathbf{n} + 2\mu\varepsilon(\mathbf{u}) \cdot \mathbf{n} = (2\mu c x_1, 2\mu c x_2, -p_1) & \mathbf{x} \in S. \end{cases} \tag{3.8}$$

Then (3.8) has a unique solution and the minimiser problem (3.7) for Ω, with $\mathbf{u}$ being the solution to (3.8), also has a solution which has a plane of symmetry containing the x_3-axis as per [6, thm 3], which is proven mainly by a geometrical argument.

The main theorem [6, thm 4] follows.

Theorem 3.3.1. *The cylinder* Ω_0 *(as defined by (3.5)) is* ***not*** *the minimiser of the problem for* Ω

$$\begin{cases} J(\mathbf{u}(\Omega), \Omega) \textit{ has a minimiser}, \\ \Omega \in \mathcal{O}_V^\varepsilon, \end{cases}$$

where $\mathbf{u}(\Omega)$ *is the solution to (3.4) and J is given by (3.3).*

Lastly, [6] give some numerical results which show that the minimiser of the problem in 3.3.1 is indeed not a cylinder and some more optimal shapes are developed through iterative methods.

3.4 Optimality of a Cylindrical Pipe

The article discussed in the previous section, [6], has established the existence of a mathematical model of viscous flow in a pipe, wherein the cylindrical pipe is not optimal under the criterion: energy dissipated by the fluid.

Here we overview [15], which is a response to [6]. [15] argues that the non-optimality claim of [6] is merely a boundary effect and a result of the special choice of boundary conditions and is not related to the shape of the pipe.

Firstly, we shall quote an argument that establishes the fact that if one considers system (3.4) then the first variation of J is dependend only on the boundary condition given on the outlet S. A perturbation of the form

$$\forall t \in \mathbb{R} : \Omega_t := (Id + t\mathbf{V})(\Omega_0),$$

where Id denotes the identity map, $\mathbf{V}$ is a smooth compactly supported vector field, i.e. $\mathbf{V} \in (C_0^\infty(\mathbb{R}^3 \setminus (\overline{E} \cup \overline{S})))^3$ (so one has $\mathbf{V} = 0$ on E and S) and Ω_0 is the cylinder given by (3.5). The first variation is then

$$\mathrm{d}J(\Omega_0, \mathbf{V}) = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} J(\mathbf{u}(\Omega_t), \Omega_t),$$

where J is the integral defined by (3.7) and $\mathbf{u}(\Omega_t)$ is the solution to (3.4) for the choice $\Omega = \Omega_t$. A volume constraint on the perturbation is assumed, by considering only such $\mathbf{V}$ that satisfy

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} |\Omega_t| = 0,$$

where $|\Omega_t|$ is the Lebesgue measure of Ω_t.

[15] shows the following expression for $\mathrm{d}J(\Omega_0, \mathbf{V})$:

$$\mathrm{d}J(\Omega_0, \mathbf{V}) = 4\mu \int_S \mathbf{u}' \cdot (\varepsilon(\mathbf{u})\mathbf{n}), \tag{3.9}$$

where $\mathbf{u}$ is given by the Poiseuille law (3.6), $\mathbf{n} = (0, 0, 1)$ is the unit outer normal vector on S, $\varepsilon(\mathbf{u})\mathbf{n}$ is to be understood in the sense of matrix-vector multiplication, the dot $\cdot$ stands for the standard Euclidean scalar product, the integral is to be taken with the 2-dimensional Lebesgue measure and $\mathbf{u}'$ is called the shape derivative of $\mathbf{u}(\Omega_t)$, defined as ($\mathbf{u}(\Omega_t)$ being the solution to (3.4) for $\Omega = \Omega_t$, of course)

$$\mathbf{u}' := \lim_{t \to 0} \frac{1}{t} (\mathbf{u}(\Omega_t) \circ (Id + t\mathbf{V}) - \mathbf{u}(\Omega_0)) - \mathbf{V} \cdot (\nabla \mathbf{u}).$$

[15] then demonstrates, that the expression (3.9) is, in effect, only dependent on $\mathbf{u} \restriction_S$ – the boundary condition imposed on S. Moreover, it is claimed, that one can do the same calculations for the cylinder Ω_0, where the boundary condition on S is perturbed (instead of the shape of the pipe, as was done here) and this leads to the same decrease of dissipated energy.

Next, [15] tackles the optimality of the cylindrical pipe. A class of admissible shapes (pipes) is considered, such that the sets are open, bounded, connected, have a Lipshitz boundary and have a fixed, finite volume $V \in \mathbb{R}$, $V > 0$, and are contained in the strip $\mathbb{R}^2 \times (0, L)$, for a real positive constant L.

As opposed to the setup of [6], the inlet E and outlet S are allowed to be any non-empty 2-dimensional (in the sense that they are embedded in three dimensions), open sets with 2-dimensional Lipschitz boundary. E and S, as before, have to be contained in the planes $\{x_3 = 0\}$ and $\{x_3 = L\}$, respectively, but it is apparent, they they need not be disks anymore, moreover, they are not necessarily of the same shape.

Additional Lipschitz regularity conditions are also required, but we shall not discuss them here. We shall denote the set of admissible pipes O_V, for its precise mathematical definition *cf.* [15, def 4.1]. Symbolically, we will use similar notation as previously, that is, for $\Omega \in O_V$

$$\begin{aligned} E &:= \overline{\Omega} \cap \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 = 0\}, \\ S &:= \overline{\Omega} \cap \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 = L\}, \\ \Gamma &:= \partial\Omega \setminus (E \cup S). \end{aligned}$$

A set of admissible velocity fields is also defined, in [15, def 4.3]. Let $\Omega \in O_V$, $\mathbf{u} := (u_1, u_2, u_3) \in C^1(\overline{\Omega})^3$ and let for a fixed $f \in \mathbb{R}$ all of the following conditions hold:

(i) $\nabla \cdot \mathbf{u} = 0$, i.e., $\mathbf{u}$ is divergence free (satisfies the continuity equation),

(ii) $\mathbf{u}\big|_\Gamma = 0$, i.e., the no-slip (Dirichlet) boundary condition,

(iii) $\int_E u_3 = f$, i.e., a fixed total inflow condition for all fields.

Note that the integral in (iii) has to be taken with the 2-dimensional Lebesgue measure. We will write $\mathbf{u} \in U_f(\Omega)$, if $\mathbf{u}$ satisfies the definition above.

We can now quote the main theorem [15, thm 4.4]:

Theorem 3.4.1. *Let $V, f \in \mathbb{R}, V > 0$ and let Ω_0 be the cylinder from (3.5) for such constants R and L that we can write $V = \pi R^2 L$. Denote $\mathbf{u}_0 =: ((\mathbf{u}_0)_1, (\mathbf{u}_0)_2, (\mathbf{u}_0)_3)$ the Poiseuille flow from (3.6) on Ω_0, with c chosen such that $\int_E (\mathbf{u}_0)_3 = f$.*

Then $\Omega_0 \in O_V$ and $\mathbf{u}_0 \in U_f(\Omega_0)$ and we have

$$\forall \Omega \in O_V : \forall \mathbf{u} \in U_f(\Omega) : \left(\int_\Omega \nabla \mathbf{u} : \nabla \mathbf{u} \geq \int_{\Omega_0} \nabla \mathbf{u}_0 : \nabla \mathbf{u}_0 \right)$$

Remark 3.4.1.1. We remark that $\mathbf{u}$ from Theorem 3.4.1 need not at all be a solution to the Navier-Stokes system (3.1). The only differential eqation it is required to solve is the continuity equation $\nabla \cdot \mathbf{u} = 0$.

One could add the condition for $\mathbf{u}$ to be the solution (3.1) and since the Poiseuille flow is also a solution to the Navier-Stokes system, the theorem would still hold. This would, nevertheless, only be a restriction.

Remark 3.4.1.2. Note the resemblance of the integral in Theorem 3.4.1 to the integral from the Dirichlet principle from Appendix B.

Theorem 3.4.1 provides an interesting inequality, however, it is not yet apparent that the Poiseuille flow of the cylindrical pipe indeed does minimise the energy dissipated by the viscous fluid. The following lemma, that can be shown using integration by parts and Gauss theorem, from [15, lemma 4.8], helps put this unclarity into perspective.

Lemma 3.4.1.1. *Let $\Omega \subset \mathbb{R}^3$ be an open bounded set with Lipschitz boundary and let $\mathbf{u} \in W^{2,2}(\Omega)^3$ satisfy $\nabla \cdot \mathbf{u} = 0$. Then we can write*

$$\int_\Omega \varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u}) = \frac{1}{2} \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{u} + \int_{\partial\Omega} \mathbf{u} \cdot (\nabla \mathbf{u})\mathbf{n},$$

where the integral over $\partial\Omega$ is to be taken with the 2-dimensional Lebesgue measure and $\mathbf{n}$ is the unit outer normal vector on $\partial\Omega$.

If one considers $\Omega \in O_V$ such that E and S are of the same shape and imposes for $\mathbf{u} \in U_f(\Omega)$ periodic boundary conditions on S and E, i.e.,

$$\mathbf{u}\big|_E = \mathbf{u}\big|_S \quad \wedge \quad \partial_3 \mathbf{u}\big|_E = \partial_3 \mathbf{u}\big|_S \tag{3.10}$$

then the last term in lemma 3.4.1.1 vanishes a we have that Poiseuille flow of a cylindrical pipe (3.6) in fact does minimise dissipation of energy by the fluid.

Same can be achieved if one considers the boundary conditions

$$\mathbf{u} \times \mathbf{n} = 0 \text{ on } E \text{ and } S. \tag{3.11}$$

(Here E and S need not be of the same shape anymore.)

We conlude by stating that the expression (3.9) offers a reason to consider that the boundary conditions (3.10) and (3.11) pose a somewhat more reasonable choice than the boundary conditions in (3.4). The model presented by [6] is, nevertheless, an interesting mathematical problem that raises the question of what is the explicit form of the minimiser in (3.7).

Conclusion

We shall now give a summary of the results produced by this work.

We have introduced, in the first chapter, a certain class of perturbations, which can be interpreted as bending and twisting of the shape of a straight coaxial capacitor. The influence of the perturbations on capacitance was inspected.

This was done by the use of a variational principle, the modified Dirichlet's principle from the second appendix, and by examination of the first and second variations of the capacitance by means of the Taylor's theorem. It has been shown that a small perturbation, as defined by us, results in an increase of the capacitance.

Next, a cylindrical quantum mechanical waveguide was taken into consideration and a twisting transformation was applied to its geometry. It was shown that the effect of twisting is such that it increases the energy of the ground-state of the waveguide, in other words, the cylindrical waveguide minimizes ground-state energy if only our transformations are taken into account. Some formulas for the first and second variation of the aforementioned energy were derived. This was done via spectral theory, often by use of the minimax theorem.

We have also offered an overview of [10], a paper that deals with similar problems concerning twisting and bending of a quantum waveguide and shown some Hardy's inequalities therefrom.

In the last part, the third chapter, an outline of two articles tackling the problem of steady viscous fluid motion was offered. We have examined two different mathematical models, from [6] and [15], each of which yielded a completely different result – the claim of [6] was that a cylindrical pipe does not minimise energy dissipated by the fluid, the second, on the other hand, has shown reasons as to why the former does not model the situation entirely correctly and that the non-optimality result is a consequence of a special choice of a boundary condition.

Furthermore, we have quoted another result of [15], in which different boundary conditions (which they deem more appropriate) are imposed and it is shown that, under these conditions, cylindrical pipe does, in fact, minimise dissipated energy.

We conclude with some open problems raised by this work.

In view of the first chapter, it is natural to ask if it is indeed possible to consider a broader class of transformations that increase capacitance, for example the one in [10], which is admits rotation of the cross-section.

Perturbation of shapes other than a cylinder might also prove to be insightful.

Concerning the second chapter, our main interest is whether it is possible to show positivity of the second variation of the ground state energy using the formulas derived.

Other boundary conditions, for example periodic, might also be considered. The question then is whether this would change any of the results that we have shown.

As per the third chapter, an explicit form of the energy-dissipation-minimising shape from [6], is desirable.

Since pipes used for fluid transport are not always straight and often have to bend, an investigation of the optimal shape of a bend pipe could help to illuminate the role of the circular cross-section, which is the usual technical solution.

Appendices

Appendix A

Remarks on Notation

Here we explain the symbols used throughout the work. Most of the notation is standard and requires no explanation. This includes arithmetic operations and elemental functions.

We note that multiplication of numbers is usualy denoted without any symbol, and is done simply by placing two numbers adjacent to each other.

A.1 Logic and Definitions

$\wedge$	and
$\vee$	or
$\Leftrightarrow$	equivalence
$\Rightarrow$	implication
$\forall$	the universal quantifier
$\exists$	the existential quantifier
$:$	quantifier-quantifier and quantifier-predicate separator
$:=$	the left object is defined by the right object
$:\Leftrightarrow$	the left predicate is defined by the right predicate

A.2 Sets

$\{\}$	set brackets
$\emptyset$	the empty set
...	a part of a sequence whose pattern is apparent
$\{x_n\}_{n=1}^{\infty}$	the infinite set $\{x_1, x_2, ...\}$, also used for an ordered sequence
$\mathbb{N}$	the set of all natural numbers, **not** including zero
$\mathbb{R}$	the set of all real numbers

$\mathbb{C}$	the set of all complex numbers
$\in$	set membership
$\overset{a.e.}{\in}$	set membership almost everywhere
$\cup$	set union
$\cap$	set intersection
$\subset$	set inclusion, is applicable even if sets are equal
$\setminus$	set difference
$\times$	cartesian product
M^n	the n-th cartesian power of a set M
$[a, b)$	interval from a to b, including $a \in \mathbb{R}$, not including $b \in \mathbb{R}$ (other combinations of [,], (,) are possible and unlisted)
$\hat{n}$	the set $\{1, 2, ..., n\}$ for some $n \in \mathbb{N}$
sup	supremum of a set
inf	infimum of a set
min	minimum of a set
max	maximum of a set
$\overline{M}$	topological closure of set M
∂M	topological boundary of set M
i	imaginary unit
$\Re$	real part of a complex number
$\bar{z}$	complex conjugate of $z \in \mathbb{C}$

We also use

$$\{x \in M : P(x)\}$$

to denote the set of all $x \in M$ (for some set M) such that they satisfy predicate P (i.e. $P(x)$ is true).

A.3 Maps

The symbolic notation (definition of a map)

$$f : X \to Y$$

means that f is map that maps all elements of X (the domain of f) to (not necessarily all) elements of Y.

$$x \mapsto f(x)$$

stands for a map that maps each x from a set, that is either stated or apparent, gets mapped to $f(x)$ (value of f at x). If this symbol is adjacent to a definition of a map, it simply defines how the map operates.

If a map maps into some number set, we call it a *function*.

We also note that maps are handled in a similar way to numbers, vectors and matrices, in terms of operations. This means $f + g$ is a map $x \mapsto f(x) + g(x)$ (if it has a good sense) and similarily for other operations.

Some other notation for maps follows.

$\mathsf{D}(f)$	the domain of f
$\operatorname{supp} f$	the support of f, i.e. $\overline{\{x \in \mathsf{D}(f) : f(x) \neq 0\}}$
$\circ$	map composition
f^{-1}	the inverse of f
$f(M)$	the image of M by f, if $M \subset \mathsf{D}(f)$
$f^{-1}(M)$	the inverse image of M by f, if $M \subset f(\mathsf{D}(f))$
$\lim\limits_{x \to y} f(x)$	limit of f as x approaches y
$\stackrel{n}{\to}$	limit of a sequence as n approaches infinity
$\to$	limit of a sequence, wherein the limiting index is apparent
$C^n(M)$	set of all functions on M with n continous derivatives
$C^\infty(M)$	set of all infinitely-diffentiable functions on M
$C_0^n(M)$	set of all $f \in C^n(M)$, such that $\operatorname{supp} f$ is bounded
$C_0^\infty(M)$	set of all $f \in C^\infty(M)$, such that $\operatorname{supp} f$ is bounded
$L^2(M)$	set of all square-integrable functions
∇	the del (nabla) operator
Δ	the Laplace operator

We also use three different notations for a partial derivative:

$$\frac{\partial f}{\partial x_i} = \partial_i f = f_{,i}$$

The first one is the standard Leibniz form and is least compact. The second notation is inline and takes up much less space. The third notation is the most compact and is the most often used. The symbol ∂_i^2 means that the second partial derivative is to be taken. Similarily, $f_{,ij}$ means simply that two derivatives are to ba taken, i.e., $(f_{,i})_{,j}$.

If we write

$$f\big|_{\mathbf{x}=\mathbf{x}_0} \text{ or } f\big|_{\mathbf{x}_0}$$

then the map is to be evaluated as some point $\mathbf{x}_0$. We also use the this symbol for restrictions:

$$f\big|_M$$

for some set $M \subset \mathsf{D}(f)$ is a map with domain M that acts as $x \mapsto f(x)$.

A similar symbol, $\upharpoonright$,is used for restrictions that are defined almost everywhere. For example

$$f \upharpoonright_M = 0$$

means that f is zero on M up to a set of zero measure. However, if M were a boundary, then it would be of zero measure and the statement would be trivial. In such case, the restriction has to be understood in the sense of traces, an aspect of Sobolev spaces.

We do not deal with traces in much detail in this work, therefore we approach this notion in a formal and intuitive manner.

We use the usual Leibniz sign for integration, that is

$$\int_M f = \int_M f(x)\mathrm{d}x,$$

It is usually apparent or noted, which measure is to be used.

We also use the symbol $O(\varepsilon^n)$, which represents the Peano remainder when we use Taylor's theorem. This means we have some interval I that

$$\exists \gamma \in C^0(I) : O(\varepsilon^n) = \varepsilon^n \gamma(\varepsilon) \wedge \lim_{\varepsilon \to 0} \gamma(\varepsilon) = 0$$

We note that although the same symbol $O(\varepsilon^n)$ might be used throughout a calculation, this does not mean that the function γ remains the same.

A.4 Vector Spaces and Matrices

$\subset\subset$	subspace symbol
$\mathbb{R}^{n,n}$	the space of all $n \times n$ matrices
$\mathcal{H}$	Hilbert space
$\langle \cdot \mid \cdot \rangle$	L^2 scalar product
$\lVert \cdot \rVert$	norm induced by the L^2 scalar product
$\lvert \cdot \rvert$	euclidean norm
$(\mathbf{x})_i$	the i-th component of a vector (or vector map) $\mathbf{x}$
$(A_{ij})_{i,j=1}^n$	a square $n \times n$ matrix given by elements A_{ij}
A^T	matrix transposition of A
A^{-1}	matrix invense of A
A_{ij}	the i-th row and j-th column of the matrix A
$J^{\mathcal{L}}(\mathbf{x})$	the Jacobian matrix of the transformation $\mathcal{L}$ at the point $\mathbf{x}$
$g^{\mathcal{L}}(\mathbf{x})$	the metric tensor of the transformation $\mathcal{L}$ at the point $\mathbf{x}$

If a map has an unusual notation, then we use the dot $\cdot$ as a placeholder.

We also note that it is usually stated or apparent, on which space in particular is the norm or a scalar product taken.

The following convention is used: if M is a measurable set, $f,\ g \in L^2(M)^n$ are a square-integrable vector functions and $A,\ B \in L^2(M)^{n^2}$ are a square-integrable matrix functions, then

$$\langle f \,|\, A \,|\, g \rangle := \langle f \,|\, Ag \rangle,$$

where Ag is to be understood in a matrix-vector multiplication sense. Morover, we shall omit parentheses if more matrices are present, i.e.,

$$\langle f \,|\, A + B \,|\, g \rangle := \langle f \,|\, (A + B) \,|\, g \rangle.$$

Appendix B

The Calculus of Variations

B.1 Introduction

Calculus of variations represents a branch of mathematical analysis that deals with functionals (that is, maps from given function spaces into a given number field), or rather, to be more specific, with extremes thereof. In other words, given a functional, the general idea is usually to find a function in its domain that either minimizes or maximizes the functional, either locally or globally, or to show nonexistence of such a function.

More specifically, the discipline aims to provide necessary and sufficient conditions for such functions and studies their properties.

We shall deal only with real-valued integral functionals and real-valued functions of real variables for simplicity.

In this appendix, elements of the calculus of variations are laid out.

Firstly, functionals of one-dimensional integral form are considered, derived methods are demonstrated on classic examples for motivation.

Secondly, we concern ourselves with three-dimensional integral functionals and present a principle called the Dirichlet principle. We shall also offer a modification of the Dirichlet principle that shall be utilized in Chapter 1.

B.2 Euler-Lagrange Equations

In this section, we adopt the approach that is shown in [8] and the following text is a mostly a summary of the introduction in the work. We shall introduce the problem only informally and then provide a more rigorous approach.

A classical, and perhaps even the simplest, problem in calculus of variations is to find a function $u : [a, b] \to \mathbb{R}^d$ that minimizes the integral

$$\int_a^b F(t, u(t), \dot{u}(t))\mathrm{d}t, \tag{B.1}$$

where $a, b \in \mathbb{R}$, $F : [a, b] \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ for some $d \in \mathbb{N}$ and $\dot{u}$ stands for the derivative of u. Evidently, more assumptions on both u and F have to be laid down so that the integral above is well defined.

Remark B.2.0.1. Note that F is a function of a $(2d + 1) - let$ of real numbers, but we have chosen to formally group them into three collections: a singlet and two d-lets. If we simply refer to the first, second and third variable of F we shall actually mean the aforementioned singlet, first d-let and second

d-let, respectively. On the other hand, if we refer to the i-th *real* variable of F, we have in mind the i-th component of the $(2d + 1)$-let instead.

Before any functional can be defined, one first has to choose a set of functions that it admits (its domain, also called the set of admissible functions).

One kind of constraints, when contriving such set, is that the functional has to have good sense should it be applied to any function from the domain. In case of the integral (B.1), the admissible functions have to be such that the integration is possible. If F is non-trivial in its third argument, then it also follows, that u must be differentiable, at least in a weak sense.

Another type of constraints is usually motivated by the problem at hand. Boundary conditions may be imposed or regularity requirements demanded.

We will, for simplicity, consider the following functional. Let $u_1, u_2 \in \mathbb{R}^d$, $a, b \in \mathbb{R}$, $F \in C^2([a, b] \times \mathbb{R}^d \times \mathbb{R}^d)$ for some $d \in \mathbb{N}$, and

$$\forall u \in \mathsf{D}(\mathcal{I}) : \mathcal{I}[u] := \int_a^b F(t, u(t), \dot{u}(t))\mathrm{d}t,$$

$$\mathsf{D}(\mathcal{I}) := \{u \in C^2([a, b], \mathbb{R}^d) : u(a) = u_1 \wedge u(b) = u_2\}.$$

Notice that we write $\mathcal{I}[u]$ instead of $\mathcal{I}(u)$ in order to emphasize that u is a function, not a number.

Because of the conditions imposed on $u \in \mathsf{D}(\mathcal{I})$ on the endpoints, we say that u has fixed ends. This is sometimes also referred to as the Dirichlet boudary condition.

Clearly, the domain of $\mathcal{I}$ consists of functions that represent smooth curves in d-dimensional space, and furthermore, they all originate and terminate (respectively) at the same points in space.

We have already stated informally that our goal is to find a function in $\mathsf{D}(\mathcal{I})$ so that $\mathcal{I}$ attains a minimum or a maximum. The following definition establishes this notion in more rigorous, albeit not surprising, terms

Definition B.2.1. Let $u \in M$. We say that u is a *minimiser* of $\mathcal{I}$ if, and only if,

$$\forall w \in \mathsf{D}(\mathcal{I}) : \mathcal{I}[u] \leq \mathcal{I}[w].$$

Remark B.2.1.1. An analogous definition can, of course, be established even for a maximising element, a *maximiser*. However, in our examples and proceedings we shall only deal with minimisers, moreover, if one has a maximiser of some functional J then it is a minimiser of $-J$.

Example B.2.2 (Length of a graph of a function)**.** Set $d = 1$. Now let $u \in \mathsf{D}(\mathcal{I})$ and define

$$\gamma_u : [a, b] \to \mathbb{R}^2 : t \mapsto (t, u(t)).$$

The map γ_u represents a curve along the graph of u. Setting F so that

$$\mathcal{I}[u] := \int_a^b |\dot{\gamma}_u(t)|\mathrm{d}t = \int_a^b \sqrt{1 + \dot{u}(t)^2}\mathrm{d}t$$

now causes $\mathcal{I}[u]$ to be the arc-length of γ and therefore of u (*cf.* [13, p. 136]). The minimiser of $\mathcal{I}$ is a function, whose graph starts at (a, u_1), ends at (b, u_2) and minimises arc-length – common knoweledge dictates that it is a line. It it not yet obvious, however, that it is so from the mathematical formulation here.

Example B.2.3. A famous historical example is that of the problem of the *brachystochrone*. Therein one attempts to find between two given points a path traced by a particle that is acted upon by the force of gravity, so that the particle reaches the endpoint in the fastest time.

To derive the precise formulation of the functional for this problem, one only need know that a particle that has fallen a vertical distance y, has at that point reached speed $\sqrt{2gy}$, g being the gravitational acceleration, and that a change in time is given as a ratio of the distance travelled over speed. This leads to (retaining notation for γ_u from the previous example, as $|\dot{\gamma}_u(t)|\mathrm{d}t$ is the "infinitesimal distance" travelled in the time $\mathrm{d}t$)

$$\mathcal{I}[u] := \int_a^b \frac{|\dot{\gamma}_u(t)|\mathrm{d}t}{\sqrt{2gu(t)}} = \int_a^b \sqrt{\frac{1+\dot{u}(t)^2}{2gu(t)}}\mathrm{d}t.$$

One of the most basic results in analysis of differentiable functions of one variable is the necessary condition for an extreme. Namely, if f is differentiable at $x \in \mathsf{D}(f)$ and reaches a maximum or a minimum at x, then

$$f'(x) = 0.$$

The following theorem can be regarded as an analogy of this necessary condition for the functional $\mathcal{I}$.

Theorem B.2.4. *Let $u \in \mathsf{D}(\mathcal{I})$ be a minimiser of $\mathcal{I}$. Then u is the solution of the following system of second order ordinary differential equations, called the Euler-Lagrange equations*

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{\partial F}{\partial \dot{u}}(t, u(t), \dot{u}(t))\Big) - \frac{\partial F}{\partial u}(t, u(t), \dot{u}(t)) = 0,$$

where

$$\frac{\partial F}{\partial u} = \left(\frac{\partial F}{\partial u_1}, \frac{\partial F}{\partial u_2}, ..., \frac{\partial F}{\partial u_d}\right)^T, \quad \frac{\partial F}{\partial \dot{u}} = \left(\frac{\partial F}{\partial \dot{u}_1}, \frac{\partial F}{\partial \dot{u}_2}, ..., \frac{\partial F}{\partial \dot{u}_d}\right)^T$$

and $\frac{\partial}{\partial u_i}$ is the derivative with respect to the (i+1)-th real variable and $\frac{\partial}{\partial \dot{u}_i}$ is with respect to the (i+d+1)-th real variable.

Proof. We shall prove this theorem using the necessary condition for functions of one variable mentioned above. Let $v \in C_0^2([a,b], \mathbb{R}^d)$. It then follows that $\forall s \in \mathbb{R} : u + sv \in \mathsf{D}(\mathcal{I})$. Setting $w := u + sv$ for all $s \in \mathbb{R}$ in the definition of minimiser and by defining $f : \mathbb{R} \to \mathbb{R} : s \mapsto \mathcal{I}[u + sv]$, we obtain

$$\forall s \in \mathbb{R} : f(s) \geq f(0).$$

Since the derivative of F is continuous, we get that the derivative of the integrand in f as a function of s is continuous as well, furthermore, this is true on a closed interval. Hence, f is differentiable and the order of differentiation and integration can be switched.

The above states that f realized a minimum at 0, therefore

$$f'(0) = 0.$$

We shall rewrite this expression by using the definitions of f and $\mathcal{I}$:

$$\int_a^b \frac{\partial}{\partial s}\Big|_{s=0} F(t, u(t) + sv(t), \dot{u}(t) + s\dot{v}(t))\mathrm{d}t = 0.$$

Now using the chain rule to express the derivative yields

$$\int_a^b \left(\frac{\partial F}{\partial u}(...) \cdot v(t) + \frac{\partial F}{\partial \dot{u}}(...) \cdot \dot{v}(t)\right)\mathrm{d}t = 0,$$

where $(...) := (t, u(t), \dot{u}(t))$ and the dot $\cdot$ represents the standard scalar product of the Euclidean space. Integrating the second term in the integrand by parts then yields

$$\underbrace{\left[\frac{\partial F}{\partial \dot{u}}(...) \cdot v(t)\right]_a^b}_{=0} + \int_a^b \left(\frac{\partial F}{\partial u}(...) - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial \dot{u}}(...)\right) \cdot v(t)\mathrm{d}t = 0.$$

The first term vanishes since $v(a) = 0 = v(b)$. To finish the proof we only need the following lemma. □

Lemma B.2.4.1 (Fundamental lemma of the calculus of variations)**.** *Let $h \in C^0((a,b),\mathbb{R}^d)$ and let the following condition on h hold:*

$$\forall \phi \in C_0^\infty((a,b),\mathbb{R}^d) : \int_a^b h(t) \cdot \phi(t)\mathrm{d}t = 0.$$

Then $\forall t \in (a,b) : h(t) = 0$.

Proof. We shall prove the lemma by contradiction. Assume

$$\exists t_0 \in (a,b) : h(t_0) \neq 0.$$

Therefore $\exists i_0 \in \hat{d} : h_{i_0}(t_0) \neq 0$, where h_{i_0} denotes the i_0-th component of h. By continuity of h we have

$$\exists \delta \in \mathbb{R}, \delta > 0 : (a < t_0 - \delta < t_0 + \delta < b) \wedge (\forall t \in (t_0 - \delta, t_0 + \delta) : |h_{i_0}(t)| > 0).$$

Let us now choose $\phi \in \mathbb{C}_0^\infty((a,b),\mathbb{R}^d)$ such that

$$\forall t \in (a,b) : \begin{cases} t \notin (t_0 - \delta, t_0 + \delta) \Rightarrow \phi(t) = 0, \\ t \in (t_0 - \delta, t_0 + \delta) \Rightarrow \phi_{i_0}(t) > 0, \\ \forall i \in (\hat{d} \setminus \{i_0\}) : \phi_i(t) = 0, \end{cases}$$

where, analogously to the previous case, for $j \in \hat{d}$ the symbol ϕ_j is the j-th component of the map ϕ. We can now arrive at the contradiction by writing

$$\int_a^b h(t) \cdot \phi(t)\mathrm{d}t = \int_{t_0-\delta}^{t_0+\delta} h(t) \cdot \phi(t)\mathrm{d}t \neq 0,$$

where the non-equality comes from the fact that both h and ϕ are non-zero and don't change their sign on the interval (a,b). □

Remark B.2.4.1. A skeptical reader of the previous proof might, however, doubt whether such function ϕ, as described above, truly exists. Nevertheless, the function $\Psi : \mathbb{R} \to \mathbb{R}$ defined as

$$\forall t \in \mathbb{R} : \Psi(x) = \begin{cases} \exp\left(-\frac{1}{1-t^2}\right) & \text{if } t \in (-1,1), \\ 0 & \text{otherwise}, \end{cases}$$

is in fact smooth, as can be checked by taking its derivative (at $t = -1, 1$, one has to take single-sided derivatives from both sides and show them to be the same) and then by induction proving that all higher derivatives are continuous.

The function Ψ can be used for contruction of ϕ_{i_0} by setting (retaining notation from proof above)

$$\forall t \in (a,b) : \phi_{i_0}(t) = \Psi(\frac{t - (t_0 - \delta)}{2\delta} - \frac{(t_0 + \delta) - t}{2\delta}).$$

Remark B.2.4.2. This lemma can, in fact, be generalized to admit functions of more than one variable. The set $[a, b]$ would then have to be replaced with a closure of a non-empty open set. A proof for the lemma for a closed bounded region and a function of two variables, which can be trivially extended to any number of variables and any closure of a non-empty open set can be found in [5, p. 22].

We can now return to examples B.2.2 and B.2.3 and try to solve the Euler-Lagrange equations in order to obtain what might be minimizers of the respective forms of $\mathcal{I}$.

Example B.2.5. Continuing in example B.2.2, we have (here $u, \dot{u}$ are only symbols for the meanwhile)

$$\forall t \in [a,b] : u, \dot{u} \in \mathbb{R} : \frac{\partial F}{\partial u}(t, u, \dot{u}) = 0 \wedge \frac{\partial F}{\partial \dot{u}}(t, u, \dot{u}) = \frac{\dot{u}}{\sqrt{1 + \dot{u}^2}}.$$

At this point we have to substitute the actual uknown functions u and $\dot{u}$ evaluated at t into both expressions and compute the derivative with respect to t of the second expression. We get

$$\forall t \in [a,b] : \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial F}{\partial \dot{u}}(t, u(t), \dot{u}(t))\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\dot{u}(t)}{\sqrt{1 + \dot{u}(t)^2}}\right) = \frac{\ddot{u}(t)}{(1 + \dot{u}(t)^2)^{\frac{1}{2}}} - \frac{\dot{u}(t)^2\ddot{u}(t)}{(1 + \dot{u}(t)^2)^{\frac{3}{2}}} = \frac{\ddot{u}(t)}{(1 + \dot{u}(t)^2)^{\frac{3}{2}}},$$

so by theorem B.2.4 the Euler-Lagrange equation for u is

$$-\frac{\ddot{u}}{(1 + \dot{u}^2)^{\frac{3}{2}}} = 0$$

which is equivalent to $\ddot{u} = 0$, the solution being, as was expected, a linear function – a line.

Example B.2.6. To continue with example B.2.3, we can utilize the fact that, in this particular case, F does not explicitly depent on the first variable t. This means we can write (we omit the arguments of functions, as they stay the same throughout all calculations and should by this time be obvious)

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(F - \dot{u}\frac{\partial F}{\partial \dot{u}}\right) = \frac{\partial F}{\partial u}\dot{u} + \frac{\partial F}{\partial \dot{u}}\ddot{u} - \ddot{u}\frac{\partial F}{\partial \dot{u}} + \dot{u}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial \dot{u}} = \dot{u}\left(\frac{\partial F}{\partial u} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial \dot{u}}\right) = 0,$$

where the Euler-Lagrange equation was used in the last equality. Note that $\dot{u} = 0$ would also imply that equality, so one would have to check by plugging directly into the Euler-Lagrange equation whether that is a solution thereof.

Integrating the left-most and right-most side yields

$$F - \dot{u}\frac{\partial F}{\partial \dot{u}} = const := \lambda.$$

So in our specific case of $F = \sqrt{\frac{1+\dot{u}^2}{2gu}}$, $\frac{\partial F}{\partial \dot{u}} = \frac{\dot{u}}{\sqrt{2gu(1+\dot{u}^2)}}$ we get

$$\sqrt{\frac{1 + \dot{u}^2}{2gu}} - \frac{\dot{u}^2}{\sqrt{2gu(1 + \dot{u}^2)}} = \lambda \Leftrightarrow u(1 + \dot{u}^2) = \frac{1}{2g\lambda^2}.$$

We remind that although $u = \frac{1}{2g\lambda^2}$ is a solution of the equation above, it is not necessarily a solution to the Euler-Lagrange equation. In many cases, in fact, a constant solution would not even satisfy the boundary conditions.

Lastly we note that although in both examples we have obtained either an explicit solution or at least a differential equation for the solution. However, the Euler-Lagrange equations pose only a necessary condition for a minimiser of $\mathcal{I}$, thus we do not actually know if the function in example B.2.2 and any solution of equation derived in B.2.3 is an actual minimiser. We do know however, that any other function cannot be a minimiser of $\mathcal{I}$.

In order to show that a function is a minimiser of $\mathcal{I}$, we can again turn to the classical analysis of functions of one variable and use the sufficient condition for a minimum. It states that if a function f has a continuous derivative on some neighbourhood of $x \in \mathsf{D}(f)$, has a second derivative at x and satisfies

$$f'(x) = 0 \wedge f''(x) > 0,$$

then it achieves a local minimum a x.

Example B.2.7. Getting back to example B.2.2, we can readily prove that a linear function (that satisfies the boundary conditions, of course) is in fact a minimiser of the functional $\mathcal{I}$ from that example. We shall adopt a similar strategy as in the proof of B.2.4.

Let $v \in C_0^1([a,b]), v \neq 0$ and let u be a linear function such that $u \in \mathsf{D}(\mathcal{I})$, i.e. u satisfies the boundary conditions and the Euler-Lagrange equation for the functional from example B.2.2. We will plug $u + sv \in \mathsf{D}(\mathcal{I})$ into $\mathcal{I}$ and take the second derivative with respect to s at zero. Explicitly

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}s^2}\Big|_{s=0}\mathcal{I}[u+sv] &= \int_a^b \frac{\partial^2}{\partial s^2}\Big|_{s=0}\left(\sqrt{1+(\dot{u}(t)+s\dot{v}(t))^2}\right)\mathrm{d}t \\ &= \int_a^b \frac{\partial}{\partial s}\Big|_{s=0}\left(\frac{\dot{v}\dot{u}+s\dot{v}^2}{\sqrt{1+(\dot{u}+s\dot{v})^2}}\right)\mathrm{d}t = \int_a^b\left(\frac{\dot{v}^2}{\sqrt{1+\dot{u}^2}} - \frac{\dot{v}^2\dot{u}^2}{(1+\dot{u}^2)^{\frac{3}{2}}}\right)\mathrm{d}t \\ &= \int_a^b \frac{\dot{v}^2}{\sqrt{1+\dot{u}^2}}\left(1-\frac{\dot{u}^2}{1+\dot{u}^2}\right)\mathrm{d}t = \int_a^b \frac{\dot{v}(t)^2}{(1+\dot{u}(t)^2)^{\frac{3}{2}}}\mathrm{d}t > 0.\end{aligned}$$

(Throughout the calculation, we have written $\dot{v}$ instead of $\dot{v}(t)$ and the same for $\dot{u}$ for the sake of brevity.) The strictnes of the inequality comes from the fact that $\dot{v}$ cannot be zero, as that would imply v is constant, however, we have $v(a) = 0$ so v would be zero, which is a contradiction with the assumption that we have made at the very beginning.

Since u satisfies the Euler-Lagrange equations, we have that

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\mathcal{I}[u+sv] = 0,$$

as is obvious from the proof of B.2.4. One can check this by an explicit computation of the derivative and thereafter integrating by parts and using the fact that $\dot{u}$ is a constant and that v vanishes a the boundaries.

Because u is a unique solution to the Euler-Lagrange equation, we know that that the function $\mathcal{I}[u + sv]$ (as a function of s) has only one minimum, hence it must be a global one. Therefore we can write

$$\forall s \in \mathbb{R} : \forall v \in C_0^1([a,b]) : \mathcal{I}[u+sv] \geq \mathcal{I}[u].$$

Now let $w \in \mathsf{D}(\mathcal{I})$. We have $u - w \in C_0^1([a,b])$. Set $v := u - w$, $s := 1$ and the above then becomes

$$\forall w \in \mathsf{D}(\mathcal{I}) : \mathcal{I}[w] \geq \mathcal{I}[u],$$

so u is indeed a minimiser of $\mathcal{I}$.

B.3 Dirichlet's Principle

This section will present the Dirichlet's principle as stated in [3]. Thereafter we shall provide a modified version of the Dirichlet's principle, which is used in Chapter 1 that deals with the capacitance of a coaxial capacitor.

Henceforth in this section, let Λ denote an open bounded set such that its boundary $\partial\Lambda$ is a boundary of class C^1 and $g \in C^0(\partial\Lambda)$ and $f \in C^0(\Lambda)$. The functional $\mathcal{D}$ that we shall concern ourselves with shall be defined as follows.

$$\forall \phi \in \mathsf{D}(\mathcal{D}) : \mathcal{D}[\phi] := \int_\Lambda \left(\frac{1}{2}|\nabla\phi|^2 - \phi f\right),$$
$$\mathsf{D}(\mathcal{D}) := \{\phi \in C^2(\Lambda) \cap C^0(\overline{\Lambda}) : \phi\big|_{\partial\Lambda} = g\}.$$

Next we shall present a Dirichlet boundary condition problem, the Poisson equation with Dirichlet boundary condition, that will be later shown to be closely related to $\mathcal{D}$.

Definition B.3.1 (Poisson equation with Dirichlet boundary condition)**.** We say that $\phi \in C^2(\Lambda) \cap C^0(\overline{\Lambda})$ is a solution to the Poisson equation with Dirichlet boundary value g with the right side f, precisely when the function ϕ satisfies

$$\begin{cases} -\Delta\phi = f & \mathbf{x} \in \Lambda, \\ \phi = g & \mathbf{x} \in \partial\Lambda. \end{cases} \tag{B.2}$$

Theorem B.3.2. *There exists at most one solution $\psi \in C^2(\Lambda) \cap C^0(\overline{\Lambda})$ to the boundary problem (B.2).*

Proof. Assume that $\psi, \tilde{\psi} \in C^2(\Lambda) \cap C^0(\overline{\Lambda})$ are two solutions of of (B.2). Denote $w := \psi - \tilde{\psi}$. It follows that $\Delta w = 0$ and one can therefore write

$$0 = -\int_\Lambda w\Delta w = -\underbrace{\int_{\partial\Lambda} w\nabla w \cdot n}_{=0} + \int_\Lambda |\nabla w|^2,$$

where the second equality follows from integration by parts and Gauss theorem, n denotes the unit outer normal vector. The underbraced term is zero because $w\big|_{\partial\Lambda} = 0$. Hence $\nabla w = 0$ and $w\big|_{\partial\Lambda} = 0$ then implies

$$w = 0.$$

□

Theorem B.3.3 (Dirichlet's principle)**.** *Let $\psi \in C^2(\Lambda) \cap C^0(\overline{\Lambda})$ be a function such that it solves (B.2). Then*

$$\mathcal{D}[\psi] = \min_{\phi \in \mathsf{D}(\mathcal{D})} \mathcal{D}[\phi]. \tag{B.3}$$

Conversely, if ψ satisfies (B.3), then ψ is a solution to (B.2).

Proof. Firstly, we prove the first statement. Let $\phi \in \mathsf{D}(\mathcal{D})$. Then by (B.2) we can write

$$0 = \int_\Lambda (\psi - \phi)(-\Delta\psi - f) = -\int_\Lambda (\psi - \phi)\Delta\psi - \int_\Lambda (\psi - \phi)f,$$

since ψ solves (B.2). Integrating the first term by parts leads to

$$0 = -\underbrace{\int_{\partial\Lambda} (\psi - \phi)\nabla\psi \cdot n}_{=0} + \int_\Lambda \nabla(\psi - \phi) \cdot \nabla\psi - \int_\Lambda (\psi - \phi)f,$$

where n denotes the unit outer normal vector and the boundary term vanishes because $(\psi - \phi)\big|_{\partial\Lambda} = 0$. We can now rearrange to obtain

$$\int_\Lambda (|\nabla\psi|^2 - \psi f) = \int_\Lambda \nabla\phi \cdot \nabla\psi - \int_\Lambda \phi f.$$

Next, we shall use an upper bound estimate, a consequence of the Schwarz inequality along with a trivial inequality (that follows from $|\nabla\psi + \nabla\phi| \geq 0$), respectively, which combined reads

$$|\nabla\phi \cdot \nabla\psi| \leq |\nabla\phi||\nabla\psi| \leq \frac{1}{2}|\nabla\phi|^2 + \frac{1}{2}|\nabla\psi|^2.$$

Hence we can write

$$\int_\Lambda (|\nabla\psi|^2 - \psi f) = \int_\Lambda \nabla\phi \cdot \nabla\psi - \int_\Lambda \phi f \leq \int_\Lambda \frac{1}{2}|\nabla\phi|^2 + \int_\Lambda \frac{1}{2}|\nabla\psi|^2 - \int_\Lambda \phi f,$$

which can be rearranged to finally get

$$\mathcal{D}[\psi] \leq \mathcal{D}[\phi].$$

To prove the converse statement, we shall proceed using a variational method, analogous to that which was employed in the previous section.

Suppose (B.3) holds. Let $\eta \in C_0^2(\Lambda)$ and define $h : \mathbb{R} \to \mathbb{R}$ as

$$\forall s \in \mathbb{R} : h(s) := \mathcal{D}[\psi + s\eta].$$

Using (B.3) we get that h has a minimum at $s = 0$. If it were differentiable at 0, then we would have

$$h'(0) = 0.$$

Let us rewrite $h(s)$ for any $s \in \mathbb{R}$ using the definition of $\mathcal{D}$:

$$\begin{aligned} h(s) &= \int_\Lambda \left(\frac{1}{2}|\nabla\psi + s\nabla\eta|^2 - (\psi + s\eta)f\right) \\ &= \int_\Lambda \left(\frac{1}{2}|\nabla\psi|^2 - \psi f\right) + s\int_\Lambda (\nabla\psi \cdot \nabla\eta - \eta f) + \frac{s^2}{2}\int_\Lambda |\nabla\psi|^2. \end{aligned}$$

It can be seen that h is a polynomial, therefore it is differentiable. Taking its derivative evaluated at zero then yields

$$0 = h'(0) = \int_\Lambda (\nabla\psi \cdot \nabla\eta - \eta f) = \int_\Lambda (-\Delta\psi - f)\,\eta,$$

where integration by parts was employed to obtain the last equality, the boundary term vanished as a consequence of Gauss theorem and because η vanishes at the boundary.

Using the Fundamental lemma of the calculus of variations B.2.4.1 with regard to remark B.2.4.2 we get that $-\Delta\psi = f$, so ψ satisfies (B.3). □

Remark B.3.3.1. If we set $f = 0$ in the boundary value problem (B.2), it becomes the Laplace equation i.e., the equation for electrostatic potential in vacuum. The Dirichlet boundary condition then represents a requirement for a prescribed potential on the boundary.

The gradient of the electrostatic potential is defined to be the electric field $\mathbf{E}$ and its square $\mathbf{E}^2$ is the electrostatic energy per unit volume, the electrostatic energy density. This means that $\mathcal{D}[\phi]$ can be interpreted as the total electrostatic energy of the system with potential ϕ. The Dirichlet's principle then states that the potential that is realized in physical reality (as per equation (B.2)) is such that it minimizes the energy of the system.

Remark B.3.3.2. Throughout this section, we have assumed for simplicity that $\mathsf{D}(\mathcal{D})$ consists of twice differentiable functions. It can be shown, however, that if one extends the domain to the set $g + W_0^{1,2}(\Lambda)$, then a minimiser of $\mathcal{D}$ exists [3, thm. 4.3.1], moreover, such a minimiser is a solution to (B.2), but only in a weak sense.

We have formulated the Dirichlet's principle for the boundary problem (B.2), wherein only a Dirichlet boundary value is imposed. Sometimes, when dealing with mathematical models that involve unbounded domains of a periodic shape, it proves convenient to instead consider a bounded domain and a problem with periodic boundary conditions.

Such approach will be taken advantage of in Chapter 1. For this purpose, we can modify the Dirichlet's principle for such functions and problems.

Firstly, we shall define a bounded set that is suitable for imposing a periodic boundary condition.

Definition B.3.4. Let $L \in \mathbb{R}$, $\Omega \subset [-L, L] \times \mathbb{R}^2$ be a open bounded set. Denote

$$\omega(l) = \left\{ \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \in \mathbb{R}^2 : \begin{pmatrix} x_1 \\ x_2 \\ l \end{pmatrix} \in \Omega \right\} \quad \text{for } l \in \{-L, L\},$$

$$\Gamma = \partial\Omega \setminus (\omega(-L) \cup \omega(L)).$$

We will say that Ω is a *tube cell*, precisely when both of the following apply

(i) $\omega(-L) = \omega(L) \neq \emptyset$,

(ii) Γ is a boundary of class C^1.

The sets $\omega(-L) = \omega(L)$ and Γ shall be called the *connector* and *lateral surface* of Ω, respectively. The number L we refer to as the *extent* of Ω

Next, we shall define the set of admissible functions, i.e. the set of functions satisfying the boundary conditions. Since we are interested in problems with a guaranteed solution, we shall, with regard to remark B.3.3.2, formulate the following only in a weak sense, using the theory of Sobolev spaces.

Definition B.3.5. Let Ω be a tube cell of extent L and denote ω and Γ the connector and lateral surface thereof, respectively. Let $\phi \in W^{2,2}(\Omega)$ and $G \in C^0(\Gamma)$. We say that ϕ satisfies the *periodic boundary conditions* of Ω with respect to G and write $\phi \in \mathcal{A}_G^\Omega$ if, and only if,

$$\phi \restriction_\Gamma = G \quad \wedge \quad \left(\forall \mathbf{x}' \overset{a.e.}{\in} \omega : \phi(-L, \mathbf{x}') = \phi(L, \mathbf{x}') \wedge \phi_{,1}(-L, \mathbf{x}') = \phi_{,1}(L, \mathbf{x}') \right).$$

Theorem B.3.6. *Let Ω be a tube cell with lateral surface Γ and $G \in C^0(\Gamma)$. Moreover, let ψ be the solution to the following weak periodic and Dirichlet boundary condition problem:*

$$\forall \phi \in \mathcal{A}_0^\Omega : \langle \nabla\phi \,|\, \nabla\psi \rangle = 0 \quad \wedge \quad \psi \in \mathcal{A}_G^\Omega. \tag{B.4}$$

Then ψ also satisfies

$$\int_\Omega |\nabla\psi|^2 = \min_{\phi \in \mathcal{A}_G^\Omega} \int_\Omega |\nabla\phi|^2. \tag{B.5}$$

Also conversely, any $\psi \in \mathcal{A}_G^\Omega$ that is the minimiser in (B.5) is also a solution to the weak boundary value problem (B.4).

Remark B.3.6.1. We shall not prove this theorem, as the proof is completely analogous to the proof of theorem B.3.3 with the formal substitutions.

$$f \leftrightarrow 0, \quad \mathsf{D}(\mathcal{D}) \leftrightarrow \mathcal{A}_G^\Omega, \quad C_0^2(\Lambda) \leftrightarrow \mathcal{A}_0^\Omega, \quad \mathcal{D}[\cdot] \leftrightarrow \int_\Omega |\nabla \cdot|^2$$

We also note that the boundary integrals, that arise from integration by parts and use of the Gauss theorem, vanish as a consequence of the boundary conditions given by $\mathcal{A}_G^\Omega$ and $\mathcal{A}_0^\Omega$.

Remark B.3.6.2. As per the boundary conditions, we can write

$$\forall \psi \in \mathcal{A}_G^\Omega : \forall \phi \in \mathcal{A}_0^\Omega : \langle \nabla\phi \,|\, \nabla\psi \rangle = -\langle \phi \,|\, \Delta\psi \rangle.$$

Appendix C

Spectral Theory

C.1 Linear Operators

Definition C.1.1. Let $(\mathcal{H}, \langle \cdot \,|\, \cdot \rangle)$ be a Hilbert space over $\mathbb{C}$ and $D \subset\subset \mathcal{H}$. We shall call any linear map $A : D \to \mathcal{H}$ an *operator on* $\mathcal{H}$. Additionaly, we say that

(i) D is the domain of A, denoted $\mathsf{D}(A)$,

(ii) A is *bounded* $:\Leftrightarrow \exists C \in \mathbb{R}, C > 0 : \forall \psi \in \mathsf{D}(A) : \|A\psi\|^2 \leq C\|\psi\|^2$,

(iii) A is *densely defined* $:\Leftrightarrow \overline{\mathsf{D}(A)} = \mathcal{H}$,

(iv) A is *non-negative* $:\Leftrightarrow \forall \psi \in \mathsf{D}(A) : 0 \leq \langle \psi \,|\, A\psi \rangle \in \mathbb{R}$,

(v) A is *bounded from below* $:\Leftrightarrow \exists C \in \mathbb{R} : \forall \psi \in \mathsf{D}(A) : C\|\psi\|^2 \leq \langle \psi \,|\, A\psi \rangle \in \mathbb{R}$

(vi) A is *closed* $:\Leftrightarrow \forall \{\psi_n\}_{n=1}^{\infty} \subset \mathsf{D}(A), \psi, \phi \in \mathcal{H} : \ \big(\psi_n \to \psi \wedge A\psi_n \to \phi\big) \ \Rightarrow \ \big(\psi \in \mathsf{D}(A) \wedge \phi = A\psi\big)$.

Remark C.1.1.1. The map $A : D \to \mathcal{H}$ is linear if it satisfies

$$\forall \psi, \phi \in \mathsf{D}(A) : \forall \alpha \in \mathbb{C} : A(\psi + \alpha\phi) = A\psi + \alpha A\phi.$$

We see that this is only possible if $\mathsf{D}(A)$ is a subspace of $\mathcal{H}$.

Remark C.1.1.2. By $\|\cdot\|$ we denote the map $\mathcal{H} \to \mathbb{R} : \psi \mapsto \sqrt{\langle \psi \,|\, \psi \rangle}$, which is the norm induced by the scalar product $\langle \cdot \,|\, \cdot \rangle$.

Definition C.1.2. Let $(\mathcal{H}, \langle \cdot \,|\, \cdot \rangle)$ be a Hilbert space and A, B operators thereon. We say that the operator B is *adjoint* to the operator A $:\Leftrightarrow$

$$\begin{cases} \mathsf{D}(B) = \{\phi \in \mathcal{H} : (\exists \eta \in \mathcal{H} : \forall \psi \in \mathsf{D}(A) : \langle \phi \,|\, A\psi \rangle = \langle \eta \,|\, \psi \rangle)\}, \\ \forall \phi \in \mathsf{D}(B) : B\phi = \eta, \end{cases}$$

where η in the second row is the same one as in the definition of $\mathsf{D}(B)$.

Remark C.1.2.1. In view of the Riezs representation theorem (*cf.* [14, thm 4.5.1]), we have that every densely defined operator has a unique adjoint operator. This permits the use of notation, wherein for an arbitrary densely defined operator A, the adjoint operator is denoted $A^\star$. For some basic properties of adjoint operators further confer [14].

Definition C.1.3. Let A be an operator on $\mathcal{H}$. We say that A is *self-adjoint*, precisely when both of the following apply:

(i) A is densely defined

(ii) $A = A^\star$

Remark C.1.3.1. We note that for any self-adjoint operator A and a function $\psi \in \mathsf{D}(A)$ we have

$$\langle \psi \,|\, A\psi \rangle = \langle A^\star \psi \,|\, \psi \rangle = \langle A\psi \,|\, \psi \rangle = \overline{\langle \psi \,|\, A\psi \rangle}$$

and thus $\langle \psi \,|\, A\psi \rangle \in \mathbb{R}$.

Definition C.1.4. Let A be a closed operator on a Hilbert space $\mathcal{H}$. We define the *resolvent set* of A as

$$\rho(A) := \{\lambda \in \mathbb{C} : (A - \lambda I) \text{ is a bijection } \}$$

The *spectrum* of A is then defined as the complement of the resolvent set in $\mathbb{C}$, that is

$$\sigma(A) := \mathbb{C} \setminus \rho(A)$$

We shall also adopt a way of classifying the points in the spectrum, in particular, the notions of the *discrete* and *essential spectrum* (*cf.* [2, 4.1]).

Definition C.1.5. Let A be a closed self-adjoint operator on $\mathcal{H}$. We say that $\lambda \in \mathbb{C}$ is an *eigenvalue* of A precisely when the following applies:

$$\exists \psi \in \mathsf{D}(A) : A\psi = \lambda\psi.$$

We shall say that ψ is an *eigenfunction* corresponding to λ, furthermore, we shall call an eigenvalue λ *isolated*, if there exists a neighbourhood U of λ in $\mathbb{C}$ such that $U \cap \sigma(A) = \{\lambda\}$

Then the *discrete spectrum* of A can be defined as

$$\sigma_d(A) := \{\lambda \in \sigma(A) : \lambda \text{ is an isolated eigenvalue of } A \ \wedge \dim\ker(A - \lambda I) < \infty\}.$$

The complement of $\sigma_d(A)$ in $\sigma(A)$ will be called the *essential spectrum*:

$$\sigma_e(A) := \sigma(A) \setminus \sigma_d(A).$$

Remark C.1.5.1. Note that the definition of the spectrum implies:

$$\lambda \in \mathbb{C} \text{ is an eigenvalue of } A \Rightarrow \lambda \in \sigma(A).$$

Remark C.1.5.2. If $\lambda \in \mathbb{C}$ is an eigenvalue of A then the number $\dim\ker(A - \lambda I)$ is often called the *geometric multiplicity* of λ as it corresponds to the maximum number of possible linearly independent eigenfunctions corresponding to the eigenvalue λ.

The discrete spectrum thus has similar properties as in the case of finitely-dimensional operators.

C.2 Sesquilinear Forms

Definition C.2.1 (Sesquilinear and Quadratic forms)**.**
Let $\mathcal{H}$ be a Hilbert space over $\mathbb{C}$, $D \subset\subset \mathcal{H}$ and $h : D \times D \to \mathbb{C}$ satisfying:

(i) $\forall \alpha \in \mathbb{C}, \forall x, y, z \in D : h(\alpha x + y, z) = \overline{\alpha} h(x, z) + h(y, z)$

(ii) $\forall \beta \in \mathbb{C}, \forall x, y, z \in D : h(x, \beta y + z) = \beta h(x, y) + h(x, z)$

Then h shall be called a *sesquilinear form* on $\mathcal{H}$. We say that h is (i) antilinear in the first argument and (ii) linear in the second argument.

Now consider the natural map $[\cdot] : D \to D \times D : x \mapsto (x, x)$. We say that the composite map $q = h \circ [\cdot] : D \to \mathbb{C} : x \mapsto h(x, x)$ is a *quadratic form* associated to h and we write $h[x]$ instead of $(h \circ [\cdot])(x)$. Alternatively, we can call q the *diagonal* of h.

Remark C.2.1.1. For a sesquilinear form h on $\mathcal{H}$, we write $\mathsf{D}(h)$ to denote the set D from above. Note that the domain of h is actually $\mathsf{D}(h) \times \mathsf{D}(h)$, but we shall not need the domain itself, the set $\mathsf{D}(h)$ proves to be satisfactory when working with sesquilinear forms.

The definition of a quadratic form makes it apparent that given a sesquilinear form, the associated quadratic form is easily constructed. The next proposition will admit a converse construction, that is, a retrieval of a sesquilinear form from a quadratic one. Proof can be found in [9, I. 6].

Proposition C.2.2 (Polarization identity)**.**
Let h be a sesquilinear form on $\mathcal{H}$. Then we have

$$\forall x, y \in \mathsf{D}(h) : h(x, y) = \frac{1}{4}(h[x + y] - h[x - y] + i\, h[x - i\, y] - i\, h[x + i\, y])$$

In quantum mechanics and spectral theory, a particular class of sesquilinear forms is utilized more often than not, the class of symmetric sesquilinear forms.

Definition C.2.3 (Symmetric forms)**.**
A sesquilinear form h on $\mathcal{H}$ is said to be *symmetric* when it satisfies that
$\forall x, y \in \mathsf{D}(h) : h(x, y) = \overline{h(y, x)}$.

Proposition C.2.4 (Alternative definition of a symmetric form)**.**
A quadratic form h on $\mathcal{H}$ is symmetric if and only if

$$\forall \phi \in \mathsf{D}(h) : h[\phi] \in \mathbb{R}$$

Proof. The necessary condition follows from definition of symmetric form and the trivial implication

$$\forall z \in \mathbb{C} : z = \overline{z} \Rightarrow z \in \mathbb{R}$$

The sufficient condition is a consequence of the polarization identity. □

Definition C.2.5. Let $h, \tilde{h}$ be sesquilinear forms on $\mathcal{H}$. We say that

(i) h is *densely defined* $:\Leftrightarrow \overline{\mathsf{D}(h)} = \mathcal{H}$,

(ii) h is *bounded from below* $:\Leftrightarrow$ h is symmetric and $\exists C \in \mathbb{R} : \forall \psi \in \mathsf{D}(h) : h[\psi] \geq C\|\psi\|^2$

(iii) h is *closed* $:\Leftrightarrow \forall\{\psi_n\}_{n=1}^{\infty} \subset \mathsf{D}(h), \psi \in \mathsf{D}(h)$:

$$\left(\psi_n \xrightarrow{n} \psi \wedge h[\psi_m - \psi_n] \xrightarrow{m,n} 0\right) \quad \Rightarrow \quad \left(\psi \in \mathsf{D}(h) \wedge a[\psi_n - \psi] \xrightarrow{n} 0\right),$$

(iv) $\tilde{h}$ is an *extension* of $h :\Leftrightarrow (\mathsf{D}(h) \subset \mathsf{D}(\tilde{h}) \wedge \forall\phi \in \mathsf{D}(h) : h[\phi] = \tilde{h}[\phi])$,

(v) h is *closable* $:\Leftrightarrow$ a closed extension of h exists,

(vi) $\tilde{h}$ is a *closure* of $h :\Leftrightarrow h$ is closable and $\tilde{h}$ is defined as

$$\begin{cases} \mathsf{D}(\tilde{h}) := \{\psi \in \mathcal{H} : \exists\{\psi_n\}_{n=1}^{\infty} \subset \mathsf{D}(h) : \psi_n \xrightarrow{n} \psi \wedge h[\psi_m - \psi_n] \xrightarrow{m,n} 0\}, \\ \forall\psi \in \mathsf{D}(\tilde{h}) : \tilde{h}[\psi] := \lim_{n\to\infty} \psi_n, \end{cases}$$

where ψ_n in the second row is the same as in the definition of $\mathsf{D}(\tilde{h})$ from the first row.

C.3 Important Theorems

C.3.1 The Representation Theorem

Definition C.3.1. Let $\mathcal{H}$ be a Hilbert space and A, a an operator and a form thereon, respectively. We say that A is an operator *corresponding* to the form a, or equivalently, a is a form *corresponding* to the operator A, precisely when all of the following hold:

(i) $\mathsf{D}(A) \subset \mathsf{D}(a)$

(ii) $\forall\phi \in \mathsf{D}(a), \psi \in \mathsf{D}(A) : h(\phi, \psi) = \langle\phi\,|\,A\psi\rangle$.

The following theorem, proof of which can be found in [9, chapter VI, thm 2.6, 2.7] provides a connection between certain operators and sesquilinear forms, that will be useful to us in the future.

Theorem C.3.2. *Let t be a densely defined, closed, symmetric, sesquilinear form bounded from below. Then there exists a unique self-adjoint operator T bounded from below, corresponding to the form t.*

Also conversely, for any self-adjoint operator T bounded from below, there exists a unique densely defined, closed, symmetric sesquilinear form bounded from below, corresponding to the operator T. Moreover, such a form is a closure of a sesquilinear form t_0, defined as

$$\begin{cases} \mathsf{D}(T) = \mathsf{D}(t_0), \\ \forall\phi \in \mathsf{D}(t_0) : t_0[\phi] = \langle\phi\,|\,T\phi\rangle. \end{cases}$$

Remark C.3.2.1. Given the one-to-one correspondence between self-adjoint operators bounded from below and closed, symmetric, sesquilinear forms bounded from below, we shall utilize the notation

$$T \xleftrightarrow{1:1} t$$

which simply means that the above theorem is being used, either to retrieve a sesquilinear form from an operator, or vice versa.

C.3.2 The Minimax Theorem

The following theorem, proof of which can be found in [2, 4.5.1, 4.5.2], offers variational formulae for eigenvalues of non-negative, self-adjoint operators.

Theorem C.3.3. *Let A be a non-negative self-adjoint operator on $\mathcal{H}$. For any finitely-dimensional subspace $L \subset\subset \mathcal{H}$ define*

$$\lambda(L) := \sup\{\frac{\langle\psi\,|\,A\psi\rangle}{||\psi||^2} : \psi \in L \wedge \psi \neq 0\}$$

and then for any $n \in \mathbb{N}$ let λ_n be such that

$$\lambda_n := \inf\{\lambda(L) : L \subset\subset \mathcal{H} \wedge \dim L = n\}.$$

Then precisely one of the following holds:

(i) $\lambda_n \overset{n}{\to} \infty$. Then $\sigma_e(A) = \emptyset$ and $\sigma(A) = \sigma_d(A)$. The numbers λ_n (for all $n \in \mathbb{N}$) are then the eigenvalues of A, each repeated according to its multiplicity.

(ii) $\exists\lambda_\infty \in \mathbb{R} : (\forall m \in \mathbb{N} : \lambda_m < \lambda_\infty) \wedge \lambda_n \overset{n}{\to} \lambda_\infty$. Then λ_∞ is the smallest number in the essential spectrum of A and the part of spectrum of A in $[0, \lambda_\infty)$ consists of eigenvalues λ_n (for all $n \in \mathbb{N}$), each repeated according to its multiplicity.

(iii) $\exists\lambda_\infty \in \mathbb{R} : \exists N \in \mathbb{N} : \lambda_N < \lambda_\infty \wedge (\forall m \in \mathbb{N}, m > N : \lambda_m = \lambda_\infty)$. Then λ_∞ is the smallest number in the essential spectrum of A and the part of spectrum of A in $[0, \lambda_\infty)$ consists of eigenvalues $\lambda_1, \lambda_2, ..., \lambda_N$, each repeated according to its multiplicity.

Remark C.3.3.1. With regard to Remark C.1.3.1, we can see that $\sigma(A) \subset \mathbb{R}$ for any A defined as above.

Remark C.3.3.2. If we denote the form corresponding to A as a then one can reformulate the minimax theorem by setting

$$\lambda(L) := \sup\{\frac{a[\psi]}{||\psi||^2} : \psi \in L \wedge \psi \neq 0\}$$

and the statement will still hold (*cf.* [2, thm 4.5.3])

Corollary C.3.3.1. *Let A be as in the theorem above. Then*

$$\inf\sigma(A) = \inf\{\frac{\langle\psi\,|\,A\psi\rangle}{||\psi||^2} : \psi \in \mathsf{D}(A) \wedge \psi \neq 0\} = \inf\{\frac{a[\psi]}{||\psi||^2} : \psi \in \mathsf{D}(a) \wedge \psi \neq 0\} \geq 0$$

C.4 Sobolev Spaces

When dealing with partial differential equations and their weak forms, the notion of the L^2 spaces proves to be not entirely satisfactory. Instead, certain subspaces of L^2, equipped with a different norm, called Sobolev spaces, are more advantageous. Although Sobolev spaces are an important tool used in Chapter 2, we shall introduce them only in a concise manner without much circumambulation.

Firstly, we shall adopt the notion of a weak derivative, and to that end, multiindexes will be defined.

Definition C.4.1. Let $n \in \mathbb{N}$, $\alpha := (\alpha_1, ..., \alpha_n) \in \mathbb{N}^n$. We call α a *multiindex* and the number

$$|\alpha| := \sum_{i=1}^{n} \alpha_i$$

will be called the *order* of α.

Now let $k \in \mathbb{N}$, α be a multiindex of order k, $U \subset \mathbb{R}^n$, $\varphi \in C^k(U)$. We will use the following notation for partial derivatives:

$$D^\alpha \varphi := \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_n}}{\partial x_n^{\alpha_n}} \varphi$$

and say that $D^\alpha \varphi$ is the partial derivative of φ with respect to α.

Definition C.4.2. Let α be a multiindex, $U \subset \mathbb{R}^n$, $n \in \mathbb{N}$, $\psi, \eta \in L^1_{loc}(U)$. We say that η is the α-th *weak derivative* of ψ precisely when

$$\forall \varphi \in C_0^\infty(U) : \int_U \psi D^\alpha \varphi = (-1)^{|\alpha|} \int_U \eta \varphi.$$

We will write $D^\alpha \psi := \eta$.

Remark C.4.2.1. The motivation for this definition comes from the fact that for $\psi \in C^1(U)$ and $\varphi \in C_0^\infty(U)$ we can write, using integration by parts and Gauss theorem

$$\forall i \in \hat{n} : \int_U \psi \frac{\partial \varphi}{\partial x_i} = - \int_U \frac{\partial \psi}{\partial x_i} \varphi$$

and even so for higher derivatives, assuming ψ is differentiable enough. There is no boundary term, since φ vanishes at the boundary.

Remark C.4.2.2. The weak derivative retains many properties that of its usual (often called strong) counterpart. We shall not list them all here, for more details *cf.* [3, subsection 5.2.1].

Thereon in this subsection, let U be a domain in $\mathbb{R}^n, n \in \mathbb{N}$ and $k, p \in \mathbb{N}$.

Definition C.4.3. Let the Sobolev space $W^{k,p}(U)$ be defined as the set of all functions $\psi \in L^1_{loc}(U)$ such that for any multiindex α of order less than, or equal to k, $D^\alpha \psi$ exists in a weak sense and belongs to $L^p(U)$.

We shall endow the set $W^{k,p}(U)$ with the following norm:

$$\forall \psi \in W^{k,p}(U) : ||\psi||_{W^{k,p}(U)} := \left(\sum_{|\alpha| \leq k} ||D^\alpha \psi||^p_{L^p(U)} \right)^{\frac{1}{p}},$$

where the sum is being taken over the set of all multiindexes of order less than or equal to k.

Remark C.4.3.1. The set $L^1_{loc}(U)$ is the set of all functions, whose absolute value is integrable for each point in U on some neighbourhood of that point.

Remark C.4.3.2. It can be shown (*cf.* [3, thm 5.2.2]) that the space $(W^{k,p}(U), ||\psi||_{W^{k,p}(U)})$ is a Banach space, in particular, for $p = 2$ (we will make use of such Sobolev spaces later), it is a Hilbert space.

Definition C.4.4. We shall also define the set

$$W_0^{k,p}(U)$$

to be the closure of $C_0^\infty(U)$ in $W^{k,p}(U)$

Remark C.4.4.1. One can interpret the set $W_0^{k,p}(U)$ to contain functions that vanish on the boundary. This is not, however, true in a strict sense, as boundaries of functions from Sobolev spaces have to be understood in a sense of traces (*cf.* [3, section 5.5]). In this work, we shall not delve into the theory of traces, and only approach boundaries in an intuitive sense.

C.5 The Principal Eigenvalue of a Laplacian

For a closed operator A on $\mathcal{H}$, we shall call the smallest value of its discrete spectrum (if it indeed exists) the *principal* (or *first*) eigenvalue.

In this section, we will briefly deal with some properties of the principal eigenvalue of the Laplacian operator, in particular, its existence, simplicity (that is, its multiplicity being one) and existence of a positive eigenfunction. It is known (*cf.* [3, thm 6.5.2]), for example, that the Laplacian operator, defined such that it operates on functions whose domain is a bounded region and that vanish at the boundary (Dirichlet boundary condition) has a principal eigenvalue, it is indeed simple and the corresponding eigenfunction can be normed so that it is positive.

If one chooses a different boundary condition, e.g. the Neumann boundary condition, which is satisfied when a functions derivative at the boundary with respect to the outer normal of that boundary is zero, then boundedness requirement is not sufficient and one has to additionaly assume some regularity of the boundary.

It is also possible to impose the Dirichlet boundary condition on one part of the boundary and Neumann boundary condition on the complement part (this will be done in Chapter 2). Such boundary condition is sometimes called a mixed boundary condition. In [1], such case is treated in even broader generality and the following theorem is a simpler version of [1, thm 10, 12], combined with [2, cor 4.2.3]

Theorem C.5.1. *Let Ω be a bounded domain in $\mathbb{R}^n, n \in \mathbb{N}$, such that $\partial\Omega$ is a boundary of class C^2 and let $\Gamma_D, \Gamma_N \subset \partial\Omega, \Gamma_D = \partial\Omega \setminus \Gamma_N$. We define a sesquilinear form h as*

$$\begin{cases} \mathsf{D}(h) := \{\phi \in W^{1,2}(\Omega) : \phi \restriction_{\Gamma_D} = 0\}, \\ \forall \phi \in \mathsf{D}(h) : h[\phi] = \|\nabla\phi\|^2. \end{cases}$$

Then there exists a unique positive solution ψ of the mixed boundary condition problem

$$\begin{cases} \forall \phi \in \mathsf{D}(h) : h(\phi, \psi) = \lambda\langle\phi \,|\, \psi\rangle, \\ \psi \in W^{2,2}(\Omega) \wedge \psi \restriction_{\Gamma_D} = 0 \wedge \psi_{,n} \restriction_{\Gamma_N} = 0, \|\psi\|^2 = 1 \\ \lambda = \inf\{h[\phi] : \psi \in \mathsf{D}(h) \wedge \|\psi\|^2 = 1\}, \end{cases}$$

where $\psi_{,n}$ stands for the derivative of ψ with respect to the outer normal of the boundary Γ_N.

Moreover, if we denote the operator associated with h as H, then $\sigma(H) = \sigma_d(H)$ and there exists a complete orthonormal set in $L^2(\Omega)$, consisting of eigenfunctions of H.

Remark C.5.1.1. The form h is closely related to the Laplacian operator, as one can, using integration by parts, Gauss theorem and boundary conditions, show that

$$\forall \phi \in \mathsf{D}(h) : h(\phi, \psi) = \langle\nabla\phi \,|\, \nabla\psi\rangle = -\langle\phi \,|\, \Delta\psi\rangle$$

Remark C.5.1.2. The reason we have $\psi \in W^{2,2}(\Omega)$ instead of $\psi \in W^{1,2}(\Omega)$ is that we require the existence of a boundary normal derivative. In Sobolev spaces, the symbol $\psi_{,n} \restriction_{\Gamma_N}$ has to be understood in a sense of traces, otherwise it would be trivially true (*cf.* [3, thm 5.5.1]).

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