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ON CONVERGENCE IN ELLIPTIC SHAPE OPTIMIZATION*

KARSTEN EPPLER[†], HELMUT HARBRECHT[‡], AND REINHOLD SCHNEIDER[‡]

Abstract. The present paper aims at analyzing the existence and convergence of approximate solutions in shape optimization. Motivated by illustrative examples, an abstract setting of the underlying shape optimization problem is suggested, taking into account the so-called two norm discrepancy. A Ritz–Galerkin-type method is applied to solve the associated necessary condition. Existence and convergence of approximate solutions are proved, provided that the infinite dimensional shape problem admits a stable second order optimizer. The rate of convergence is confirmed by numerical results.

Key words. shape optimization, shape calculus, existence and convergence of approximate solutions, optimality conditions

AMS subject classifications. 49Q10, 49K20, 49M15, 65K10

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1. Introduction. Shape optimization is quite important for aircraft design, bridge construction, electromagnetic shaping, etc. Many problems that arise in applications, particularly in structural mechanics, can be formulated as the minimization of functionals defined over a class of admissible domains. Such problems have been intensively studied in the literature in the past 25–30 years (see [14, 33, 35, 44, 47] and the references therein). In the majority of papers, the undiscretized problem has been studied. Only a few papers deal with the convergence of approximate solutions to the solution of the original shape optimization problem. For example, in [6, 7, 8] the question of convergence is considered on the fully discretized level. Therein, a grid is fixed in advance on the hold all and the admissible shapes are allowed to vary only *on* this predefined grid. Consequently, a *discrete* optimization problem has to be solved next. Further investigations on convergence of approximate solutions have been reported in [33, 44].

In [18, 19, 20, 22, 23, 24, 25], we considered the numerical solution of several elliptic shape optimization problems. Boundary variations were used to derive boundary integral representations of the shape gradient and the shape Hessian. This approach allows the embedding of a shape problem into a Banach space by identifying the domain with the parametrization of its boundary, i.e., with a function. Solving the shape optimization problem becomes equivalent to finding the parametrization of the minimizing domain. We applied a Ritz–Galerkin-type method to approximate this parametrization. All ingredients of the shape gradient and Hessian that arise from the state equation were computed with sufficiently high accuracy by a fast wavelet boundary element method. In this way, the discretization of the shape is decoupled

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[†]Institute of Numerical Mathematics, TU Dresden, Zellescher Weg 12–14, 01069 Dresden, Germany (karsten.eppler@tu-dresden.de).

[‡]Institut für Informatik und Praktische Mathematik, Christian–Albrechts–Universität zu Kiel, Olshausenstr. 40, 24098 Kiel, Germany (hh@numerik.uni-kiel.de, rs@numerik.uni-kiel.de).

from the discretization of the state equation. Consequently, we may distinguish two types of errors.

First, the discretization error of the shape refers to the approximation error and determines the best possible rate of convergence. The present paper mainly tackles this issue by proving *existence* and *convergence* of approximate solutions. To this end, it is assumed that the objective, the constraints, and the state are given exactly.

Second, solving the state equation numerically induces a consistency error. Consistency errors are also caused by the approximate computation of the objective and constraints by, e.g., numerical quadrature. We present a Strang-type lemma to incorporate the error arising from numerical approximation. It gives a sufficient condition for realizing the best order of convergence.

When identifying the boundary of the regular $C^{k,\alpha}$-domain with its parametrization with respect to a fixed reference manifold $\widehat{\Gamma}$, a shape calculus based on boundary variational fields of prescribed smoothness leads to a second order Frechét calculus in a Banach space. For applications of interest, the space $C^{2,\alpha}(\widehat{\Gamma})$ for a certain $\alpha \in (0,1]$ is appropriate; cf. [15, 16, 17]. Since shape optimization problems are highly nonlinear, we are looking for domains that satisfy the first order necessary condition. These solutions are called stationary domains. To verify their local optimality, the second order Frechét derivative has to be coercive. However, for *integral objectives* in elliptic shape optimization it turns out that coercivity cannot be expected in the norm of the space of differentiation $C^{2,\alpha}(\widehat{\Gamma})$. Instead, coercivity of the shape Hessian at $\Omega^\star$ can be usually shown only in a *weaker* Sobolev space $H^s(\widehat{\Gamma})$. This *lack of coercivity* is known from other PDE-constrained optimal control problems as the so-called *two norm discrepancy*; cf. [4, 5, 28, 29]. The two norm discrepancy in shape optimization was first observed in [10, 11, 12, 15, 17]. It will play a key role in our convergence analysis.

Our investigations concentrate on the optimization of shapes and are not applicable to dealing with topological changes. Certainly, dealing with variable topologies is of enormous practical interest, and much important work has been done for the theoretical foundation and development of algorithms; see the monograph [3] for the state of the art. The so-called topological derivative has been addressed in [27, 31, 37, 39, 48, 49, 39] (we mention only some of the related papers). Related necessary optimality conditions for simultaneous shape and topology optimization have been investigated in [50], but the study of sufficient optimality conditions seems to be a challenging problem.

Concerning the present paper, section 2 is dedicated to a summary of second order shape calculus. Additionally, some examples are presented to illustrate the two norm discrepancy. First, we consider shape functionals based on a simple domain or boundary integral. Then, we treat PDE-constrained shape optimization problems by means of elliptic free boundary problems. In addition to the problem with simple constraints on the domain, we also discuss shape optimization problems subject to further functional constraints.

Motivated by these examples, we present in section 3 an abstract setting for the investigation of the second order sufficient optimality condition to verify stable minimizers. Then we introduce suitable trial spaces to discretize the shape optimization problem by means of a Ritz–Galerkin method for solving the necessary condition. The Ritz–Galerkin method solves a finite dimensional optimization problem that arises from restricting the class of admissible domains to domains given by the trial space. We show that there exist approximate solutions, provided that the level of discretization is sufficiently large, and prove convergence of the approximate solutions $\Omega_N^\star$ to

$\Omega^\star$, the optimal solution of the original infinite dimensional shape problem. The approximate solution behaves like the best approximation in the trial space to $\Omega^\star$, with respect to the natural space of coercivity of the shape Hessian. Therefore, the computation of the rate of convergence is along the lines of conventional approximation theory.

In section 4, we present two numerical examples that confirm our analysis. The first one is a simple shape problem based on a domain integral minimization, which is mainly incorporated for illustration. The second is a more advanced PDE-constrained shape optimization problem, with several additional functional constraints. Both examples are chosen such that the optimal domain is known a priori. We observe rates of convergence which verify the present theory.

2. Motivation and background.

2.1. Shape calculus. Shape optimization is concerned with the minimization of the shape functional

$$J(\Omega) = \int_\Omega j(u, \nabla u, \mathbf{x}) d\mathbf{x} \to \min, \qquad \Omega \in \Upsilon, \tag{2.1}$$

where Υ is a suitable class of admissible domains $\Omega \in \mathbb{R}^n$. The so-called *state* u satisfies an abstract boundary value problem

$$\mathcal{A}u = f \text{ in } \Omega, \qquad \mathcal{B}u = g \text{ on } \Gamma, \tag{2.2}$$

where $\mathcal{A}$ corresponds to a well-posed elliptic partial differential operator in the domain Ω, and $\mathcal{B}$ operates on the functions supported at the free boundary $\Gamma \subset \partial\Omega$. For the sake of simplicity, we restrict ourselves to finding solutions with known topology and assume that all involved functions and data are sufficiently smooth.

Generally, problem (2.1) is highly implicit, with respect to the shape of the domain, and has to be solved iteratively. The canonical way to solve the minimization problem is to determine its stationary points. Then, via the second order optimality condition, regular minimizers of second order are verified. To this end, we will briefly survey shape calculus. In particular, we refer the reader to Murat and Simon [38], Simon [46], Pironneau [44], Sokołowski and Zolésio [47], Delfour and Zolésio [14], and the references therein. Herein, two basic concepts are considered, namely, the perturbation of identity (Murat and Simon) and the speed method (Sokołowski and Zolésio).

For example, the perturbation of identity exploits a smooth perturbation field $\mathbf{U} : \Omega \to \mathbb{R}^n$ and defines the standard domain perturbation as

$$\Omega_\varepsilon[\mathbf{U}] := \{(\mathbf{I} + \varepsilon\mathbf{U})(\mathbf{x}) : \mathbf{x} \in \Omega\}.$$

Then the directional derivative of $J(\Omega)$ is computed as

$$\nabla J(\Omega)[\mathbf{U}] := \lim_{\varepsilon \to 0} \frac{J(\Omega_\varepsilon[\mathbf{U}]) - J(\Omega)}{\varepsilon}.$$

Ever since Hadamard [32] it has been known that $\nabla J(\Omega)[\mathbf{U}]$ is a distribution living only on the free boundary of the domain Ω, provided that $J(\Omega)$ is shape differentiable; see also [13].

The latter observation leads to the idea of considering only boundary variations for the update in the optimization algorithm. Therefore, we shall directly apply boundary variations for the computation of the boundary integral representations of the shape gradient and Hessian. To this end, we introduce a reference manifold $\widehat{\Gamma} \subset \mathbb{R}^n$ and consider a fixed boundary perturbation field, for example, in the direction of the outer normal $\widehat{\mathbf{n}}$. We suppose that the free boundary of each domain $\Omega \in \Upsilon$ can be parametrized via a sufficiently smooth function r in terms of

$$\boldsymbol{\gamma} : \widehat{\Gamma} \to \Gamma, \quad \boldsymbol{\gamma}(\mathbf{x}) = \mathbf{x} + r(\mathbf{x})\widehat{\mathbf{n}}(\mathbf{x}).$$

That is, we can identify a domain with the scalar function r. Defining the standard variation

$$\boldsymbol{\gamma}_\varepsilon : \widehat{\Gamma} \to \Gamma_\varepsilon, \quad \boldsymbol{\gamma}_\varepsilon(\mathbf{x}) := \boldsymbol{\gamma}(\mathbf{x}) + \varepsilon dr(\mathbf{x})\widehat{\mathbf{n}}(\mathbf{x}),$$

where dr is again a sufficiently smooth scalar function, we obtain the perturbed domain Ω_ε. Consequently both the shape and its increment can be seen as elements of a Banach space X. We will specify the notion of "sufficiently smooth" in the next subsections.

2.2. Optimization of domain or boundary integrals. First, we introduce some notation. For a given domain $D \in \mathbb{R}^n$, the space $C^2(\overline{D})$ consists of all two times continuously differentiable functions $f : \overline{D} \to \mathbb{R}^m$. A function $f \in C^2(\overline{D})$ belongs to $C^{2,\alpha}(\overline{D})$ if the (spatial) Hessian $\nabla^2 f$ is Hölder continuous with coefficient $0 < \alpha \leq 1$. A domain $D \in \mathbb{R}^n$ is of class $C^{2,\alpha}$ if for each $\mathbf{x} \in \partial D$ a neighborhood $U(\mathbf{x}) \subseteq \partial\Omega$ and a diffeomorphism $\boldsymbol{\gamma} : [0,1]^{n-1} \to \overline{U(\mathbf{x})}$ exist such that $\boldsymbol{\gamma} \in C^{2,\alpha}([0,1]^{n-1})$; see [52], for example.

For the sake of clearness, we present here two elementary shape problems, since both the shape calculus and the analysis become much more evident in comparison with the more advanced shape optimization problems presented in the subsequent subsections. To this end, let $n = 2$, $\Omega \in C^1$, and consider the following shape optimization problem of domain integral type:

$$J(\Omega) = \int_\Omega h(\mathbf{x})d\mathbf{x} \to \min, \tag{2.3}$$

where $h \in C^1(\mathbb{R}^2)$ are given data. We choose the class of admissible domains as the set of all domains that are star-shaped with respect to the origin. Then we can choose $\widehat{\Gamma}$ as the unit circle. Equivalently, we can parametrize $\Gamma = \partial\Omega$ via polar coordinates

$$\Gamma := \left\{ \boldsymbol{\gamma}(\phi) = r(\phi)\left[\begin{smallmatrix}\cos\phi\\ \sin\phi\end{smallmatrix}\right] : \phi \in [0, 2\pi] \right\},$$

where $r \in C^1_{\text{per}}([0,2\pi])$ is a positive function. Here and in what follows, the space $C^{k,\alpha}_{\text{per}}$ is defined as

$$C^{k,\alpha}_{\text{per}}([0,2\pi]) = \{ f \in C^{k,\alpha}([0,2\pi]) : f^{(i)}(0) = f^{(i)}(2\pi) \text{ for all } i = 0,\dots,k \},$$

and likewise $C^k_{\text{per}}([0,2\pi])$. Let us further remark that the tangent and the outward normal at Γ are computed by

$$\mathbf{t} = \frac{r'\left[\begin{smallmatrix}\cos\phi\\ \sin\phi\end{smallmatrix}\right] + r\left[\begin{smallmatrix}-\sin\phi\\ \cos\phi\end{smallmatrix}\right]}{\sqrt{r^2 + r'^2}}, \qquad \mathbf{n} = \frac{r'\left[\begin{smallmatrix}\sin\phi\\ -\cos\phi\end{smallmatrix}\right] + r\left[\begin{smallmatrix}\cos\phi\\ \sin\phi\end{smallmatrix}\right]}{\sqrt{r^2 + r'^2}}. \tag{2.4}$$

We consider $dr \in C^1_{\text{per}}([0,2\pi])$ as a standard variation for perturbed domains Ω_ε, respectively, boundaries Γ_ε, defined by $r_\varepsilon(\phi) = r(\phi) + \varepsilon dr(\phi)$, where $\boldsymbol{\gamma}_\varepsilon(\phi) = r_\varepsilon(\phi)\widehat{\mathbf{n}}(\phi)$

is always a Jordan curve. Herein, $\widehat{\mathbf{n}}(\phi) = [\cos\phi, \sin\phi]^T$ denotes the outward normal vector to the reference manifold $\widehat{\Gamma}$.

LEMMA 2.1 (see [16]). *The shape functional from* (2.3) *is twice Frechét differentiable with respect to* $C^1_{\mathrm{per}}([0,2\pi])$*, where the shape gradient and Hessian read as*

$$\nabla J(\Omega)[dr] = \int_0^{2\pi} r(\phi)dr(\phi)h\big(r(\phi),\phi\big)d\phi,$$

$$\nabla^2 J(\Omega)[dr_1, dr_2] = \int_0^{2\pi} dr_1(\phi)dr_2(\phi)\left\{h\big(r(\phi),\phi\big) + r(\phi)\frac{\partial h}{\partial \widehat{\mathbf{n}}}\big(r(\phi),\phi\big)\right\}d\phi.$$

Consider now a stationary domain $\Omega^\star$, which means $\nabla J(\Omega^\star)[dr] = 0$ for all $dr \in C^1([0,2\pi])$. Of course, the latter equation implies that $h|_{\Gamma^\star} \equiv 0$. Hence, as one readily verifies, it holds that

$$\nabla^2 J(\Omega^\star)[dr_1, dr_2] = \int_0^{2\pi} dr_1(\phi)dr_2(\phi)\left\{\frac{r^{\star 2}(\phi)}{\sqrt{r^{\star 2}(\phi) + r^{\star\prime 2}(\phi)}}\frac{\partial h}{\partial \mathbf{n}}\big(r^\star(\phi),\phi\big)\right\}d\phi.$$

Optimality usually can be guaranteed by coercivity of the second order Frechét derivative. However, it is impossible to realize coercivity with respect to $C^1_{\mathrm{per}}([0,2\pi])$; only an estimate

$$\nabla^2 J(\Omega^\star)[dr, dr] \geq c_E \|dr\|^2_{L^2([0,2\pi])}$$

for some $c_E > 0$ can be expected. Note that we have such an estimate if $(\partial h/\partial \mathbf{n})|_{\Gamma^\star} \geq c_E > 0$. This lack of regularity is known from other control problems as the so-called *two norm discrepancy*. Nevertheless, the bilinear form imposed by the shape Hessian $\nabla^2 J(\Omega)$ is obviously also continuous on $L^2([0,2\pi]) \times L^2([0,2\pi])$, that is,

$$|\nabla^2 J(\Omega)[dr_1, dr_2]| \leq c_S(\Omega)\|dr_1\|_{L^2([0,2\pi])}\|dr_2\|_{L^2([0,2\pi])}$$

for all $dr_1, dr_2 \in L^2([0,2\pi])$. Notice that it is generally impossible to extend the domain of definition $C^1([0,2\pi])$ to $L^2([0,2\pi])$. In other words, J is only densely defined with respect to $L^2([0,2\pi])$.

Also, in the case of a shape optimization problem of boundary integral type

$$J(\Omega) = \int_\Gamma g(\mathbf{x})d\sigma \to \min, \tag{2.5}$$

where $g \in C^2(\mathbb{R}^2)$ are given data, one makes the above observations concerning the coercivity. Similarly to above, coercivity cannot be realized in $C^1_{\mathrm{per}}([0,2\pi])$. The energy space of the bilinear form imposed by the shape Hessian $\nabla^2 J(\Omega)$ is the Sobolev space $H^1_{\mathrm{per}}([0,2\pi])$; see [16] for details.

2.3. PDE-constrained shape optimization problems. We shall consider free elliptic boundary problems as the most illustrative model problem for PDE-constrained shape optimization problems. Let $T \subset \mathbb{R}^n$ denote a bounded domain with boundary $\partial T = \Gamma$. Inside the domain T we assume the existence of a simply connected subdomain $S \subset T$ with fixed boundary $\partial S = \Sigma$. We denote the annular domain $T \setminus \overline{S}$ by Ω; see also Figure 2.1.

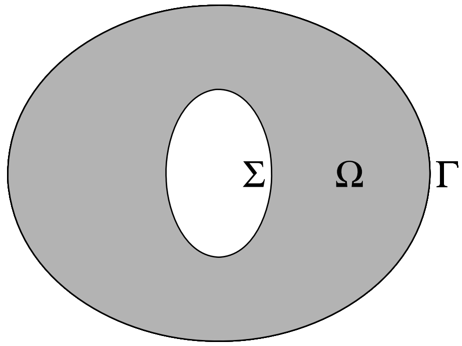

FIG. 2.1. *The domain Ω and its boundaries Γ and Σ.*

We consider the following overdetermined boundary value problem in the annular domain Ω:

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ \|\nabla u\| &= g && \text{on } \Gamma, \\ u &= 0 && \text{on } \Gamma, \\ u &= h && \text{on } \Sigma, \end{aligned} \tag{2.6}$$

where $f \geq 0$ and $g, h > 0$ are sufficiently smooth functions such that the shape differentiability of the objective (2.7) is provided up to second order. We like to stress that the positivity of the data implies that u is positive in Ω. Hence, there holds the identity

$$\|\nabla u\| \equiv -\frac{\partial u}{\partial \mathbf{n}} \qquad \text{on } \Gamma$$

since u admits homogeneous Dirichlet data on Γ.

We arrive at a free boundary problem if the boundary Γ is the unknown. In other words, we seek a domain Ω with fixed boundary Σ and unknown boundary Γ such that the overdetermined boundary value problem (2.6) is solvable. For the existence of solutions we refer the reader to, e.g., [1, 26].

Shape optimization provides an efficient tool for solving such free boundary value problems; cf. [14, 34, 47, 51]. Considering the cost functional

$$J(\Omega) = \int_\Omega \|\nabla u\|^2 - 2fu + g^2 d\mathbf{x} \tag{2.7}$$

with underlying *state equation*

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ u &= 0 && \text{on } \Gamma, \\ u &= h && \text{on } \Sigma, \end{aligned} \tag{2.8}$$

the solution of the free boundary problem is equivalent to the shape optimization problem

$$J(\Omega) \to \min. \tag{2.9}$$

This issues from the necessary condition of a minimizer to the cost functional (2.7); that is,

$$\nabla J(\Omega)[\mathbf{U}] = \int_\Gamma \langle \mathbf{U}, \mathbf{n}\rangle \left\{ g^2 - \left[\frac{\partial u}{\partial \mathbf{n}}\right]^2 \right\} d\sigma = 0 \tag{2.10}$$

has to be valid for all sufficiently smooth perturbation fields $\mathbf{U}$. Hence, shape optimization induces a variational formulation of the condition

$$\frac{\partial u}{\partial \mathbf{n}} = -g \qquad \text{on } \Gamma. \tag{2.11}$$

However, a stationary domain $\Omega^\star$ of the minimization problem (2.7), (2.8) will be a stable minimum if and only if the shape Hessian is strictly $H^{1/2}([0, 2\pi])$-coercive at this domain (see below).

It suffices to consider $S \in C^{0,1}$, but due to a second order boundary perturbation calculus, we have to assume $T \in C^{2,\alpha}$ for some fixed $\alpha \in (0, 1)$. We assume, similarly to the previous subsection, that the domain T is star-shaped with respect to $\mathbf{0}$, and we apply the same shape calculus. The shape gradient of the cost functional in (2.7) becomes, in polar coordinates,

$$\langle \nabla J(\Omega), dr\rangle = \int_0^{2\pi} dr\, r \left\{ g^2 - \left[\frac{\partial u}{\partial \mathbf{n}}\right]^2 \right\} d\phi. \tag{2.12}$$

According to [15, 16] the shape Hessian reads as

$$\begin{aligned}\langle \nabla^2 J(\Omega)\cdot dr_1, dr_2\rangle = \int_0^{2\pi} & dr_1 dr_2 \left\{ g^2 - \left[\frac{\partial u}{\partial \mathbf{n}}\right]^2 + 2rg\langle \nabla g, \widehat{\mathbf{n}}\rangle \right. \\ & \left. - \frac{2r}{\sqrt{r^2 + r'^2}} \frac{\partial u}{\partial \mathbf{n}} \left[r\frac{\partial^2 u}{\partial \mathbf{n}^2} + r' \frac{\partial^2 u}{\partial \mathbf{n}\partial \mathbf{t}}\right] \right\} - 2r\, dr_1 \frac{\partial u}{\partial \mathbf{n}} \cdot \frac{\partial du[dr_2]}{\partial \mathbf{n}} d\phi.\end{aligned} \tag{2.13}$$

Herein, the *local shape derivative* $du = du[dr_2]$ of the state function satisfies

$$\begin{aligned} \Delta du &= 0 && \text{in } \Omega,\\ du &= 0 && \text{on } \Sigma,\\ du &= -dr_2 \langle \widehat{\mathbf{n}}, \mathbf{n}\rangle \tfrac{\partial u}{\partial \mathbf{n}} && \text{on } \Gamma. \end{aligned} \tag{2.14}$$

Notice that $\partial^2 u/\partial \mathbf{n}^2 := \langle \nabla^2 u \cdot \mathbf{n}, \mathbf{n}\rangle$ and $\partial^2 u/(\partial\mathbf{n}\partial\mathbf{t}) := \langle \nabla^2 u\cdot \mathbf{n}, \mathbf{t}\rangle$.

LEMMA 2.2 (see [15, 25]). *The shape Hessian $\nabla^2 J(\Omega)$ defines a continuous bilinear form on $H^{1/2}([0, 2\pi]) \times H^{1/2}([0, 2\pi])$; that is, there exists a constant $c_S(\Omega)$ depending only on the actual domain Ω such that*

$$|\nabla^2 J(\Omega)[dr_1, dr_2]| \le c_S(\Omega)\|dr_1\|_{H^{1/2}([0,2\pi])}\|dr_2\|_{H^{1/2}([0,2\pi])}.$$

In accordance with this lemma, we observe that the shape Hessian is a pseudodifferential operator of order one, i.e., $\nabla^2 J(\Omega) : H^{1/2}([0, 2\pi]) \to H^{-1/2}([0, 2\pi])$. In particular the last term in (2.13) implies that the shape Hessian is a nonlocal operator.

According to [25] the following sufficient criterion concerning the $H^{1/2}([0, 2\pi])$-coercivity holds.

LEMMA 2.3. *The shape Hessian $\nabla^2 J(\Omega^\star)$ is $H^{1/2}([0, 2\pi])$-coercive; that is, there exists a constant $c_E > 0$ such that*

$$\nabla^2 J(\Omega^\star)[dr, dr] \ge c_E\|dr\|^2_{H^{1/2}([0,2\pi])}$$

if

$$\kappa + \left[\frac{\partial g}{\partial \mathbf{n}} - f\right] \Big/ g \geq 0 \qquad \text{on } \Gamma^\star.$$

In particular, in the case when $f \equiv 0$ and $g \equiv$ const., the shape Hessian is $H^{1/2}([0,2\pi])$-coercive if the boundary $\Gamma^\star$ is convex (seen from inside).

The problem under consideration can be viewed as the prototype of a free boundary problem arising in many applications. For example, the growth of anodes in electrochemical processing might be modeled as above with $f \equiv 0$ and $g, h \equiv 1$.

In the two-dimensional exterior magnetic shaping of liquid metals, the state equation is an exterior Poisson equation and the uniqueness is ensured by a volume constraint of the domain Ω [9, 20, 41, 43]; see also the following subsection. However, since the shape functional involves the perimeter, which corresponds to the surface tension of the liquid, the energy space of the shape Hessian will be $H^1([0,2\pi])$.

The detection of voids or inclusions in two- or three-dimensional electrical impedance tomography is slightly different since the roles of Σ and Γ are interchanged [23, 24, 45]. Particularly, this inverse problem is severely ill-posed, in contrast to the present class of problems. It has been proven in [23] that the shape Hessian is *not* strictly coercive in any $H^s([0,2\pi])$ for all $s \in \mathbb{R}$.

2.4. Shape problems with additional functional constraints. We consider the following shape optimization problem:

$$J(\Omega) = \int_\Omega j(u, \nabla u, \mathbf{x}) d\mathbf{x} \to \min,$$

subject to L domain or boundary integral equality constraints

$$\begin{aligned} J_i(\Omega) &= \int_\Omega h_i(\mathbf{x}) d\mathbf{x} = c_i, \quad 1 \leq i \leq K, \\ J_i(\Omega) &= \int_\Gamma g_i(\mathbf{x}) d\sigma = c_i, \quad K < i \leq L. \end{aligned}$$

We suppose that all functionals J and J_i, $1 \leq i \leq L$, are twice Frechét differentiable in a certain Banach space X. Moreover, let the Sobolev space H^s denote the strongest energy space of the bilinear forms imposed by the shape Hessians of *all* the above shape functionals.

Along the lines of standard optimization theory, one considers the free minimization of the Lagrangian

$$L(\Omega, \lambda_1, \ldots, \lambda_L) := J(\Omega) + \sum_{i=1}^{L} \lambda_i \big(J_i(\Omega) - c_i\big)$$

if Kuhn–Tucker regularity is provided. Hence, it is well known that the necessary and sufficient optimality condition for a regular local optimal shape $\Omega^\star$ reads as

LEMMA 2.4. *Let $\Omega^\star \in X$ satisfy*

$$\nabla L(\Omega^\star, \lambda_1^\star, \ldots, \lambda_L^\star)[dr] = 0 \quad \text{for all } dr \in X$$

for certain $\lambda_i^\star \in \mathbb{R}$. Moreover, define the linearizing cone

$$Y := \{dr \in X : \nabla J_i(\Omega^\star)[dr] = 0 \text{ for all } 1 \leq i \leq L\} \subset X,$$

and assume the linear independence of all gradients $\nabla J_i(\Omega^\star)$ at $\Omega^\star$.

Then $\Omega^\star$ is a regular local minimizer of second order if and only if the following coercivity condition is satisfied:

$$\nabla^2 L(\Omega^\star, \lambda_1^\star, \dots, \lambda_L^\star)[dr, dr] \geq c_E \|dr\|_{H^s}^2 \quad \textit{for all } dr \in Y.$$

Here, the techniques of the proof from [17, subsection 4.3] remain directly applicable, including the case of integral constraints that depend again on a PDE solution.

Remark 2.5. The linear independent constraint qualification (LICQ) implies in particular that the (vector valued) gradient of the constraints is a mapping onto $\mathbb{R}^L$. Hence, Y is a closed subspace of X of finite codimension L.

Consequently, the general concept developed in section 3 keeps applicable with respect to the Banach space Y. We mention that the treatment of inequality constraints is obvious and related modifications are well established in theory.

3. Approximation theory in shape optimization.

3.1. Assumptions on the optimization problem. Let us first introduce the abstract setting needed for our theory. To this end, let X denote a Banach space, where we shall denote the ball $\{h \in X : \|r - h\|_X < \delta\}$ by $B_\delta^X(r)$.

We consider the following optimization problem in the Banach space X:

$$(P) \qquad J(r) \to \min, \qquad r \in X.$$

Herein, $J : X \mapsto \mathbb{R}$ defines a two times continuously differentiable functional; i.e., the gradient $\nabla J(r) \in X^\star$ as well as the Hessian $\nabla^2 J(r) \in L(X, X^\star)$ exist for all $r \in X$, and the mappings $\nabla J(\cdot) : X \to X^\star$, $\nabla J^2(\cdot) : X \to L(X, X^\star)$ are continuous.

We assume that the necessary first order optimality condition holds in $r^\star$:

$$\text{(A1)} \qquad \nabla J(r^\star)[dr] = 0 \qquad \text{for all } dr \in X.$$

As illustrated in the previous section, we have to take the two norm discrepancy into account; i.e., the coercivity estimate holds only in a weaker Sobolev space $H^s \supset X$, $s \geq 0$. Therefore, we shall assume that there is a constant $c_S > 0$, depending *continuously* on the actual variable r, such that the continuous bilinear form imposed by the shape Hessian on $X \times X$ extends continuously to a bilinear form on $H^s \times H^s$, i.e.,

$$\text{(A2)} \qquad |\nabla^2 J(r)[h_1, h_2]| \leq c_S(r) \|h_1\|_{H^s} \|h_2\|_{H^s} \quad \text{for all } h_1, h_2 \in H^s,$$

if $r \in \overline{B_\delta^X(r^\star)}$. Of course, there exists an absolute constant C_S, defined by

$$(3.1) \qquad C_S := \max\left\{c_S(r) : r \in \overline{B_\delta^X(r^\star)}\right\},$$

such that $c_S(r) \leq C_S$ for all $r \in \overline{B_\delta^X(r^\star)}$. Moreover, we assume that $\nabla^2 J$ is strongly coercive at $r^\star$, that is,

$$\text{(A3)} \qquad \nabla^2 J(r^\star)[h, h] \geq c_E \|h\|_{H^s}^2 \quad \text{for all } h \in H^s$$

for some $c_E > 0$.

Remark 3.1. The existence of a continuous extension for the objective J from X to H^s is not assumed throughout this paper since this is, in general, not realistic for shape problems; cf. subsection 2.2. That is, J remains only “densely defined” with respect to H^s; this holds similarly for ∇J, $\nabla^2 J$. As it turns out, by our investigations a complete convergence analysis is possible without assuming a continuation property.

As a first consequence of our assumptions we have the following lemma concerning Lipschitz continuity of the shape gradient with respect to the topology that is induced by the coercivity space of the shape Hessian.

LEMMA 3.2. *The gradient is locally Lipschitz as a mapping in the* (H^{-s}, H^s)-*duality* $(H^{-s} := (H^s)')$, *that is,*

$$\|\nabla J(r+h) - \nabla J(r)\|_{H^{-s}} \leq C_S \|h\|_{H^s} \tag{3.2}$$

for all $r, r+h \in \overline{B_\delta^X(r^\star)}$. *Herein, the constant* C_S *is given by* (3.1).

Proof. The assertion follows immediately from the following estimate:

$$|\nabla J(r+h)[dr] - \nabla J(r)[dr]| = \left| \int_0^1 \langle \nabla^2 J(r+th) \cdot h, dr \rangle dt \right| \leq C_S \|h\|_{H^s} \|dr\|_{H^s}$$

for all $r, r+h \in \overline{B_\delta^X(r^\star)}$, and $dr \in H^s$. ◻

Notice that the twice differentiability of J provides only the Lipschitz continuity of the shape gradient in the $(X^\star, X)$-duality, i.e.,

$$\|\nabla J(r+h) - \nabla J(r)\|_{X^\star} \leq C_S \|h\|_X$$

for all $r, r+h \in \overline{B_\delta^X(r^\star)}$.

3.2. Sufficient conditions. The above assumptions allow the following statement on the regular local optimality of second order of $r^\star$. Although this is rather standard, we recall it for convenience.

THEOREM 3.3 (sufficient second order optimality condition). *Let the necessary condition* (A1) *hold for a certain* $r^\star \in X$. *For all* $r \in \overline{B_\delta^X(r^\star)}$ *suppose that the bilinear form imposed by the shape Hessian satisfies* (A2) *and the following remainder estimate:*

$$\begin{aligned} &|\nabla^2 J(r)[h_1, h_2] - \nabla^2 J(r^\star)[h_1, h_2]| \\ &\qquad \leq \eta(\|r - r^\star\|_X) \|h_1\|_{H^s} \|h_2\|_{H^s} \quad \textit{for all } h_1, h_2 \in H^s, \end{aligned} \tag{A4}$$

where $\eta : \mathbb{R}_0^+ \to \mathbb{R}_0^+$ *is a decreasing function that satisfies* $\eta(t) \to 0$ *as* $t \to 0$. *Then, the domain* $r^\star$ *is a strong regular local optimum of second order with respect to certain constants* $\widehat{c}_E > 0$,

$$J(r) - J(r^\star) \geq \widehat{c}_E \|r - r^\star\|_{H^s}^2 \quad \textit{for all } r \in \overline{B_{\widehat{\delta}}^X(r^\star)}, \tag{3.3}$$

if and only if the shape Hessian satisfies the strong coercivity estimate (A3).

Proof. For all $r = r^\star + h \in \overline{B_\delta^X(r^\star)}$ the following Taylor expansion holds:

$$J(r) - J(r^\star) = 0 + \frac{1}{2} \nabla^2 J(r^\star + \xi h)[h, h], \quad \xi \in (0, 1).$$

According to (A3) and (A4), one infers on the one hand,

$$\begin{aligned} J(r) - J(r^\star) &\geq \frac{1}{2} \nabla^2 J(r^\star)[h, h] - |\nabla^2 J(r^\star + \xi h)[h, h] - \nabla^2 J(r^\star)[h, h]| \\ &\geq \frac{1}{2} \nabla^2 J(r^\star)[h, h] - \eta(\|h\|_X) \|h\|_{H^s}^2 \\ &\geq \frac{1}{2} \big(c_E - \eta(\|h\|_X)\big) \|h\|_{H^s}^2. \end{aligned}$$

Supposing $0 < \widehat{\delta} \leq \delta$ to be chosen such that $\eta(\|r - r^\star\|_X) \leq c_E/2$ for all $r \in \overline{B^X_{\widehat{\delta}}(r^\star)}$, we arrive at

$$J(r) - J(r^\star) \geq \frac{c_E}{4}\|r - r^\star\|^2_{H^s} \quad \text{for all } r \in \overline{B^X_{\widehat{\delta}}(r^\star)}.$$

On the other hand, we choose $r = r^\star + h \in \overline{B_{\widehat{\delta}}(r^\star)}$ arbitrarily but fixed. Combining the Taylor expansion

$$J(r) - J(r^\star) = \frac{1}{2}\nabla^2 J(r^\star + \xi h)[h,h] \geq \widehat{c}_E\|h\|^2_{H^s}, \quad \xi \in (0,1),$$

with (A4) yields

$$\begin{aligned}\nabla^2 J(r^\star)[h,h] &= \nabla^2 J(r^\star + \xi h)[h,h] + \nabla^2 J(r^\star)[h,h] - \nabla^2 J(r^\star + \xi h)[h,h] \\ &\geq \big(2\widehat{c}_E - \eta(\|h\|_X)\big)\|h\|^2_{H^s}.\end{aligned}$$

Fixing, similarly to the above, $0 < \delta \leq \widehat{\delta}$ such that $\eta(\|h\|_X) \leq \widehat{c}_E/2$ yields the coercivity estimate (A3) with $c_E := 3\widehat{c}_E/2$ for all $h \in \overline{B^X_\delta(0)}$. This finishes the proof since X is dense in H^s and $\nabla^2 J(r^\star) : H^s \times H^s \to \mathbb{R}$ is bilinear. ∎

Let us remark that the verification of (A4) turns out to be rather technical in the case of PDE-constrained shape optimization problems. For the presented model problems, (A4) has been proven in [10, 11, 12], whereas the verification of (A2) is much simpler (see, e.g., [15]) but already an indicator of the two norm discrepancy.

Combining the assumptions (A2) (together with (3.1)), (A3), and (A4) leads to the following corollary by repeating a portion of the preceding proof.

COROLLARY 3.4. *For $\widehat{\delta} > 0$ sufficiently small, the shape Hessian is strongly coercive in the whole ball $\overline{B^X_{\widehat{\delta}}(r^\star)}$, that is,*

$$\nabla^2 J(r)[h,h] \geq \frac{c_E}{2}\|h\|^2_{H^s} \quad \textit{for all } h \in H^s,\ r \in \overline{B^X_{\widehat{\delta}}(r^\star)}. \tag{3.4}$$

Moreover, with respect to the objective, the following upper and lower quadratic bound

$$\frac{c_E}{4}\|r - r^\star\|^2_{H^s} \leq J(r) - J(r^\star) \leq \frac{C_S}{2}\|r - r^\star\|^2_{H^s} \tag{3.5}$$

holds for all $r \in \overline{B^X_{\widehat{\delta}}(r^\star)}$.

3.3. Ritz–Galerkin discretization. We shall consider a Ritz–Galerkin scheme to solve the necessary condition (A1); i.e., we replace the given infinite dimensional optimization problem with a finite dimensional problem. The trial space should provide sufficient regularity in order to approximate functions in X. To this end, we introduce an appropriate Hilbert space $H^k \subset X$, continuously embedded in X, i.e.,

$$\|r\|_X \leq c_{H^k \to X}\|r\|_{H^k} \qquad \text{for all } r \in H^k. \tag{V1}$$

Then we shall consider a sequence of nested finite dimensional trial spaces,

$$V_0 \subset V_1 \subset \cdots \subset V_N \subset \cdots \subset H^k \subset X, \quad \bigcap_{N\geq 0} V_N = V_0, \quad \overline{\bigcup_{N\geq 0} V_N}^{H^k} = H^k, \tag{V2}$$

providing the following inverse estimate:

$$\|r_N\|_{H^k} \leq E(N)\|r_N\|_{H^s} \quad \text{for all } r_N \in V_N. \tag{V3}$$

Moreover, we assume that there exists an $L > k$ such that the following approximation property holds:

$$\text{(V4)} \qquad \inf_{r_N \in V_N} \|r - r_N\|_{H^s} = o\left(\frac{1}{E(N)}\right) \|r\|_{H^\ell} \quad \text{if } r \in H^\ell \ (k < \ell \leq L).$$

Herein, the Landau symbol $g(x) = o(f(x))$ means that $\lim_{x\to\infty} g(x)/f(x) = 0$.

Remark 3.5. Suppose $X = C^{2,\alpha}([0,1])$ for some $\alpha \in (0,1)$. Then the Sobolev space $H^k([0,1])$ with $3 \geq k > 2 + \alpha$ provides a continuous embedding in accordance with (V1). Choosing $V_N \subset C^{2,1}([0,1])$ as the space of smoothest cubic splines on the uniform subdivision with step width $h_N := 2^{-N}/4$, we have the approximation property

$$\inf_{r_N \in V_N} \|r - r_N\|_{H^s} \lesssim h_N^{\ell - s} \|r\|_{H^\ell} \quad \text{if } r \in H^\ell \ (k < \ell \leq 4)$$

uniformly in N, provided that $s < k$. The inverse estimate reads as

$$\|r_N\|_{H^k} \lesssim h_N^{s-k} \|r_N\|_{H^s} \quad \text{for all } r_N \in V_N$$

uniformly in N, provided that $s \leq k$. Hence, we conclude that the trial spaces $(V_N)_{N \geq 0}$ satisfy (V2)–(V4).

The Ritz–Galerkin scheme reads as follows. In order to solve

$$(P_N) \qquad J(r_N) \to \min, \qquad r_N \in V_N,$$

one seeks an approximate solution $r_N^\star \in V_N$ such that the discretized necessary condition

$$\nabla J(r_N^\star)[q_N] = 0 \tag{3.6}$$

holds for all $q_N \in V_N$.

There exist different strategies for finding $r_N \in V_N$ such that (3.6) holds. In general, suppose that r_N has N degrees of freedom; i.e., there exist $\varphi_1, \varphi_2, \ldots, \varphi_N$ such that

$$V_N = \operatorname{span}\{\varphi_1, \varphi_2, \ldots, \varphi_N\}.$$

One makes the ansatz $r_N = \sum_{i=1}^N r_i \varphi_i$ and considers an iterative scheme

$$\mathbf{r}^{(n+1)} = \mathbf{r}^{(n)} - h^{(n)} \mathbf{M}^{(n)} \mathbf{G}^{(n)}, \tag{3.7}$$

where $h^{(n)}$ is a suitable step width and

$$\mathbf{r}^{(n)} = \big(r_i^{(n)}\big)_{i=1,\ldots,N}, \quad \mathbf{G}^{(n)} := \big(\nabla J(r_N^{(n)})[\varphi_i]\big)_{i=1,\ldots,N}.$$

First order methods are the gradient method ($\mathbf{M}^{(n)} := \mathbf{I}$) and the quasi-Newton method, where $\mathbf{M}^{(n)}$ denotes a suitable approximation to the inverse shape Hessian. Choosing

$$\mathbf{M}^{(n)} := \big(\nabla^2 J(r_N^{(n)})[\varphi_i, \varphi_j]\big)_{i,j=1,\ldots,N}^{-1}$$

yields the Newton method, which converges much faster compared to first order methods; see [19] for an example.

3.4. Existence of approximate solutions. We will consider the existence of solutions of (3.6) and the question of the accuracy of approximate solutions $r_N^\star$. Since the solutions of (3.6) are only stationary points, it is reasonable to consider only local optimization problems. Therefore, we replace the global problems (P) and (P_N) with the local optimization problem

$$(P^\delta) \qquad J(r) \to \min, \quad r \in \overline{B_\delta^X(r^\star)},$$

and its discrete variant

$$(P_N^\delta) \qquad J(r_N) \to \min, \qquad r_N \in V_N \cap \overline{B_\delta^X(r^\star)},$$

where $\delta = \widehat{\delta}$ is chosen in accordance with the estimates (3.4), (3.5) and is *independent* of N. Obviously, the solution of (P^δ) is $r^\star$, since J is strictly coercive on the convex set $\overline{B_\delta^X(r^\star)}$. Moreover, we have as a first consequence the following lemma.

LEMMA 3.6. *Problem* (P_N^δ) *always admits a solution* $r_N^\star \in V_N \cap \overline{B_\delta^X(r^\star)}$. *Any point* $r_N^\star \in V_N \cap \overline{B_\delta^X(r^\star)}$ *satisfying* (3.6) *is a local regular optimizer of second order. Moreover, the coercivity implies the uniqueness of* $r_N^\star$.

Proof. The existence of $r_N^\star$ is obvious since the admissible set $V_N \cap \overline{B_\delta^X(r^\star)}$ is compact. It follows for all $r_N := r_N^\star + h_N \in V_N \cap \overline{B_\delta^X(r^\star)}$ that $r_N^\star + \xi h_N \in V_N \cap \overline{B_\delta^X(r^\star)}$ is always satisfied for all $\xi \in (0,1)$ by convexity of the admissible set. Consequently, if $r_N^\star$ also satisfies (3.6), we deduce from (3.4) that

$$J(r_N) - J(r_N^\star) = \frac{1}{2}\nabla^2 J(r_N^\star + \xi h_N)[h_N, h_N] \geq \frac{c_E}{4}\|r_N - r_N^\star\|_{H^s}^2, \quad \xi \in (0,1),$$

for all $r_N = r_N^\star + h_N \in V_N \cap \overline{B_\delta^X(r^\star)}$. Uniqueness of $r_N^\star$ is an immediate consequence of the strict convexity of J (ensured again by (3.4)) on the convex set $V_N \cap \overline{B_\delta^X(r^\star)}$. ∎

Nevertheless, if $r_N^\star$ remains at the "artificial" boundary $\partial\{V_N \cap \overline{B_\delta^X(r^\star)}\} = V_N \cap \partial B_\delta^X(r^\star)$, only a related variational inequality holds instead of (3.6). Furthermore, $\|r_N^\star - r^\star\|_X = \delta$ for $N \to \infty$ contradicts convergence on its own. Consequently, we have to ensure that $r_N^\star$ is an *interior* point of the set $V_N \cap \overline{B_\delta^X(r^\star)}$, i.e.,

$$\|r_N^\star - r^\star\|_X < \delta,$$

at least for all sufficiently large $N \geq N_0$. This result is provided by the next theorem.

THEOREM 3.7. *Let* (A1)–(A4) *and* (V1)–(V4) *hold. Then, if* $r^\star \in H^\ell$ *for some* $\ell > k$, *there exists an* N_0 *such that*

$$r_N^\star \in V_N \cap B_\delta^X(r^\star) \quad \textit{for all } N \geq N_0.$$

Proof. We split the proof into four parts.

(i) We define $P_N : L^2 \to V_N$ as the L^2-orthogonal projection onto V_N. Then, by our assumptions (V1), (V2) we have

$$\|P_N(r^\star) - r^\star\|_X \leq c_{H^k \to X}\|P_N(r^\star) - r^\star\|_{H^k} \lesssim \inf_{r_N \in V_N}\|r_N - r^\star\|_{H^k} \stackrel{N\to\infty}{\longrightarrow} 0$$

and likewise by (V4),

$$\|P_N(r^\star) - r^\star\|_{H^s} \lesssim \inf_{r_N \in V_N}\|r_N - r^\star\|_{H^s} \stackrel{N\to\infty}{\longrightarrow} 0.$$

Hence, we deduce that there exists an N_0 such that $V_N \cap \overline{B_\delta^X(r^\star)} \neq \emptyset$ for all $N \geq N_0$. Without loss of generality we assume that $N_0 = 0$.

(ii) Recall that

$$J(r^\star) = \inf\big\{J(r) : r \in \overline{B_\delta^X(r^\star)}\big\},$$
$$J(r_N^\star) = \inf\big\{J(r_N) : r_N \in V_N \cap \overline{B_\delta^X(r^\star)}\big\},$$

and define $J_\delta(N) \geq J(r_N^\star) \geq J(r^\star)$ via

$$J_\delta(N) := \inf\big\{J(r_N) : r_N \in V_N \cap \partial B_\delta^X(r^\star)\big\}.$$

Since $J\big(P_N(r^\star)\big) \geq J(r_N^\star)$, we conclude the assertion $\|r_N^\star - r^\star\|_X < \delta$ if we can prove

$$J_\delta(N) > J\big(P_N(r^\star)\big) \quad \text{for all } N \geq N_0. \tag{3.8}$$

On the one hand, (3.5) implies

$$J\big(P_N(r^\star)\big) - J(r^\star) \leq \frac{C_S}{2}\|P_N(r^\star) - r^\star\|_{H^s}^2. \tag{3.9}$$

On the other hand, by introducing the quantity

$$\begin{aligned} F_\delta^X(N) &:= \inf\big\{\|r_N - r^\star\|_{H^s} : r_N \in V_N \cap \partial B_\delta^X(r^\star)\big\} \\ &= \inf\big\{\|r_N - r^\star\|_{H^s} : r_N \in V_N \setminus B_\delta^X(r^\star)\big\}, \end{aligned}$$

we derive from (3.5)

$$J_\delta(N) - J(r^\star) \geq \frac{c_E}{4} F_\delta^X(N)^2. \tag{3.10}$$

Combining (3.9) and (3.10), we see that the inequality

$$\|P_N(r^\star) - r^\star\|_{H^s} < C^\star \cdot F_\delta^X(N), \quad C^\star := \sqrt{\frac{c_E}{2C_S}}, \tag{3.11}$$

will imply (3.8) and, thus, $\|r_N^\star - r^\star\|_X < \delta$.

(iii) We shall establish a relation between $F_\delta^X(N)$, $\|r^\star - P_N(r^\star)\|_{H^s}$, and $E(N)$ from the inverse estimate (V3). For the sake of simplicity, we assume without loss of generality that the constant $c_{H^k\to X}$ from (V1) is less than one such that

$$B_\delta^{H^k}(r^\star) \subseteq B_\delta^X(r^\star). \tag{3.12}$$

Introducing

$$\begin{aligned} F_\delta^{H^k}(N) &:= \inf\big\{\|r_N - r^\star\|_{H^s} : r_N \in V_N \cap \partial B_\delta^{H^k}(r^\star)\big\} \\ &= \inf\big\{\|r_N - r^\star\|_{H^s} : r_N \in V_N \setminus B_\delta^{H^k}(r^\star)\big\}, \end{aligned}$$

there follows from (3.12) the relation

$$F_\delta^{H^k}(N) \leq F_\delta^X(N).$$

We shall now compute a lower bound for $F_\delta^{H^k}(N)$. From

$$\|r_N - P_N(r^\star)\|_{H^s} - \|P_N(r^\star) - r^\star\|_{H^s} \leq \|r_N - r^\star\|_{H^s}$$

one infers the inequality

$$F_\delta^{H^k}(N) \geq \inf\big\{\|r_N - P_N(r^\star)\|_{H^s} : r_N \in V_N \setminus B_\delta^{H^k}(r^\star)\big\} - \|P_N(r^\star) - r^\star\|_{H^s}. \tag{3.13}$$

We choose N_0 sufficiently large to ensure

$$\|P_N(r^\star) - r^\star\|_{H^k} \leq \delta/2 \quad \text{for all } N \geq N_0.$$

Then it holds that $B_{\delta/2}^{H^k}\big(P_N(r^\star)\big) \subset B_\delta^{H^k}(r^\star)$, and we arrive at

$$\begin{aligned}
\inf\big\{&\|r_N - P_N(r^\star)\|_{H^s} : r_N \in V_N \setminus B_\delta^{H^k}(r^\star)\big\} \\
&\geq \inf\big\{\|r_N - P_N(r^\star)\|_{H^s} : r_N \in V_N \setminus B_{\delta/2}^{H^k}\big(P_N(r^\star)\big)\big\} \\
&\geq \inf_{r_N \in V_N}\{\|r_N\|_{H^s} : \|r_N\|_{H_k} = \delta/2\} \\
&\geq \frac{\delta}{2E(N)}.
\end{aligned}$$

Inserting this estimate into (3.13), we deduce

$$F_\delta^X(N) \geq F_\delta^{H^k}(N) \geq \frac{\delta}{2E(N)} - \|P_N(r^\star) - r^\star\|_{H^s} \quad \text{for all } N \geq N_0. \tag{3.14}$$

(iv) Observing

$$\|P_N(r^\star) - r^\star\|_{H^s} \lesssim \inf_{r_N \in V_N} \|r_N - r^\star\|_{H^s},$$

we infer from (V4) that we can increase N_0 such that

$$\|P_N(r^\star) - r^\star\|_{H^s} < \frac{\delta}{2E(N)} \cdot \frac{C^\star}{C^\star + 1} \quad \text{for all } N \geq N_0.$$

Thus, in view of (3.14), we arrive at

$$\|P_N(r^\star) - r^\star\|_{H^s} < C^\star\left(\frac{\delta}{2E(N)} - \|P_N(r^\star) - r^\star\|_{H^s}\right) < C^\star F_\delta^X(N),$$

that is, (3.11), for all $N \geq N_0$, which finishes the proof according to part (ii). ∎

Remark 3.8. Obviously, by means of standard optimization theory, (3.3) and (3.6) imply well-posedness of the finite dimensional optimization problem; that is, existence and (local) uniqueness of minimizers are ensured. In particular, the strict coercivity of (P_N^δ), induced by the coercivity of (P^δ), provides the convergence

$$r_N^{(n)} \to r_N^\star \quad \text{as } n \to \infty$$

of the iterative scheme (3.7); see, e.g., [30, 40].

3.5. Convergence. The above theorem ensures the *existence* of an approximate solution $r_N^\star$ to the finite dimensional problems (P_N^δ) that satisfies the necessary condition (3.6), provided that N is sufficiently large. The next theorem estimates the distance $\|r_N^\star - r^\star\|_{H^s}$.

THEOREM 3.9. *The approximate solution $r_N^\star$ of the finite dimensional problem (P_N^δ) satisfies the error estimate*

$$\|r_N^\star - r^\star\|_{H^s} \leq \frac{2C_S}{c_E} \inf_{r_N \in V_N} \|r_N - r^\star\|_{H^s}$$

uniformly with the number of unknowns N.

Proof. For the sake of clearness in the representation, let $\langle \cdot, \cdot \rangle$ denote the duality pairing between H^s and its dual space H^{-s}.

On the one hand, observing (3.2), Galerkin orthogonality implies

$$\begin{aligned}\langle \nabla J(r_N^\star) - \nabla J(r^\star), r_N^\star - r^\star \rangle &= \langle \nabla J(r_N^\star) - \nabla J(r^\star), r_N - r^\star \rangle \\ &\leq C_S \|r_N^\star - r^\star\|_{H^s} \|r_N - r^\star\|_{H^s}\end{aligned}$$

for all $r_N \in V_N$. On the other hand, by introducing

$$j(t) := \langle \nabla J\big(t r_N^\star + (1-t) r^\star\big), r_N^\star - r^\star \rangle,$$

we derive the estimate

$$\begin{aligned}\langle \nabla J(r_N^\star) - \nabla J(r^\star), r_N^\star - r^\star \rangle &= j(1) - j(0) = \int_0^1 j'(t)\, dt \\ &= \int_0^1 \langle \nabla^2 J(t r_N^\star + (1-t) r^\star\big) \cdot (r_N^\star - r^\star), r_N^\star - r^\star \rangle \, dt \geq \frac{c_E}{2} \|r_N^\star - r^\star\|_{H^s}^2.\end{aligned}$$

Combining both estimates yields

$$\|r_N^\star - r^\star\|_{H^s}^2 \leq \frac{2C_S}{c_E} \|r_N^\star - r^\star\|_{H^s} \|r_N - r^\star\|_{H^s}$$

for all $r_N \in V_N$, which is equivalent to the assertion. ∎

Of course, from this theorem one can determine the *rate of convergence* if one estimates $\inf_{r_N \in V_N} \|r_N - r^\star\|_{H^s}$.

3.6. The fully discretized problem. Up to now, we investigated only the discretization with respect to the shape. Hence, we neglected consistency errors arising from the approximate solution of the state equation or from computing the objective and constraints by, e.g., quadrature. Consequently, we shall focus on the following further modification of problem (P_N^δ):

$$(P_{N\epsilon}^\delta) \quad \text{seek } r_{N\epsilon}^\star \in V_N \cap \overline{B_\delta^X(r_N^\star)} \quad \text{such that } \langle \nabla J_\epsilon(r_N^\star), q_N \rangle = 0 \quad \text{for all } q_N \in V_N,$$

where ϵ is an approximation parameter referring to the inexact computation of the gradient. We prove the following Strang-type lemma which estimates the consistency error induced by solving $(P_{N\epsilon}^\delta)$.

LEMMA 3.10. *Assume that the estimate*

$$|\langle [\nabla J_\epsilon(r_N) - \nabla J(r_N)] - [\nabla J_\epsilon(q_N) - \nabla J(q_N)], s_N \rangle| \leq \epsilon \|r_N - q_N\|_{H^s} \|s_N\|_{H^s} \tag{3.15}$$

holds for all $r_N, q_N \in V_N \cap \overline{B_\delta^X(r_N^\star)}$ *and* $s_N \in V_N$. *Then, provided that* ϵ *is sufficiently small,* $(P_{N\epsilon}^\delta)$ *admits a unique solution* $r_{N\epsilon}^\star \in V_N \cap \overline{B_\delta^X(r_N^\star)}$ *which satisfies the a priori estimate*

$$\|r^\star - r_{N\epsilon}^\star\|_{H^s} \leq \left(1 + \frac{2\max\{1, C_S\}}{c_E - 2\epsilon}\right) \left\{ \|r^\star - r_N\|_{H^s} + \sup_{q_N \in V_N} \frac{\langle \nabla J(r_N) - \nabla J_\epsilon(r_N), q_N \rangle}{\|q_N\|_{H^s}} \right\}.$$

Proof. Due to our assumptions from the previous subsections, the unperturbed Richardson iteration

$$r_N^{(n+1)} = r_N^{(n)} - \alpha \sum_{i=1}^N \nabla J(r_N^{(n)})[\varphi_i]\varphi_i, \quad n = 0, 1, \ldots,$$

defines a contraction of $V_N \cap \overline{B_\delta^X(r_N^\star)}$ onto itself for a whole range of $\alpha \in [\underline{\alpha}, \overline{\alpha}]$. Estimate (3.15) ensures that the perturbed Richardson iteration

$$r_{N\epsilon}^{(n+1)} = r_{N\epsilon}^{(n)} - \alpha \sum_{i=1}^{N} \nabla J_\epsilon(r_{N\epsilon}^{(n)})[\varphi_i]\varphi_i, \quad n = 0, 1, \dots,$$

is still a contraction of $V_N \cap \overline{B_\delta^X(r_N^\star)}$ onto itself for $\alpha := (\underline{\alpha} + \overline{\alpha})/2$, provided that ϵ is sufficiently small. This proves existence and uniqueness of the perturbed solution $r_{N\epsilon}^\star$.

Next, using again (3.15), we find

$$\begin{aligned}
&\langle \nabla J_\epsilon(r_N) - \nabla J_\epsilon(q_N), r_N - q_N \rangle \\
&\qquad \geq \langle \nabla J(r_N) - \nabla J(q_N), r_N - q_N \rangle - \epsilon \|r_N - q_N\|_{H^s}^2 \\
&\qquad \geq \Big(\frac{c_E}{2} - \epsilon \Big) \|r_N - q_N\|_{H^s}^2,
\end{aligned}$$

where $\widetilde{c}_E := c_E/2 - \epsilon > 0$ holds if ϵ is sufficiently small.

Due to Galerkin orthogonality, the Ritz–Galerkin solution $r_{N\epsilon}^\star$ of $(P_{N\epsilon}^\delta)$ satisfies

$$\begin{aligned}
\widetilde{c}_E \|r_{N\epsilon}^\star - r_N\|_{H^s}^2 &\leq \langle \nabla J_\epsilon(r_{N\epsilon}^\star) - \nabla J_\epsilon(r_N), r_{N\epsilon}^\star - r_N \rangle \\
&\leq \langle \nabla J(r^\star) - \nabla J(r_N), r_{N\epsilon}^\star - r_N \rangle + \langle \nabla J(r_N) - \nabla J_\epsilon(r_N), r_{N\epsilon}^\star - r_N \rangle \\
&\leq C_S \|r^\star - r_N\|_{H^s} \|r_{N\epsilon}^\star - r_N\|_{H^s} + \langle \nabla J(r_N) - \nabla J_\epsilon(r_N), r_{N\epsilon}^\star - r_N \rangle,
\end{aligned}$$

that is,

$$\|r_{N\epsilon}^\star - r_N\|_{H^s} \leq \frac{\max\{1, C_S\}}{\widetilde{c}_E} \left\{ \|r^\star - r_N\|_{H^s} + \sup_{q_N \in V_N} \frac{\langle \nabla J(r_N) - \nabla J_\epsilon(r_N), q_N \rangle}{\|q_N\|_{H^s}} \right\}.$$

Since $r_N \in V_N \cap \overline{B_\delta^X(r_N^\star)}$ is arbitrary, we arrive at the assertion using the triangle inequality

$$\|r^\star - r_{N\epsilon}^\star\|_{H^s} \leq \|r^\star - r_N\|_{H^s} + \|r_N - r_{N\epsilon}^\star\|_{H^s}. \qquad \square$$

4. Numerical results.

4.1. An unconstrained shape optimization problem. For comparison we shall employ model problems, where the solution is known analytically. To this end, we choose the shape optimization problem (2.3) based on the domain integral

$$J(\Omega) = \int_\Omega \Big(\frac{x^2}{8} + \frac{y^2}{4} - 2 \Big) d\mathbf{x}$$

as our first numerical example. In accordance with subsection 2.2, the ellipse centered in $\mathbf{0}$ with semiaxes $2\sqrt{2}$ and 2 is a strict minimizer of second order.

The numerical setting is as follows. We subdivide the parameter interval $[0, 2\pi]$ equidistantly into N intervals. With respect to this subdivision, the radial function $r \in X := C_{\text{per}}^1([0, 2\pi])$ is then approximated periodically by N cubic B-splines B_i^3, $i = 1, \dots, N$, that is,

$$r_N = \sum_{i=1}^{N} a_i B_i^3 \in C_{\text{per}}^{2,1}([0, 2\pi]).$$

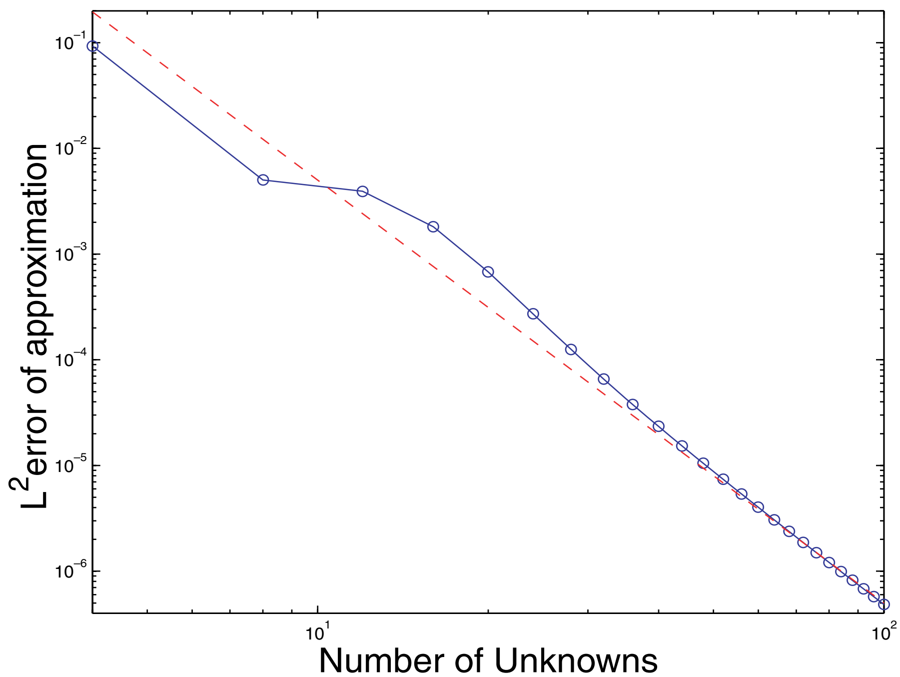

FIG. 4.1. *L^2-error of the approximate solution.*

We employ a Newton method to iteratively solve the necessary condition $\nabla J(\Omega) \equiv 0$, using the circle with radius 2 as an initial guess.

Since the energy space for the shape Hessian is $L^2([0, 2\pi])$, we measure the L^2-norm of the approximation error given by

$$\|r - r_N\|^2_{L^2([0,2\pi])} = \int_0^{2\pi} |r - r_N|^2 d\phi.$$

The measurements are shown in Figure 4.1. We observe, as predicted, the rate of convergence N^{-4}, indicated by the dashed line.

4.2. A constrained shape optimization problem. We consider next a cylindric circular bar which is homogeneous and isotropic with a planar, simply connected cross section $\Omega \in \mathbb{R}^2$. We follow Banichuk and Karihaloo [2], but normalize the shear modulus $G = 1$ and the elastic modulus $E = 1$. We want to solve the problem of maximizing the torsional rigidity of the bar subject to given equality constraints on the bending stiffness and the volume.

First, we briefly recall the mathematical formulation of the quantities. The torsional rigidity is calculated by

$$T(\Omega) = 2 \int_\Omega u(\mathbf{x}) d\mathbf{x},$$

where the stress function $u = u(\Omega)$ satisfies

$$-\Delta u = 2 \text{ in } \Omega, \qquad u = 0 \text{ on } \Gamma.$$

The bending rigidity with respect to a fixed barycenter in the origin is given by

$$B(\Omega) = \int_\Omega y^2 d\mathbf{x}.$$

The volume of the domain and its (simplified) barycenter coordinates read as

$$V(\Omega) = \int_\Omega d\mathbf{x}, \qquad S_x(\Omega) = \int_\Omega x d\mathbf{x}, \qquad S_y(\Omega) = \int_\Omega y d\mathbf{x}.$$

Consequently, we arrive at the following constraint shape optimization problem:

$$J(\Omega) := -T(\Omega) \to \min$$

subject to

$$B(\Omega) = B_0, \qquad V(\Omega) = V_0, \qquad S_x(\Omega) = 0, \qquad S_y(\Omega) = 0.$$

Choosing $B_0 = \sqrt{2}\pi/4$, $V_0 = \pi$, we see that the necessary condition is fulfilled by the ellipse with semiaxes $h_x = 2^{-1/4}$ and $h_y = 2^{1/4}$. The associated Lagrange multipliers are $\lambda_B = -4/9$, $\lambda_V = 8\sqrt{2}/9$, and $\lambda_{S_x} = \lambda_{S_y} = 0$; cf. [2]. From the identity

$$T(\Omega) = \int_\Omega \|\nabla u(\mathbf{x})\|^2 d\mathbf{x},$$

we deduce that $\nabla T(\Omega)[dr]$ and $\nabla^2 T(\Omega)[dr_1, dr_2]$ are given as in (2.12) and (2.13) with $g \equiv 0$ and

$$\Delta du = 0 \text{ in } \Omega, \qquad du = -dr_2 \langle \widehat{\mathbf{n}}, \mathbf{n} \rangle \frac{\partial u}{\partial \mathbf{n}} \text{ on } \Gamma.$$

Recall that twice differentiability needs $r \in X := C^{2,\alpha}_{\text{per}}([0, 2\pi])$; cf. subsection 2.3. The computation of the other gradients and Hessians is straightforward; see [18, 19] for the details.

We approximate the radial function r similarly to our first example by periodic cubic splines on the interval $[0, 2\pi]$. Even though the sufficient optimality condition has not yet been proven, our experience indicates coercivity in the energy space $H^{1/2}([0, 2\pi])$; cf. [18, 19, 21]. More precisely, coercivity of the Lagrangian at $(\Omega^\star, \lambda^\star)$ has to hold on the closed subspace $Y \subseteq C^{2,\alpha}_{\text{per}}([0, 2\pi])$, where

$$\begin{aligned} Y := \{dr \in C^{2,\alpha}_{\text{per}}([0, 2\pi]) : \nabla B(\Omega^\star)[dr] = 0 \wedge \nabla V(\Omega^\star)[dr] = 0 \\ \wedge \nabla S_x(\Omega^\star)[dr] = 0 \wedge \nabla S_y(\Omega^\star)[dr] = 0\}. \end{aligned}$$

However, the pure Lagrangian is introduced only for investigating the sufficient optimality condition. In order to numerically solve the discretized constrained shape optimization problem, we need to find the stationary points of the following augmented Lagrange functional:

$$L_c(\Omega, \boldsymbol{\lambda}) := -T(\Omega) + \boldsymbol{\lambda}^T \begin{bmatrix} B(\Omega) - B_0 \\ V(\Omega) - V_0 \\ S_x(\Omega) \\ S_y(\Omega) \end{bmatrix} + \frac{c}{2} \left\| \begin{bmatrix} B(\Omega) - B_0 \\ V(\Omega) - V_0 \\ S_x(\Omega) \\ S_y(\Omega) \end{bmatrix} \right\|^2,$$

where $\boldsymbol{\lambda} := (\lambda_B, \lambda_V, \lambda_{S_x}, \lambda_{S_y})$ and $c > 0$ is an appropriate chosen penalty parameter. The optimization algorithm then reads as follows:

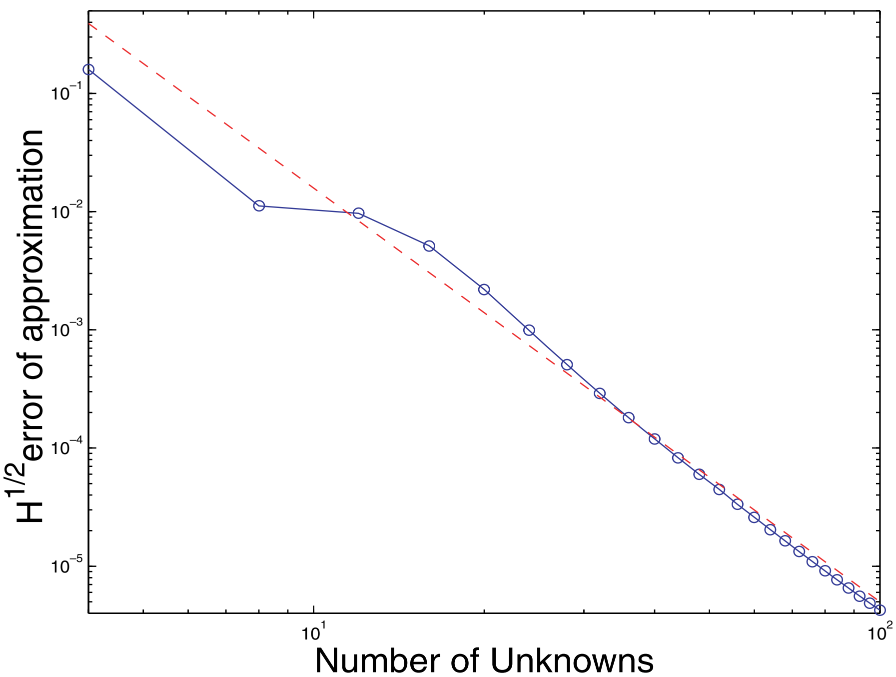

FIG. 4.2. *$H^{1/2}$-error of the approximate solution.*

- initialization: choose initial guess $(\Omega^{(0)}, \boldsymbol{\lambda}^{(0)})$ for $(\Omega^\star, \boldsymbol{\lambda}^\star)$.
- inner iteration: solve $\Omega^{(n+1)} := \operatorname{argmin} L_c(\Omega, \boldsymbol{\lambda}^{(n)})$ with initial guess $\Omega^{(n)}$.
- outer iteration: update

$$\lambda^{(n+1)} := \lambda^{(n)} - c \begin{bmatrix} B(\Omega^{(n+1)}) - B_0 \\ V(\Omega^{(n+1)}) - V_0 \\ S_x(\Omega^{(n+1)}) \\ S_y(\Omega^{(n+1)}) \end{bmatrix}.$$

In the inner iteration, we employ a Newton scheme combined with a quadratic line-search. Instead of the first order update rule described above, we use a second order Lagrange multiplier method introduced in [36] (see also [21]), which provides faster convergence of the dual parameters. The state equation is solved by using a boundary element method; cf. [18, 19] for the details. Notice that about 2000 boundary elements are required to solve the state equation sufficiently accurately if we discretize the free boundary by $N = 100$ B-splines.

According to our convergence result we shall observe the rate of convergence

$$\|r - r_N\|_{H^{1/2}([0,2\pi])} \lesssim N^{-3.5} \|r\|_{H^4([0,2\pi])}.$$

We measure this norm via the approximation

$$\|r - r_N\|^2_{H^{1/2}([0,2\pi])} \sim \|r - r_N\|^2_{L^2([0,2\pi])} + \int_0^{2\pi} |r - r_N||r' - r'_N| d\phi.$$

The results are presented in Figure 4.2. As predicted, the error decreases like $N^{-3.5}$, which is indicated by the dashed line.

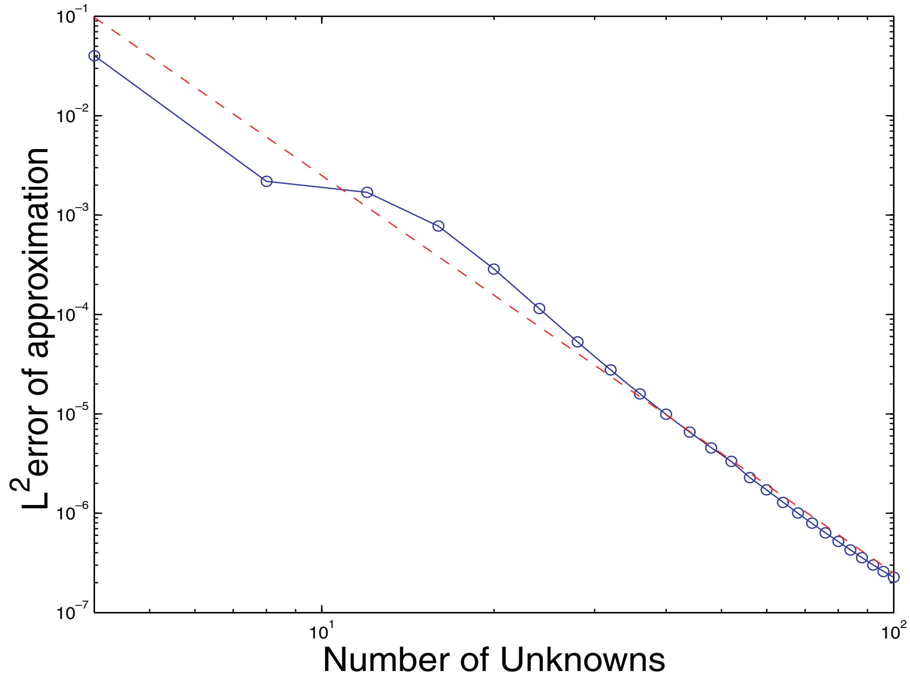

Fig. 4.3. *L^2-error of the approximate solution.*

In addition we also measured the L^2-norm of the approximation error, visualized in Figure 4.3. In fact, even though we have not proven the Aubin–Nitsche trick, we observe the higher rate of convergence N^{-4}, indicated by the dashed line.

5. Concluding remarks. In the present paper we established a complete convergence analysis for approximate solutions of shape optimization problems. In particular, we incorporated the two norm discrepancy. We presented numerical results which verify the predicted rates of convergence. We would like to point out that our analysis applies also to p-discretizations of the domain's parametrization, for example, finite dimensional Fourier sequences for the discretization of the radial function. For several applications we refer to [9, 18, 19, 20]; see also [22, 24, 42] for related problems in three dimensions.

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