ENERGY CHANGE TO INSERTION OF INCLUSIONS ASSOCIATED WITH A DIFFUSIVE/CONVECTIVE STEADY-STATE HEAT CONDUCTION PROBLEM

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Abstract. The topological derivative concept has been successfully applied in many relevant physics and engineering problems. In particular, the topological asymptotic analysis has been fully developed for a wide range of problems modeled by partial differential equations. In this paper, the topological asymptotic analysis of the energy shape functional associated with a diffusive/convective steady state heat equation is developed. The topological derivative with respect to the nucleation of a circular inclusion is derived in its closed form with help of a non-standard adjoint state. Finally, we provide the estimates for the remainders of the topological asymptotic expansion and perform a complete mathematical justification for the derived formulas. The obtained result is new and can be applied in the context of topology design of heat sinks, for instance.

1. Introduction

The topological derivative concept [16] has been successfully applied in many relevant physics and engineering problems such as inverse problems [2, 3, 12], topology optimization [8, 10], image processing [14], multi-scale constitutive modeling [9], fracture mechanics [17] and damage evolution modeling [1]. In particular, the topological asymptotic analysis has been fully developed for a wide range of problems modeled by partial differential equations. See, for instance, [4, 5, 6, 7, 11, 13, 15].

In order to introduce these ideas, let us consider an open and bounded domain $\Omega \subset \mathbb{R}^2$, which is subject to a non-smooth perturbation confined in a small region $\omega_\varepsilon(\hat{x}) = \hat{x} + \varepsilon\omega$ of size ε. Here, $\hat{x}$ is an arbitrary point of Ω and ω is a fixed domain of $\mathbb{R}^2$. We introduce a characteristic function $x \mapsto \chi(x)$, $x \in \mathbb{R}^2$, associated to the unperturbed domain, namely $\chi = \mathbb{1}_\Omega$. Then, we define a characteristic function associated to the topologically perturbed domain of the form $x \mapsto \chi_\varepsilon(\hat{x}; x)$, $x \in \mathbb{R}^2$. In the case of a hole, for example, $\chi_\varepsilon(\hat{x}) = \mathbb{1}_\Omega - \mathbb{1}_{\overline{\omega_\varepsilon}(\hat{x})}$ and the singulary perturbed domain is given by $\Omega_\varepsilon(\hat{x}) = \Omega \setminus \overline{\omega_\varepsilon}(\hat{x})$. Then, we assume that a given shape functional $\psi(\chi_\varepsilon(\hat{x}))$, associated to the topologically perturbed domain, admits the following topological asymptotic expansion

$$\psi(\chi_\varepsilon(\hat{x})) = \psi(\chi) + f(\varepsilon) D_T\psi(\hat{x}) + \mathcal{R}(f(\varepsilon)), \tag{1.1}$$

where $\psi(\chi)$ is the shape functional associated to the unperturbed domain and $f(\varepsilon)$ is a positive function such that $f(\varepsilon) \to 0$ when $\varepsilon \to 0$. The function $\hat{x} \mapsto D_T\psi(\hat{x})$ is called the topological derivative of ψ at $\hat{x}$. Finally, $\mathcal{R}(f(\varepsilon))$ is the remainder of the topological asymptotic expansion, namely $\mathcal{R}(f(\varepsilon)) = o(f(\varepsilon))$. Therefore, the term $f(\varepsilon) D_T\psi(\hat{x})$ represents a first order correction of $\psi(\chi)$ to approximate $\psi(\chi_\varepsilon(\hat{x}))$.

In this paper, the topological asymptotic analysis of the energy shape functional associated with a diffusive/convective steady state heat equation is developed. The topological derivative $D_T\psi(\hat{x})$ with respect to the nucleation of a circular inclusion $\omega_\varepsilon(\hat{x}) := B_\varepsilon(\hat{x}) = \{\|x - \hat{x}\| < \varepsilon\}$ is derived in its closed form with help of a non-standard adjoint state. Finally, we provide the estimates for the remainders of the topological asymptotic expansion and perform a complete mathematical justification for the derived formulas. The obtained result is not available in the literature yet and can be applied in the context of topology design of heat sinks, for instance.

This paper is organized as follows. In Section 2, the mathematical formulation of the diffusive/convective steady state heat problem as well as the energy shape functional are introduced

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for both, original unperturbed and topologically perturbed domains. In addition, arguments on the existence of the associated topological derivative are provided. The explicit form of the topological derivative is derived in Section 3. The estimates for the remainders of the topological asymptotic expansion are presented in Section 4. Finally, the paper ends with some concluding remarks in Section 5.

2. Model Problem

In this section the mathematical model of the diffusive/convective steady state heat problem as well as the energy shape functional are introduced. The original unperturbed and topologically perturbed problems are presented, together with arguments on the existence of the associated topological derivative.

2.1. **Unperturbed Problem.** The original unperturbed problem is stated as

$$\theta \in H_0^1(\Omega) : \int_\Omega k\nabla\theta \cdot \nabla\eta + \int_\Omega (\beta \cdot \nabla\theta)\eta = \int_\Omega b\eta, \ \forall \eta \in H_0^1(\Omega), \tag{2.1}$$

where β is a given velocity vector field and b is a heat source. In addition, we assume that β is a divergence-free vector field, namely $\mathrm{div}(\beta) = 0$. The energy shape functional is defined by

$$\psi(\chi) := \mathcal{J}(\theta) = \frac{1}{2}\int_\Omega k\|\nabla\theta\|^2. \tag{2.2}$$

In order to simplify further analysis, we introduce the adjoint problem

$$\varphi \in H_0^1(\Omega) : \int_\Omega k\nabla\varphi \cdot \nabla\eta + \int_\Omega (\beta \cdot \nabla\eta)\varphi = -\int_\Omega k\nabla\theta \cdot \nabla\eta, \ \forall \eta \in H_0^1(\Omega). \tag{2.3}$$

2.2. **Perturbed Problem.** The topological perturbation is defined as

$$\gamma_{\omega_\varepsilon} = \gamma_{\omega_\varepsilon}(x) := \begin{cases} 1 & \text{if } x \in \Omega \setminus \overline{\omega_\varepsilon} \\ \gamma & \text{if } x \in \omega_\varepsilon \end{cases}, \tag{2.4}$$

where $0 < \gamma < \infty$ is the contrast parameter and $\omega_\varepsilon(\hat{x}) := B_\varepsilon(\hat{x}) = \{\|x - \hat{x}\| < \varepsilon\}$ for $\hat{x} \in \Omega$. By setting $k_\varepsilon = \gamma_{\omega_\varepsilon} k$ and $b_\varepsilon = \gamma_{\omega_\varepsilon} b$, the topologically perturbed problem is stated as

$$\theta_\varepsilon \in H_0^1(\Omega) : \int_\Omega k_\varepsilon\nabla\theta_\varepsilon \cdot \nabla\eta + \int_\Omega (\beta \cdot \nabla\theta_\varepsilon)\eta = \int_\Omega b_\varepsilon\eta, \ \forall \eta \in H_0^1(\Omega). \tag{2.5}$$

The topologically perturbed counterpart of the shape functional is given by

$$\psi(\chi_\varepsilon(\hat{x})) := \mathcal{J}_\varepsilon(\theta_\varepsilon) = \int_\Omega k_\varepsilon\|\nabla\theta_\varepsilon\|^2. \tag{2.6}$$

For the sake of simplicity, we assume that k, β and b behave like a constant in the neighborhood of $B_\varepsilon(\hat{x})$. So that $k(x) = k(\hat{x})$, $\beta(x) = \beta(\hat{x})$ and $b(x) = b(\hat{x})$ in $B_\varepsilon(\hat{x})$.

2.3. **Preliminaries.** Let us subtract (2.1) from (2.5). After some manipulations taking into account the contrast (2.4), there are:

$$\int_\Omega k\nabla(\theta_\varepsilon - \theta) \cdot \nabla\eta + \int_\Omega (\beta \cdot \nabla(\theta_\varepsilon - \theta))\eta = (1-\gamma)\int_{B_\varepsilon} k\nabla\theta_\varepsilon \cdot \nabla\eta - (1-\gamma)\int_{B_\varepsilon} b\eta, \tag{2.7}$$

and equivalently

$$\int_\Omega k_\varepsilon\nabla(\theta_\varepsilon - \theta) \cdot \nabla\eta + \int_\Omega (\beta \cdot \nabla(\theta_\varepsilon - \theta))\eta = (1-\gamma)\int_{B_\varepsilon} k\nabla\theta \cdot \nabla\eta - (1-\gamma)\int_{B_\varepsilon} b\eta. \tag{2.8}$$

By setting $\eta = \theta_\varepsilon - \theta$ as test function in (2.8), we have the equality

$$\int_\Omega k_\varepsilon\|\nabla(\theta_\varepsilon - \theta)\|^2 + \int_\Omega (\beta \cdot \nabla(\theta_\varepsilon - \theta))(\theta_\varepsilon - \theta) = (1-\gamma)\int_{B_\varepsilon} k\nabla\theta \cdot \nabla(\theta_\varepsilon - \theta) - (1-\gamma)\int_{B_\varepsilon} b(\theta_\varepsilon - \theta). \tag{2.9}$$

Since $\theta_\varepsilon - \theta = 0$ on $\partial\Omega$ and $\mathrm{div}(\beta) = 0$ by assumption, the second term on the left hand side of (2.9) vanishes. So that we obtain the following important result

$$\int_\Omega k_\varepsilon \|\nabla(\theta_\varepsilon - \theta)\|^2 = (1-\gamma)\int_{B_\varepsilon} k\nabla\theta \cdot \nabla(\theta_\varepsilon - \theta) - (1-\gamma)\int_{B_\varepsilon} b(\theta_\varepsilon - \theta). \tag{2.10}$$

2.4. **Existence of the Topological Derivative.** The original and perturbed shape functionals in which we are dealing with were introduced through equations (2.2) and (2.6), respectively. Now we are in position to state the following import result associated with the existence of the topological derivative for the problem under analysis:

Lemma 1. *Let θ_ε and θ be solutions to the perturbed* (2.5) *and original* (2.1) *variational problems, respectively. Then, the following estimate hold true*

$$\|\theta_\varepsilon - \theta\|_{H^1(\Omega)} \leq C\varepsilon, \tag{2.11}$$

where C is used to denote a generic constant independent of the control parameter ε.

Proof. Let us consider the equality (2.10). From the Cauchy-Schwarz inequality we obtain

$$\int_\Omega k_\varepsilon \|\nabla(\theta_\varepsilon - \theta)\|^2 \leq C_1\|\nabla\theta\|_{L^2(B_\varepsilon)}\|\nabla(\theta_\varepsilon - \theta)\|_{L^2(B_\varepsilon)} + C_2\|b\|_{L^2(B_\varepsilon)}\|\theta_\varepsilon - \theta\|_{L^2(B_\varepsilon)}. \tag{2.12}$$

The interior elliptic regularity of θ yields,

$$\int_\Omega k_\varepsilon \|\nabla(\theta_\varepsilon - \theta)\|^2 \leq C_3\varepsilon\,\|\theta_\varepsilon - \theta\|_{H^1(\Omega)}, \tag{2.13}$$

since by assumption $b(x) = b(\hat{x})$ in the neighborhood of $B_\varepsilon(\hat{x})$. From the Poincaré inequality on the left hand side of (2.13), there is

$$c\|\theta_\varepsilon - \theta\|^2_{H^1(\Omega)} \leq \int_\Omega k_\varepsilon \|\nabla(\theta_\varepsilon - \theta)\|^2, \tag{2.14}$$

which leads to the result with the constant $C = C_3/c$ independent of the small parameter ε. □

3. Topological Asymptotic Analysis

By subtracting (2.2) from (2.6) and using (2.10), it follows

$$\psi(\chi_\varepsilon(\hat{x})) - \psi(\chi) = \int_\Omega k\nabla\theta \cdot \nabla(\theta_\varepsilon - \theta) - \frac{1-\gamma}{2}\int_{B_\varepsilon} k\nabla\theta_\varepsilon \cdot \nabla\theta - \frac{1-\gamma}{2}\int_{B_\varepsilon} b(\theta_\varepsilon - \theta). \tag{3.1}$$

Let us set $\eta = \theta_\varepsilon - \theta$ in (2.3). Then we have the following equality

$$\int_\Omega k\nabla\varphi \cdot \nabla(\theta_\varepsilon - \theta) + \int_\Omega (\beta \cdot \nabla(\theta_\varepsilon - \theta))\varphi = -\int_\Omega k\nabla\theta \cdot \nabla(\theta_\varepsilon - \theta). \tag{3.2}$$

By setting $\eta = \varphi$ solution to the adjoint problem (2.3) in (2.7) we obtain the equality

$$\int_\Omega k\nabla(\theta_\varepsilon - \theta) \cdot \nabla\varphi + \int_\Omega (\beta \cdot \nabla(\theta_\varepsilon - \theta))\varphi = (1-\gamma)\int_{B_\varepsilon} k\nabla\theta_\varepsilon \cdot \nabla\varphi - (1-\gamma)\int_{B_\varepsilon} b\varphi. \tag{3.3}$$

After comparing (3.2) with (3.3), together with (3.1), we obtain the following import result

$$\psi(\chi_\varepsilon(\hat{x})) - \psi(\chi) = -\frac{1-\gamma}{2}\int_{B_\varepsilon} k\nabla\theta_\varepsilon \cdot \nabla(\theta + 2\varphi) + (1-\gamma)\int_{B_\varepsilon} b\varphi - \frac{1-\gamma}{2}\int_{B_\varepsilon} b(\theta_\varepsilon - \theta). \tag{3.4}$$

3.1. **Asymptotic Analysis of the Solution.** Let us introduce the following ansätz for the solution θ_ε to the perturbed boundary value problem (2.5)

$$\theta_\varepsilon(x) = \theta(x) + \varepsilon\vartheta(x/\varepsilon) + \tilde{\theta}_\varepsilon(x). \tag{3.5}$$

Some terms in the above expansions require explanations. Function θ is solution to the unperturbed boundary value problem (2.1), while function ϑ is solution to an exterior boundary value problem and $\tilde{\theta}_\varepsilon$ is the remainder. The strong form of problem (2.5) reads: Find θ_ε, such that

$$\left\{\begin{array}{rcll} -\mathrm{div}(k_\varepsilon \nabla\theta_\varepsilon) + \beta\cdot\nabla\theta_\varepsilon &=& b_\varepsilon & \text{in} \quad B_\varepsilon \cup (\Omega\setminus B_\varepsilon), \\ \theta_\varepsilon &=& 0 & \text{on} \quad \partial\Omega, \\ [\![\theta_\varepsilon]\!] &=& 0 & \multirow{2}{*}{\}\ \text{on} \quad \partial\omega_\varepsilon.} \\ [\![k_\varepsilon\nabla\theta_\varepsilon]\!]\cdot n &=& 0 & \end{array}\right. \tag{3.6}$$

After introducing the ansätz (3.5) in (3.6), we obtain

$$-\varepsilon\,\mathrm{div}(k_\varepsilon\nabla\vartheta) - \mathrm{div}(k_\varepsilon\nabla\tilde{\theta}_\varepsilon) + \varepsilon(\beta\cdot\nabla\vartheta) + \beta\cdot\nabla\tilde{\theta}_\varepsilon = 0, \tag{3.7}$$

since θ is solution to (2.1). Now, let us consider a change of variables of the form $x = \varepsilon y$, which implies $\nabla_y\vartheta(y) = \varepsilon\nabla\vartheta(x/\varepsilon)$. Therefore, in the fast variable y the first term of the above equation has order $O(\varepsilon^{-1})$, allowing us to choose ϑ such that

$$\mathrm{div}_y(\gamma_\omega k\nabla_y\vartheta) = 0 \quad \text{in} \quad B_1 \cup (\mathbb{R}^2\setminus B_1), \tag{3.8}$$

where $\omega = B_1$, with B_1 used to denote a ball of unitary radius and

$$\gamma_\omega = \left\{\begin{array}{ll} 1 & \text{in} \quad \mathbb{R}^2\setminus\omega, \\ \gamma & \text{in} \quad \omega. \end{array}\right. \tag{3.9}$$

Now, let us consider the transmission conditions on $\partial\omega_\varepsilon = \partial B_\varepsilon$ that appear in (3.6). In particular, taking into account that the outward unit normal to the boundary ∂B_ε can be written as $n = (x-\hat{x})/\varepsilon$, we have

$$(1-\gamma)\nabla\theta(\hat{x})\cdot n + [\![\gamma_\omega k\nabla_y\vartheta(y)]\!]\cdot n + \varepsilon(1-\gamma)(\nabla\nabla\theta(\xi))n\cdot n + [\![k_\varepsilon\nabla\tilde{\theta}_\varepsilon(x)]\!]\cdot n = 0, \tag{3.10}$$

where $\nabla\theta(x)$ have been expanded in Taylor series around $\hat{x}$, so that ξ is used to denote an intermediate point between x and $\hat{x}$. After collecting the terms of the same power of ε, we obtain the following exterior problems for $\varepsilon\to 0$ defined in the new variable $y = x/\varepsilon$

$$\left\{\begin{array}{rcll} \mathrm{div}_y(\gamma_\omega k\nabla_y\vartheta) &=& 0 & \text{in} \quad B_1\cup(\mathbb{R}^2\setminus B_1), \\ \vartheta &\to& 0 & \text{at} \quad \infty, \\ [\![\vartheta]\!] &=& 0 & \\ [\![\gamma_\omega k\nabla_y\vartheta]\!]\cdot n &=& g_0 & \Big\}\ \text{on} \quad \partial\omega, \end{array}\right. \tag{3.11}$$

with $g_0 = -(1-\gamma)\nabla\theta(\hat{x})\cdot n$. Finally, the remainder $\tilde{\theta}_\varepsilon$ is solution to a boundary value problem that compensates for the discrepancies introduced by the boundary layers ϑ and by the higher order terms of the Taylor series expansion of $\nabla\theta(x)$ around the point $\hat{x}\in\Omega$, namely

$$\left\{\begin{array}{rcll} \mathrm{div}(k_\varepsilon\nabla\tilde{\theta}_\varepsilon) - \beta\cdot\nabla\tilde{\theta}_\varepsilon &=& \varepsilon(\beta\cdot\nabla\vartheta) & \text{in} \quad B_\varepsilon\cup(\Omega\setminus B_\varepsilon), \\ \tilde{\theta}_\varepsilon &=& \varepsilon^2\theta_0 & \text{on} \quad \partial\Omega, \\ [\![\tilde{\theta}_\varepsilon]\!] &=& 0 & \\ [\![k_\varepsilon\nabla\tilde{\theta}_\varepsilon]\!]\cdot n &=& \varepsilon g_1 & \Big\}\ \text{on} \quad \partial\omega_\varepsilon, \end{array}\right. \tag{3.12}$$

where $\theta_0 := -\varepsilon^{-1}\vartheta_{|\partial\Omega}$, $g_1 = -(1-\gamma)(\nabla\nabla\theta(\xi))n\cdot n$, with ξ used to denote an intermediate point between x and $\hat{x}$.

Lemma 2. *Let $\tilde{\theta}_\varepsilon$ be solution to* (3.12). *Then, the estimate $\|\tilde{\theta}_\varepsilon\|_{H^1(\Omega)} = o(\varepsilon)$ holds true.*

Proof. The proof is left to Section 4.1 □

3.2. **Topological Derivative Calculation.** We replace (3.5) into (3.4) to obtain the following result,

$$\psi(\chi_\varepsilon(\hat{x})) - \psi(\chi) = -\frac{1-\gamma}{2}\int_{B_\varepsilon} k(\hat{x})(\nabla\theta\cdot\nabla(\theta+2\varphi))(\hat{x}) - \frac{1-\gamma}{2}\varepsilon\int_{B_\varepsilon} k(\hat{x})\nabla\vartheta\cdot\nabla(\theta+2\varphi)(\hat{x}) + (1-\gamma)\int_{B_\varepsilon}(b\varphi)(\hat{x}) + \mathcal{E}(\varepsilon), \quad (3.13)$$

where $\mathcal{E}(\varepsilon) = \sum_{i=1}^{5}\mathcal{E}_i(\varepsilon) = o(\varepsilon^2)$ as can be seen in Section 4.2, with:

$$\mathcal{E}_1(\varepsilon) = -\frac{1-\gamma}{2}\int_{B_\varepsilon} k(\hat{x})\nabla\tilde{\theta}_\varepsilon\cdot\nabla(\theta+2\varphi), \quad (3.14)$$

$$\mathcal{E}_2(\varepsilon) = -\frac{1-\gamma}{2}\int_{B_\varepsilon} k(\hat{x})[\nabla\theta\cdot\nabla(\theta+2\varphi) - (\nabla\theta\cdot\nabla(\theta+2\varphi))(\hat{x})], \quad (3.15)$$

$$\mathcal{E}_3(\varepsilon) = -\varepsilon\frac{1-\gamma}{2}\int_{B_\varepsilon} k(\hat{x})[\nabla\vartheta\cdot(\nabla(\theta+2\varphi) - \nabla(\theta+2\varphi)(\hat{x}))], \quad (3.16)$$

$$\mathcal{E}_4(\varepsilon) = +(1-\gamma)\int_{B_\varepsilon} b(\hat{x})(\varphi - \varphi(\hat{x})), \quad (3.17)$$

$$\mathcal{E}_5(\varepsilon) = -\frac{1-\gamma}{2}\int_{B_\varepsilon} b(\hat{x})(\theta_\varepsilon - \theta), \quad (3.18)$$

since $k(x) = k(\hat{x})$, $\beta(x) = \beta(\hat{x})$ and $b(x) = b(\hat{x})$ in $B_\varepsilon(\hat{x})$ by assumption. Let us consider again a change of variable in the form $x = \varepsilon y$. Then, the difference (3.13) can be written as:

$$\psi(\chi_\varepsilon(\hat{x})) - \psi(\chi) = -\varepsilon^2\frac{1-\gamma}{2}\int_{B_1} k(\hat{x})(\nabla\theta\cdot\nabla(\theta+2\varphi))(\hat{x}) - \varepsilon^2\frac{1-\gamma}{2}\int_{B_1} k(\hat{x})\nabla_y\vartheta(y)\cdot\nabla(\theta+2\varphi)(\hat{x}) + \varepsilon^2(1-\gamma)\int_{B_1}(b\varphi)(\hat{x}) + \mathcal{E}(\varepsilon). \quad (3.19)$$

The solution to the exterior problem (3.11) is known in the literature since it has exactly the same structure as the Laplace boundary value problem. In addition, for the particular case associated with circular inclusions such solution is explicitly known (see for instance [5] and [16, Ch. 5, pp. 144]). Namely, the solution to (3.11) in B_1 is given by

$$\vartheta(y)_{|B_1} = \frac{1-\gamma}{1+\gamma}\nabla\theta(\hat{x})\cdot(y-\hat{y}). \quad (3.20)$$

Now, let us consider this last result in (3.19), which allows us to evaluate the integral over B_1 explicitly, leading to

$$\psi(\chi_\varepsilon(\hat{x})) - \psi(\chi) = -\pi\varepsilon^2\frac{1-\gamma}{1+\gamma}k(\hat{x})\nabla\theta(\hat{x})\cdot\nabla(\theta+2\varphi)(\hat{x}) + \pi\varepsilon^2(1-\gamma)b(\hat{x})\varphi(\hat{x}) + \mathcal{E}(\varepsilon). \quad (3.21)$$

Finally, we have all necessary elements to state the main result of the paper, which is:

Theorem 3. *Let $\mathcal{J}_\varepsilon(\theta_\varepsilon)$ be the topologically perturbed energy shape functional given by* (2.6)*. Then, it admits the topological asymptotic expansion of the form*

$$\mathcal{J}_\varepsilon(\theta_\varepsilon) = \mathcal{J}(\theta) - \pi\varepsilon^2\rho\|\nabla\theta\|^2 - 2\pi\varepsilon^2\rho\nabla\theta\cdot\nabla\varphi + \pi\varepsilon^2(1-\gamma)b\,\varphi + \mathcal{E}(\varepsilon), \quad (3.22)$$

with the function $f(\varepsilon) = \pi\varepsilon^2$, $\mathcal{E}(\varepsilon) = o(\varepsilon^2)$ according to Section 4.2 and the topological derivative given by

$$D_T\mathcal{J}(\hat{x}) = -\rho\|\nabla\theta(\hat{x})\|^2 - 2\rho\nabla\theta(\hat{x})\cdot\nabla\varphi(\hat{x}) + (1-\gamma)b(\hat{x})\varphi(\hat{x}), \quad (3.23)$$

where θ and φ are solutions to the direct (2.1) *and adjoint* (2.3) *problems, respectively, both associated to the original unperturbed domain Ω. Finally, $\rho = k(\hat{x})(1-\gamma)/(1+\gamma)$.*

4. Estimation for the Remainders

In this section, the proof of Lemma 2 and the estimation for the remainder $\mathcal{E}(\varepsilon)$ left in the asymptotic expansion (3.13) are presented. We assume that the topological perturbation $B_\varepsilon(\hat{x})$ doesn't touch the boundary $\partial\Omega$, namely, $\overline{B_\varepsilon}(\hat{x}) \Subset \Omega$.

4.1. **Proof of Lemma 2 .** For the sake of completeness, we introduce the explicit solution to the scalar exterior problem (3.11), which can be found in many references (see for instance [16, Ch. 5, pp. 144]). Namely,

$$\vartheta(x/\varepsilon)_{|\Omega\setminus\overline{B_\varepsilon}} = \frac{\varepsilon}{\|x-\hat{x}\|^2}\nabla\theta(\hat{x})\cdot(x-\hat{x}) \tag{4.1}$$

$$\vartheta(x/\varepsilon)_{|B_\varepsilon} = \varepsilon^{-1}\nabla\theta(\hat{x})\cdot(x-\hat{x}). \tag{4.2}$$

From the above formulas, we observe that $\vartheta_{|\partial\Omega} = -\varepsilon\theta_0$, with function θ_0 independent of the small parameter ε. In addition, from a simple calculation there are $\|\vartheta\|_{L^2(\partial B_\varepsilon)} = O(\sqrt{\varepsilon})$, $\|\vartheta\|_{L^2(B_\varepsilon)} = O(\varepsilon)$ and $\|\vartheta\|_{L^2(\Omega)} = O(\varepsilon\sqrt{|\log\varepsilon|}) = o(\varepsilon^\delta)$, with $\delta < 1$. Now, we have all elements to proof Lemma 2. We start by decomposing the solution to (3.12) as $\tilde{\theta}_\varepsilon = \tilde{\theta}_\varepsilon^h + \tilde{\theta}_\varepsilon^p$. Therefore:

Lemma 4. *Let $\tilde{\theta}_\varepsilon^h$ be solution to the following variational problem:*

$$\tilde{\theta}_\varepsilon^h \in \tilde{\mathcal{U}}_\varepsilon : \int_\Omega k_\varepsilon \nabla\tilde{\theta}_\varepsilon^h \cdot \nabla\eta + \int_\Omega (\beta\cdot\nabla\tilde{\theta}_\varepsilon^h)\eta = \varepsilon\int_{\partial B_\varepsilon} g_1\eta, \ \forall\eta\in H_0^1, \tag{4.3}$$

where $\tilde{\mathcal{U}}_\varepsilon = \{\varphi\in H^1(\Omega) : \varphi|_{\partial\Omega} = \varepsilon^2\theta_0\}$. Then, the estimate $\|\tilde{\theta}_\varepsilon^h\|_{H^1(\Omega)} = O(\varepsilon^2)$ holds true.

Proof. By taking $\eta = \tilde{\theta}_\varepsilon^h - \varepsilon^2\varphi_\theta$ in (4.3), we have the equality

$$\int_\Omega k_\varepsilon\nabla\tilde{\theta}_\varepsilon^h\cdot\nabla\tilde{\theta}_\varepsilon^h + \int_\Omega(\beta\cdot\nabla\tilde{\theta}_\varepsilon^h)\tilde{\theta}_\varepsilon^h = \varepsilon\int_{\partial B_\varepsilon} g_1\,\tilde{\theta}_\varepsilon^h + \varepsilon^2\int_{\partial\Omega} k(\nabla\tilde{\theta}_\varepsilon^h\cdot n)\theta_0, \tag{4.4}$$

where $\varphi_\theta\in H^1(\Omega)$ is the lifting of the Dirichlet boundary data θ_0. The second term on the left hand side of (4.4) can be replace by

$$\int_\Omega(\beta\cdot\nabla\tilde{\theta}_\varepsilon^h)\tilde{\theta}_\varepsilon^h = \frac{\varepsilon^2}{2}\int_{\partial\Omega}(\beta\cdot n)\theta_0\,\tilde{\theta}_\varepsilon^h, \tag{4.5}$$

since $\mathrm{div}(\beta) = 0$ by assumption and $\tilde{\theta}_\varepsilon^h = \varepsilon^2\theta_0$ on $\partial\Omega$. Therefore,

$$\int_\Omega k_\varepsilon\nabla\tilde{\theta}_\varepsilon^h\cdot\nabla\tilde{\theta}_\varepsilon^h = \varepsilon\int_{\partial B_\varepsilon} g_1\,\tilde{\theta}_\varepsilon^h + \varepsilon^2\int_{\partial\Omega} k(\nabla\tilde{\theta}_\varepsilon^h\cdot n)\theta_0 - \frac{\varepsilon^2}{2}\int_{\partial\Omega}(\beta\cdot n)\theta_0\,\tilde{\theta}_\varepsilon^h, \tag{4.6}$$

From the Cauchy-Schwarz inequality we obtain

$$\int_\Omega k_\varepsilon\nabla\tilde{\theta}_\varepsilon^h\cdot\nabla\tilde{\theta}_\varepsilon^h \le \varepsilon^2 C_1\|\tilde{\theta}_\varepsilon^h\|_{H^{1/2}(\partial B_\varepsilon)} + \varepsilon^2 C_2\|\partial_n\tilde{\theta}_\varepsilon^h\|_{H^{-1/2}(\partial\Omega)} + \varepsilon^2 C_3\|\tilde{\theta}_\varepsilon^h\|_{H^{1/2}(\partial\Omega)}, \tag{4.7}$$

where we have used the interior elliptic regularity of function θ. Taking into account the trace theorem, we have

$$\int_\Omega k_\varepsilon\,\nabla\tilde{\theta}_\varepsilon^h\cdot\nabla\tilde{\theta}_\varepsilon^h \le \varepsilon^2 C_4\|\tilde{\theta}_\varepsilon^h\|_{H^1(\Omega)}. \tag{4.8}$$

Finally, from the Poincaré inequality on the left hand side of (4.8), namely,

$$c\|\tilde{\theta}_\varepsilon^h\|_{H^1(\Omega)}^2 \le \int_\Omega k_\varepsilon\,\nabla\tilde{\theta}_\varepsilon^h\cdot\nabla\tilde{\theta}_\varepsilon^h, \tag{4.9}$$

we have,

$$\|\tilde{\theta}_\varepsilon^h\|_{H^1(\Omega)} \le C\varepsilon^2, \tag{4.10}$$

which leads to the result, with $C = C_4/c$ independent of ε. ☐

Lemma 5. *Let $\tilde{\theta}^p_\varepsilon$ be solution to the following variational problem:*

$$\tilde{\theta}^p_\varepsilon \in H^1_0 : \int_\Omega k_\varepsilon \nabla\tilde{\theta}^p_\varepsilon \cdot \nabla\eta + \int_\Omega (\beta\cdot\nabla\tilde{\theta}^p_\varepsilon)\eta = -\varepsilon\int_\Omega(\beta\cdot\nabla\vartheta)\eta,\ \forall\eta\in H^1_0. \tag{4.11}$$

Then, the estimates $\|\tilde{\theta}^p_\varepsilon\|_{H^1(\Omega)} = o(\varepsilon)$ holds true.

Proof. By setting $\eta = \tilde{\theta}^p_\varepsilon$ in (4.11), we have the equality

$$\int_\Omega k_\varepsilon\nabla\tilde{\theta}^p_\varepsilon\cdot\nabla\tilde{\theta}^p_\varepsilon + (\beta\cdot\nabla\tilde{\theta}^p_\varepsilon)\tilde{\theta}^p_\varepsilon = -\varepsilon\int_\Omega(\beta\cdot\nabla\vartheta)\tilde{\theta}^p_\varepsilon. \tag{4.12}$$

The second term on the left hand side of (4.12) vanishes, since $\tilde{\theta}^p_\varepsilon = 0$ on $\partial\Omega$ and $\operatorname{div}(\beta)=0$ by assumption. Let us consider the right hand side of (4.12). Integration by parts yields

$$\int_\Omega(\beta\cdot\nabla\vartheta)\tilde{\theta}^p_\varepsilon = (1-\gamma)\int_{\partial B_\varepsilon}(\beta\cdot n)\vartheta\,\tilde{\theta}^p_\varepsilon + (1-\gamma)\int_{B_\varepsilon}(\beta\cdot\nabla\tilde{\theta}^p_\varepsilon)\vartheta - \int_\Omega(\beta\cdot\nabla\tilde{\theta}^p_\varepsilon)\vartheta, \tag{4.13}$$

From the Cauchy-Schwarz inequality

$$\int_\Omega(\beta\cdot\nabla\vartheta)\tilde{\theta}^p_\varepsilon \le C_1\|\tilde{\theta}^p_\varepsilon\|_{L^2(\partial B_\varepsilon)}\|\vartheta\|_{L^2(\partial B_\varepsilon)} + C_2\|\nabla\tilde{\theta}^p_\varepsilon\|_{L^2(B_\varepsilon)}\|\vartheta\|_{L^2(B_\varepsilon)} + C_3\|\nabla\tilde{\theta}^p_\varepsilon\|_{L^2(\Omega)}\|\vartheta\|_{L^2(\Omega)}, \tag{4.14}$$

and the trace theorem, we obtain

$$\int_\Omega(\beta\cdot\nabla\vartheta)\tilde{\theta}^p_\varepsilon \le C_4\|\tilde{\theta}^p_\varepsilon\|_{H^1(B_\varepsilon)}\|\vartheta\|_{L^2(\partial B_\varepsilon)} + C_5\|\tilde{\theta}^p_\varepsilon\|_{H^1(\Omega)}\|\vartheta\|_{L^2(\Omega)} \le C_6\varepsilon^{1/2}\|\tilde{\theta}^p_\varepsilon\|_{H^1(\Omega)}, \tag{4.15}$$

since $\|\vartheta\|_{L^2(\partial B_\varepsilon)} = O(\sqrt{\varepsilon})$ and $\|\vartheta\|_{L^2(\Omega)} = o(\varepsilon^\delta)$, with $\delta < 1$. Then, from the above results we obtain

$$\int_\Omega k_\varepsilon\nabla\tilde{\theta}^p_\varepsilon\cdot\nabla\tilde{\theta}^p_\varepsilon \quad\le\quad C_6\varepsilon^{3/2}\|\tilde{\theta}^p_\varepsilon\|_{H^1(\Omega)}. \tag{4.16}$$

From the Poincaré inequality on the left hand side of (4.16), namely,

$$c\|\tilde{\theta}^p_\varepsilon\|^2_{H^1(\Omega)} \le \int_\Omega k_\varepsilon\nabla\tilde{\theta}^p_\varepsilon\cdot\nabla\tilde{\theta}^p_\varepsilon, \tag{4.17}$$

we finally obtain

$$\|\tilde{\theta}^p_\varepsilon\|_{H^1(\Omega)} \le C\varepsilon^{3/2}, \tag{4.18}$$

which leads to the result, with $C = C_6/c$ independent of ε. □

Finally, the proof of Lemma 2 follows immediately from the results of Lemma 4 and Lemma 5.

4.2. **Estimation for the Remainder $\mathcal{E}(\varepsilon)$.** Let us start by considering the remainder $\mathcal{E}_1(\varepsilon)$ given by (3.14), namely

$$\mathcal{E}_1(\varepsilon) = (1-\gamma)\int_{B_\varepsilon} k(\hat{x})\nabla\tilde{\theta}_\varepsilon\cdot(\nabla(\theta+2\varphi)\pm\nabla(\theta+2\varphi)(\hat{x})). \tag{4.19}$$

Taking into account the Cauchy-Schwartz inequality, we have

$$\mathcal{E}_1(\varepsilon) \le C_0\left(\|\nabla(\theta+2\varphi)-\nabla(\theta+2\varphi)(\hat{x})\|_{L^2(B_\varepsilon)}\|\nabla\tilde{\theta}_\varepsilon\|_{L^2(B_\varepsilon)} + \|\nabla(\theta+2\varphi)(\hat{x})\|_{L^2(B_\varepsilon)}\|\nabla\tilde{\theta}_\varepsilon\|_{L^2(B_\varepsilon)}\right). \tag{4.20}$$

From the interior elliptic regularity of functions φ and θ there is $\|\nabla(\theta+2\varphi)-\nabla(\theta+2\varphi)(\hat{x})\| \le c_1\|x-\hat{x}\|$ in $B_\varepsilon(\hat{x})$, where c_1 is a constant independent of ε. Then, in view of Lemma 2, there is

$$\mathcal{E}_1(\varepsilon) \le C_1\varepsilon\|\nabla\tilde{\theta}_\varepsilon\|_{L^2(B_\varepsilon)} \le C_1\varepsilon\|\tilde{\theta}_\varepsilon\|_{H^1(\Omega)} = o(\varepsilon^2), \tag{4.21}$$

where we have used the fact that $\|\nabla(\theta+2\varphi)(\hat{x})\|_{L^2(B_\varepsilon)} = O(\varepsilon)$ and $\|x-\hat{x}\|_{L^2(B_\varepsilon)} = O(\varepsilon^2)$. Regarding the remainder $\mathcal{E}_2(\varepsilon)$ given by (3.15), let us introduce the notation $h_2 = k(\hat{x})\nabla\theta\cdot\nabla(\theta+$

$2\varphi)$. From the interior elliptic regularity of functions θ and φ, we have $\|h_2(x)-h_2(\hat{x})\| \le c_2\|x-\hat{x}\|$ in $B_\varepsilon(\hat{x})$, where c_2 is a constant independent of ε. Therefore,

$$\mathcal{E}_2(\varepsilon) = -\frac{1-\gamma}{2}\int_{B_\varepsilon} (h_2(x) - h_2(\hat{x})) \le C_2 \int_{B_\varepsilon} \|x-\hat{x}\| = o(\varepsilon^2). \tag{4.22}$$

We introduce the notations $G_3 = k(\hat{x})\nabla\vartheta$ and $H_3 = \nabla(\theta + 2\varphi)$. Once again, from the interior elliptic regularity of the functions φ and θ, there is $\|H_3(x) - H_3(\hat{x})\| \le c_3\|x-\hat{x}\|$ in $B_\varepsilon(\hat{x})$, where c_3 is a constant independent of ε. Thus the remainder $\mathcal{E}_3(\varepsilon)$ given by (3.16) can be bounded as

$$\mathcal{E}_3(\varepsilon) = -\varepsilon\frac{1-\gamma}{2}\int_{B_\varepsilon} G_3\cdot(H_3(x) - H_3(\hat{x})) \le \varepsilon C_3\|G_3\|_{L^2(B_\varepsilon)}\|x-\hat{x}\|_{L^2(B_\varepsilon)} = o(\varepsilon^2), \tag{4.23}$$

where we have used the explicit solution to ϑ. From the interior elliptic regularity of function φ, there is $\|\varphi(x) - \varphi(\hat{x})\| \le c_4\|x-\hat{x}\|$, with constant c_4 independent of ε. So that the remainder $\mathcal{E}_4(\varepsilon)$ given by (3.17) can be bounded as follows

$$\mathcal{E}_4(\varepsilon) \le C_4\|b(\hat{x})\|_{L^2(B_\varepsilon)}\|\varphi - \varphi(\hat{x})\|_{L^2(B_\varepsilon)} = o(\varepsilon^2), \tag{4.24}$$

where we have used again $\|b(\hat{x})\|_{L^2(B_\varepsilon)} = O(\varepsilon)$ and $\|x-\hat{x}\|_{L^2(B_\varepsilon)} = O(\varepsilon^2)$. Finally, let us consider the remainder $\mathcal{E}_5(\varepsilon)$ given by (3.18). From the Hölder inequality and the Sobolev embedding theorem, it comes for any $p > 1$

$$\mathcal{E}_5(\varepsilon) \le C_5\varepsilon^{1+1/p}\|\theta_\varepsilon - \theta\|_{L^{2p/(p-1)}(B_\varepsilon)} \le C_6\varepsilon^{1+1/p}\|\theta_\varepsilon - \theta\|_{H^1(\Omega)} = o(\varepsilon^2), \tag{4.25}$$

where we have used Lemma 1.

5. Conclusions

In this paper the topological derivative for the energy shape functional associated with the diffusive/convective steady state heat equation has been derived in its closed form. In particular, the existence of the topological derivative has been proved and precise estimates for the remainders have been derived. The obtained result is new and can be used in many applications such as topology design of heat sinks, for instance.

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