Shape derivatives of the probability to find a fixed number of electrons chemically characterized by a wave function

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Abstract

In Quantum Chemistry, researchers are interested in finding new ways to describe well the electronic structures of molecules and their interactions. The model of Maximal Probability Domains (MPDs) is a developing method based on probabilities that allows such a geometrical and spatial characterization of the electronic structures of chemical systems.

In this article, we consider quantum systems of n electrons chemically characterized by general wave functions. For any integer $k \geqslant 1$, we derive a formula for the k-th-order shape derivative of the functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$, with $p_\nu(\Omega)$ the probability to find exactly a fixed number ν of electrons in a given spatial region $\Omega \subseteq \mathbb{R}^3$, where *exactly* means that the $n-\nu$ remaining ones are located in the complement $\mathbb{R}^3\backslash\Omega$.

This explicit formula is computable by Quantum Monte-Carlo methods and it holds true with respect to the $W^{1,\infty}$-perturbations of a measurable domain for H^k-regular wave functions. Then, by restricting our analysis to the first- and second-order shape derivatives, we can make our statement more precise with respect to the regularity of the domain, and recover the usual structure expected from shape derivatives.

The main ingredient of the proof consists in generalizing at any higher order the well-known expressions for the first- and second-order shape derivatives of a volume integral. Although we only need to assume that the domain is measurable to get the shape differentiability of a volume integral at any order, we also prove that the $C^{1,1}$-regularity is enough to provide a notion of partial derivative with respect to the domain at any order (shape gradient, Hessian,...).

Keywords : shape optimization, shape derivatives, volume integral, maximal probability domains, geometry of wave functions, quantum chemistry.

AMS classification : 49K40, 49M15, 49M05, 81Q99, 92E99, 81V99, 51M04, 51M16.

1 Introduction

On the one hand, the traditional chemical intuition i.e. the way chemists understand how molecules interact together has been deeply influenced by a localized vision of electrons around the cores. Indeed, it yields to fruitful concepts [23, 29, 38] firmly rooted to the models because it can simply explain many different experimental manifestations. On the other hand, Quantum Mechanics [21, 32, 41] allows the electrons to be delocalized over the whole space. Indeed, a chemical system of n electrons is completely characterized by its wave function, *a priori* defined everywhere.

Hence, there is a loss of chemical informations that Quantum Chemistry tries to recover in several manners. Interpretative methods (valence bond theory, molecular orbitals) work in the Fock space when the correlation between electrons is small, while topological approaches try to partition directly the physical space into regions with a chemical meaning [2, 3, 15, 31, 35, 39].

One way to reconnect the usual expectations of chemists with the results of accurate quantum mechanical calculations consists in removing the problematical high-dimensionality of the wave function by averaging it correctly over the positions of electrons [11, 19, 30]. More precisely, computing the probability $p_\nu(\Omega)$ to find exactly a fixed number ν of electrons in a given spatial region $\Omega \subseteq \mathbb{R}^3$, where *exactly* means that the $n-\nu$ remaining ones are located in the complement part $\mathbb{R}^3\backslash\Omega$, one can try to solve the following shape optimization problem:

$$\sup_{\Omega \subseteq \mathbb{R}^3} p_\nu(\Omega). \tag{1}$$

*Centro de Modelamiento Matemático (CMM), Facultad de Ciencas Físicas y Matemáticas (FCFM), UMR 2071 CNRS-Universidad de Chile, Beauchef 851, Santiago, Chile (jdalphin@dim.uchile.cl).

Suggested by Savin in [34], the model of Maximal Probability Domains (MPDs) i.e. searching for the local/global maximizers and the critical points of (1) is a developing method based on probabilities that allows a geometrical and spatial characterization of the electronic structures of molecules and their interactions. Indeed, it has shown to provide vivid images of cores and valence regions of atoms [7, 34], lone and bonding pairs [26], and domains in which can move the electrons in a simple molecule [20, 24, 25], a liquid [1], a crystal [9, 10], or in an inorganic compound [8].

Therefore, MPDs may become a rigorous entry point to recover standard chemical concepts from the quantum informations of the systems gathered in the wave functions. For example, the domains that locally maximize the probability to find exactly two electrons can be directly related to the Lewis' concept of electron pair [23] and it provides a visual representation of this chemical interaction in the physical three-dimensional space.

The mathematical existence and regularity of maximizers for (1) are difficult and open problems, even for simple analytic wave functions such as a two-electron molecule. Indeed, the direct method from Calculus of Variations does not apply here. Roughly speaking, there is a lack of continuity and compactness due to the poor control we have on the perimeter of a minimizing sequence. The boundary can oscillate severely, reveal some cracks and cusps, or simply become unbounded.

From a numerical point of view, it is still an on-going effort to develop algorithms and programs that are able to efficiently optimize the domains solving (1). The gradient and Newton methods heavily rely on the concept of shape derivatives [7, 25], where mesh adaptation techniques seem necessary to ensure a certain confidence in the numerical MPDs obtained. We also mention [36, 37] where a Quantum Monte-Carlo approach is used to obtain some MPDs.

The goal of this article is to properly derive formulas for the shape derivatives of the functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$ with general wave functions. To our knowledge, such a theoretical study has not been carried out in its generality, although some expressions were obtained at the Hartree-Fock level [7, 25]. In particular, the first- and second-order shape derivatives are fundamental in the numerical implementation but also to gain theoretical informations about the nature of MPDs.

In this paper, our first main contribution is to study the (Fréchet) differentiability properties of the map $p_{\nu,\Omega} : \theta \mapsto p_\nu[(I+\theta)(\Omega)]$ associated with the shape functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$ for general wave functions Ψ. Under the H^k-regularity of Ψ, we get that $p_{\nu,\Omega}$ is of class C^k around the origin for any integer $k \geqslant 0$ and for any measurable subset Ω of $\mathbb{R}^3$. The results with their precise references in the text are sum up in Table 1, where $\mathbb{B}^{0,1}$ refers to the set of Lipschitz contractions.

$\Omega \subseteq \mathbb{R}^3$	Ψ	$\theta : \mathbb{R}^3 \to \mathbb{R}^3$	**Regularity of** $p_{\nu,\Omega} : \theta \mapsto p_\nu\left[(I+\theta)(\Omega)\right]$	**Proof**
Measurable	L^2		The map $p_\nu : \Omega \mapsto p_\nu(\Omega)$ is well defined.	Definition 2.2
Measurable	L^2	$C^{0,1}$	$p_{\nu,\Omega}$ is well defined on $\mathbb{B}^{0,1}$.	Lemma 2.6
Measurable	L^2	$W^{1,\infty}$	$p_{\nu,\Omega}$ is of class C^0 on $\mathbb{B}^{0,1} \cap W^{1,\infty}$.	Lemma 2.6
Measurable	H^1	$W^{1,\infty}$	$p_{\nu,\Omega}$ is of class C^1 on $\mathbb{B}^{0,1} \cap W^{1,\infty}$.	Corollary 2.9
Lipschitz	H^1	$W^{1,\infty}$	p_ν has a well-defined shape gradient.	Theorem 2.8
Measurable	H^2	$W^{1,\infty}$	$p_{\nu,\Omega}$ is of class C^2 on $\mathbb{B}^{0,1} \cap W^{1,\infty}$.	Corollary 2.11
Lipschitz	H^2	$W^{1,\infty} \cap C^1$	$p_{\nu,\Omega}$ is of class C^2 on $\mathbb{B}^{0,1} \cap W^{1,\infty} \cap C^1$.	Corollary 2.11
$C^{1,1}$-domain	H^2	$W^{1,\infty} \cap C^1$	p_ν has a well-defined shape Hessian.	Theorem 2.10
Measurable	H^k	$W^{1,\infty}$	$p_{\nu,\Omega}$ is of class C^k on $\mathbb{B}^{0,1} \cap W^{1,\infty}$.	Theorem 2.7

Table 1: *Summary of the regularity results concerning the functional* $p_{\nu,\Omega} : \theta \mapsto p_\nu[(I+\theta)(\Omega)]$.

The main achievement of Theorem 2.7 is to get an explicit formula (21) for the k-th-order shape derivative of p_ν i.e. the k-th-order (Fréchet) differential of $p_{\nu,\Omega}$ at the origin for any integer $k \geqslant 1$. The counterpart of this general result is the poor structure we get for the shape derivatives of p_ν. Hence, by restricting our analysis to the low-order ones, our second main contribution consists in recovering the shape gradient and Hessian form that are expected from more regular domains [28] [22, Section 5.9] [6].

In Theorem 2.8, we show that if the domain has a Lipschitz boundary, then the functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$ of Definition 2.2 has a first-order shape derivative of the following form:

$$\forall \theta \in W^{1,\infty}\left(\mathbb{R}^3, \mathbb{R}^3\right), \qquad D_{\mathbf{0}} p_{\nu,\Omega}(\theta) = \int_{\partial\Omega} \frac{\partial p_\nu}{\partial \Omega}(\mathbf{x})\, \theta_{\mathbf{n}}(\mathbf{x})\, dA(\mathbf{x}), \tag{2}$$

where the integration on the boundary $\partial\Omega$ is done with respect to the two-dimensional Hausdorff measure referred to as $A(\bullet)$, where $(\bullet)_{\mathbf{n}} := \langle(\bullet) \mid \mathbf{n}_\Omega\rangle$ is the normal component of a vector field, with $\mathbf{n}_\Omega(\mathbf{x})$ the unit vector normal to the boundary $\partial\Omega$ at the point $\mathbf{x}$ and pointing outwards Ω, and where the following map is well defined by (26):

$$\frac{\partial p_\nu}{\partial\Omega} : \partial\Omega \longrightarrow \mathbb{R}.$$

It depends on the domain Ω but *not* on the perturbation θ. Hence, by analogy with the finite-dimensional case, it is called the shape gradient of p_ν.

Similarly, in Theorem 2.10, we prove that if the domain has a $C^{1,1}$-boundary, then the functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$ of Definition 2.2 has a second-order shape derivative of the following form:

$$\begin{aligned}\forall(\theta,\tilde{\theta}) \in \left(W^{1,\infty}\cap C^1\right)^2, \quad D^2_{\mathbf{0}}p_{\nu,\Omega}(\theta,\tilde{\theta}) = &\int_{\partial\Omega} \frac{\partial^2 p_\nu}{\partial\Omega^2}(\mathbf{x})\,\theta_{\mathbf{n}}(\mathbf{x})\,\tilde{\theta}_{\mathbf{n}}(\mathbf{x})\,dA(\mathbf{x}) \\ &+ \int_{\partial\Omega}\int_{\partial\Omega} K_\Omega(\mathbf{x},\mathbf{y})\,\theta_{\mathbf{n}}(\mathbf{x})\,\tilde{\theta}_{\mathbf{n}}(\mathbf{y})\,dA(\mathbf{x})\,dA(\mathbf{y}) \\ &- \int_{\partial\Omega} \frac{\partial p_\nu}{\partial\Omega}(\mathbf{x})\,Z[\theta,\tilde{\theta}](\mathbf{x})\,dA(\mathbf{x}).\end{aligned} \tag{3}$$

We mention that in (3) the perturbations θ and $\tilde{\theta}$ must be continuously differentiable since the expression of Z involves the derivatives of θ and $\tilde{\theta}$ whose values are computed on the boundary. The first term of (3) can be interpreted as the Hessian part of the second-order shape derivative. Indeed, the following map is well defined by (35):

$$\frac{\partial^2 p_\nu}{\partial\Omega^2} : \partial\Omega \longrightarrow \mathbb{R}.$$

It depends on Ω but *not* on the perturbations $(\theta,\tilde{\theta})$. By analogy with the finite-dimensional case, it is called the shape Hessian of p_ν. However, the second term in (3) also plays an important role. It has the form of a kernel and the following map is well defined by (34):

$$K_\Omega : \partial\Omega \times \partial\Omega \longrightarrow \mathbb{R}.$$

Again, the kernel K_Ω depends on Ω but *not* on the perturbations θ and $\tilde{\theta}$. Finally, note that the last term in (3) depends on the shape gradient. In particular, if Ω is a critical shape for p_ν i.e. if $D_{\mathbf{0}}p_{\nu,\Omega} \equiv 0$, then $\frac{\partial p_\nu}{\partial\Omega} = 0$ and this term is equal to zero. It also depends on the vector field:

$$Z[\theta,\tilde{\theta}] := \mathbf{II}_\Omega\left[\tilde{\theta}_{\partial\Omega},\theta_{\partial\Omega}\right] + \left\langle \nabla_{\partial\Omega}(\theta_{\mathbf{n}}) \mid \tilde{\theta}_{\partial\Omega}\right\rangle + \left\langle \nabla_{\partial\Omega}(\tilde{\theta}_{\mathbf{n}}) \mid \theta_{\partial\Omega}\right\rangle, \tag{4}$$

where $(\bullet)_{\partial\Omega} := (\bullet) - (\bullet)_{\mathbf{n}}\mathbf{n}_\Omega$ refers to the tangential component of a vector field, and in particular $\nabla_{\partial\Omega}(\bullet) := \nabla(\bullet) - \langle\nabla(\bullet) \mid \mathbf{n}_\Omega\rangle\mathbf{n}_\Omega$ is the tangential component of the gradient operator, where $\mathbf{II}_\Omega(\bullet,\bullet) := -\langle D_{\partial\Omega}\mathbf{n}_\Omega(\bullet) \mid (\bullet)\rangle$ is the second fundamental form associated to the $C^{1,1}$-surface $\partial\Omega$, which is a symmetric bilinear form on the tangent space, with $D_{\partial\Omega}(\bullet) := D(\bullet) - D(\bullet)\mathbf{n}_\Omega[\mathbf{n}_\Omega]^T$ denoting the tangential component of the differential operator on vector fields. In particular, if the perturbations θ and $\tilde{\theta}$ are normal to the boundary $\partial\Omega$ i.e. if $\theta_{\partial\Omega} = \tilde{\theta}_{\partial\Omega} = 0$, then $Z[\theta,\tilde{\theta}] \equiv 0$ and the last term in (3) is again equal to zero in this case.

The method used for the proof of Theorem 2.7 consists in expressing $p_{\nu,\Omega}$ as a volume integral on an higher-dimensional space. The first- and second-order shape derivatives of a volume integral are well known in the context of shape calculus [16, Chapter 9] [22, Chapter 5] [40, Chapter 2]. However, the differentiability results of a shape functional $F : \Omega \mapsto F(\Omega)$ are usually stated and proved in terms of directional derivatives $t \in \mathbb{R} \mapsto F[(I + t\theta)(\Omega)]$ rather than Fréchet differential.

Indeed, we usually have $F(\Omega) := \int_\Omega f$, where the integrand f can depend on Ω, for example through the solutions of partial differential equations (PDEs), or can only be defined on Ω, making difficulties in defining f on the domain perturbations. Hence, in this case, it is easier to handle a real variable t than a space of vector fields θ. Since the two viewpoints are not entirely equivalent, we emphasize that we consider here the Fréchet setting for the derivatives.

Moreover, the shape derivatives of order higher than two are little studied [22, Section 5.9.7] although some structure theorems are available [28] [22, Section 5.9.4] [6]. Indeed, the second-order shape derivative is usually enough to conclude about the optimality of a shape [13, 14], and even in this case, the theoretical/numerical computation are difficult, especially when PDEs are involved.

In our situation, things are much simpler because the integrand f is defined on the whole space and does not depend on the domain Ω. Therefore, our third main contribution in this paper is stated in Theorem 3.2. We prove that for any integer $k \geqslant 0$, if $f \in W^{k,1}$ and if Ω is measurable, then the associated map $F_\Omega : \theta \in W^{1,\infty} \mapsto \int_{(I+\theta)(\Omega)} f$ is of class C^k around the origin.

The main achievement of Theorem 3.2 is to obtain an explicit formula (43) for the k-th-order shape derivative of F i.e. for the k-th-order differential of F_Ω at the origin for any integer $k \geqslant 1$. In Theorem 3.3, we also manage to express (43) into a divergence form. Consequently, if Ω has a Lipschitz boundary, then the shape derivatives of F are expressed as boundary integrals (49)–(50). In particular, in Corollary 3.5, we recover the well-known structure of shape gradient for the first-order shape derivative of F:

$$\forall \theta \in W^{1,\infty}, \quad D_{\mathbf{0}} F_\Omega(\theta) = \int_{\partial\Omega} f \theta_{\mathbf{n}} dA.$$

Furthermore, in Theorem 3.6, we show that for any integer $k \geqslant 2$, if Ω is a $C^{1,1}$-domain and if the perturbations are normal to the boundary (this hypothesis is fundamental here), then the k-th-order shape derivative of F has the following structure:

$$\forall (\theta^1, \ldots, \theta^k) \in \left(W^{1,\infty} \cap C^1\right)^k, \qquad D^k_{\mathbf{0}} F_\Omega \left(\theta^1, \ldots, \theta^k\right) = \int_{\partial\Omega} \frac{\partial^k F}{\partial \Omega^k}(\mathbf{x}) \left(\prod_{i=1}^k \theta^i_{\mathbf{n}}(\mathbf{x}) \right) dA(\mathbf{x}). \quad (5)$$

The well-defined map $\frac{\partial^k F}{\partial \Omega^k} : \partial\Omega \to \mathbb{R}$ depends on f and Ω but *not* on the perturbations $(\theta^1, \ldots, \theta^k)$. Hence, by analogy with the finite-dimensional case, it is called the k-th-order partial derivative of F with respect to the domain Ω. In addition, it has an explicit expression which is given by:

$$\frac{\partial^k F}{\partial \Omega^k} = \sum_{i_1,\ldots,i_{k-1}=1}^{n} \sum_{l=0}^{k-1} \sum_{\substack{I_l \subseteq [\![1,k-1]\!] \\ \text{card } I_l = l}} \sum_{p \in \mathcal{S}_{I_l}} s(p) \frac{\partial^{k-1-l} f}{\prod\limits_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} \partial \mathbf{x}_{i_j}} \prod_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} [\mathbf{n}_\Omega]_{i_j} \prod_{j \in I_l} [D_{\partial\Omega} \mathbf{n}_\Omega]_{i_j i_{p(j)}}, \quad (6)$$

where $\mathcal{S}_{I_l}$ is the set of permutations on I_l i.e. of the bijective maps from I_l into I_l, and where $s : \mathcal{S}_{I_l} \to \{-1, 1\}$ denotes the signature associated with permutations. In order to get back to the usual case of permutations on $[\![1, l]\!]$, we recall that the signature of a permutation $p \in \mathcal{S}_{I_l}$ is defined as $s(p) := s(p_{I_l}^{-1} \circ p \circ p_{I_l})$, where p_{I_l} is the unique strictly increasing map from $[\![1, l]\!]$ into I_l. We also emphasize the fact that the boundary values of the partial derivatives of f have to be understood in the sense of trace. In particular, the map (6) is uniquely determined on $\partial\Omega$ up to a set of zero $A(\partial\Omega \cap \bullet)$-measure, and as a consequence, it is correct to speak about *the* partial derivatives of F with respect to the domain Ω.

The formula (6) is very well known for little value of k but to our knowledge, such a general expression is new in its generality. We refer to Corollary 3.7 for a precise statement concerning the case $k = 2$ and for practical purpose, we compute the first partial derivatives:

$$\begin{cases} \frac{\partial F}{\partial \Omega} = f \\ \\ \frac{\partial^2 F}{\partial \Omega^2} = \langle \nabla f \mid \mathbf{n}_\Omega \rangle \ + \ H_\Omega \ f \\ \\ \frac{\partial^3 F}{\partial \Omega^3} = \langle \text{Hess } f\left(\mathbf{n}_\Omega\right) \mid \mathbf{n}_\Omega \rangle + 2 H_\Omega \ \langle \nabla f \mid \mathbf{n}_\Omega \rangle + f \left[H_\Omega^2 - \text{trace}\left(D_{\partial\Omega} \mathbf{n}_\Omega^2 \right) \right], \end{cases} \quad (7)$$

where $H_\Omega := \text{div}_{\partial\Omega} \mathbf{n}_\Omega$ is the scalar mean curvature associated with the $C^{1,1}$-(hyper)surface $\partial\Omega$, with $\text{div}_{\partial\Omega}(\bullet) := \text{div}(\bullet) - \langle D(\bullet)\mathbf{n}_\Omega \mid \mathbf{n}_\Omega \rangle = \text{trace}[D_{\partial\Omega}(\bullet)]$ denoting the tangential component of the divergence operator.

To conclude this introduction, let us now explain how the paper is organized. In Section 2, we obtain the shape derivatives of $p_\nu : \Omega \to p_\nu(\Omega)$ for general wave functions. First, we define the probability as a shape functional in Section 2.1. In Section 2.2, we give the general differentiability result for p_ν while in Section 2.3 (respectively Section 2.4), we treat the specific case of the first- (resp. second-)order shape derivative of p_ν. Then, in Section 3, we study the shape derivatives of a volume integral $F : \Omega \mapsto \int_\Omega f$. We treat the measurable case in Section 3.1, the Lipschitz regularity in Section 3.2 and the $C^{1,1}$-domains in Section 3.3. Finally, Section 4 is an appendix that gathers all the material and the proofs of standard results needed throughout the article.

2 Shape differentiability for general wave functions

2.1 On the expression of the probability for general wave functions

Let $n \geqslant 2$ be an integer henceforth set. In this article, we consider a quantum system of n electrons whose chemical state is assumed to be entirely characterized by a given well-defined wave function [32, Section 1.1.1]:

$$\begin{array}{cccc} \Psi : & \left(\mathbb{R}^3 \times \{-\frac{1}{2},\frac{1}{2}\}\right)^n & \longrightarrow & \mathbb{C} \\ & \left[\begin{pmatrix} \mathbf{x}_1 \\ \sigma_1 \end{pmatrix}, \ldots, \begin{pmatrix} \mathbf{x}_n \\ \sigma_n \end{pmatrix}\right] & \longmapsto & \Psi\left[\begin{pmatrix} \mathbf{x}_1 \\ \sigma_1 \end{pmatrix}, \ldots, \begin{pmatrix} \mathbf{x}_n \\ \sigma_n \end{pmatrix}\right], \end{array} \tag{8}$$

where $\mathbf{x}_i$ and σ_i respectively refer to the space and spin variables of the i-th electron, for any $i \in [\![1,n]\!]$. Since we are dealing with fermions, we assume the antisymmetry of the wave function [41, Section 2.1.3], and we set $L^2((\mathbb{R}^3 \times \{-\frac{1}{2},\frac{1}{2}\})^n, \mathbb{C})$ as the complex separable Hilbert space of all possible quantum states. However, we do not impose here a unitary L^2-norm condition on the wave function as it is often the case. In other words, we make the following hypothesis.

Assumption 2.1. *The map Ψ is a skew-symmetric form i.e. for any $(i,j) \in [\![1,n]\!]^2$ such that $i \neq j$, and for any $(\sigma_i,\sigma_j) \in \{-\frac{1}{2},\frac{1}{2}\}^2$ and any $(\mathbf{x}_i,\mathbf{x}_j) \in \mathbb{R}^3 \times \mathbb{R}^3$, we have:*

$$\Psi\left[\ldots, \begin{pmatrix} \mathbf{x}_i \\ \sigma_i \end{pmatrix}, \ldots, \begin{pmatrix} \mathbf{x}_j \\ \sigma_j \end{pmatrix}, \ldots\right] = -\Psi\left[\ldots, \begin{pmatrix} \mathbf{x}_j \\ \sigma_j \end{pmatrix}, \ldots, \begin{pmatrix} \mathbf{x}_i \\ \sigma_i \end{pmatrix}, \ldots\right]. \tag{9}$$

Moreover, the map Ψ is measurable and square integrable i.e. for any $(\sigma_1,\ldots,\sigma_n) \in \{-\frac{1}{2},\frac{1}{2}\}^n$, the following map belongs to $L^2((\mathbb{R}^3)^n, \mathbb{C})$:

$$\begin{array}{cccc} \Psi^{(\sigma_1,\ldots,\sigma_n)} : & \mathbb{R}^3 \times \ldots \times \mathbb{R}^3 & \longrightarrow & \mathbb{C} \\ & (\mathbf{x}_1,\ldots,\mathbf{x}_n) & \longmapsto & \Psi\left[\begin{pmatrix} \mathbf{x}_1 \\ \sigma_1 \end{pmatrix}, \ldots, \begin{pmatrix} \mathbf{x}_n \\ \sigma_n \end{pmatrix}\right]. \end{array} \tag{10}$$

Finally, in addition to be well defined and finite, we assume that the following normalizing constant is a positive quantity i.e. it is not equal to zero:

$$c_0 := \sum_{(\sigma_1,\ldots,\sigma_n)\in\{-\frac{1}{2},\frac{1}{2}\}^n} \int_{(\mathbb{R}^3)^n} \left| \Psi\left[\begin{pmatrix} \mathbf{x}_1 \\ \sigma_1 \end{pmatrix}, \ldots, \begin{pmatrix} \mathbf{x}_n \\ \sigma_n \end{pmatrix}\right] \right|^2 d\mathbf{x}_1 \ldots d\mathbf{x}_n. \tag{11}$$

Hence, assuming that the wave function Ψ given in (8) satisfies Assumption 2.1, we can now use the traditional probabilistic interpretation of the wave function [32, Section 1.1.1] in order to define the shape functional in which we will be interested throughout the article. Indeed, the probability to find for any $i \in [\![1,n]\!]$ the electron i of spin σ_i in a domain Ω_i is proportional to:

$$\int_{\Omega_1\times\ldots\times\Omega_n} \left| \Psi^{(\sigma_1,\ldots,\sigma_n)} \right|^2,$$

where $\Psi^{(\sigma_1,\ldots,\sigma_n)}$ is defined by (10). Since $\Psi^{(\sigma_1,\ldots,\sigma_n)}$ is measurable, the above quantity is well defined for any (Lebesgue) measurable subsets $\Omega_1,\ldots,\Omega_n$ of $\mathbb{R}^3$, and it is finite since $\Psi^{(\sigma_1,\ldots,\sigma_n)}$ is square integrable. In particular, the probability to find n electrons in a measurable set $\Omega \subseteq \mathbb{R}^3$, regardless of their spins, is proportional to:

$$\sum_{(\sigma_1,\ldots,\sigma_n)\in\{-\frac{1}{2},\frac{1}{2}\}^n} \int_{\Omega^n} \left| \Psi\left[\begin{pmatrix} \mathbf{x}_1 \\ \sigma_1 \end{pmatrix}, \ldots, \begin{pmatrix} \mathbf{x}_n \\ \sigma_n \end{pmatrix}\right] \right|^2 d\mathbf{x}_1 \ldots d\mathbf{x}_n.$$

The constant of proportionality is determined by the fact that we expect to find n electrons in the whole space $\mathbb{R}^3$ with probability one. Hence, let $c_0 > 0$ be as in (11) and the probability $p_n(\Omega)$ to find n electrons in a measurable subset Ω of $\mathbb{R}^3$ is given by the following well-defined quantity:

$$p_n(\Omega) := \frac{1}{c_0} \sum_{(\sigma_1,\ldots,\sigma_n)\in\{-\frac{1}{2},\frac{1}{2}\}^n} \int_{\Omega^n} \left| \Psi\left[\begin{pmatrix} \mathbf{x}_1 \\ \sigma_1 \end{pmatrix}, \ldots, \begin{pmatrix} \mathbf{x}_n \\ \sigma_n \end{pmatrix}\right] \right|^2 d\mathbf{x}_1 \ldots d\mathbf{x}_n. \tag{12}$$

Similarly, the probability $p_0(\Omega)$ to find zero electron in a measurable subset Ω of $\mathbb{R}^3$ is defined as:

$$p_0\left(\Omega\right) := p_n\left(\mathbb{R}^3\backslash\Omega\right). \tag{13}$$

We now set $\nu \in [\![1, n-1]\!]$ and search for the probability to find exactly ν electrons in Ω, where *exactly* means that the $n-\nu$ remaining ones are located in the complement $\mathbb{R}^3\backslash\Omega$. The associated event can be interpreted as the reunion of the events *finding exactly electrons* $i_1,\ldots,i_\nu$ *in* Ω, taken among all the subsets $\{i_1,\ldots,i_\nu\}$ of ν pairwise distinct elements of $[\![1,n]\!]$. Hence, for any subset $I_\nu \subset [\![1,n]\!]$ of ν elements i.e. such that card $I_\nu = \nu$, we introduce the set $\Omega_{I_\nu} := \prod_{i=1}^n A_i$, where $A_i = \Omega$ if $i \in I_\nu$ otherwise $A_i = \mathbb{R}^3\backslash\Omega$. Following the same arguments than for p_n and p_0, the probability $p_\nu(\Omega)$ to find exactly ν electrons in a measurable subset Ω of $\mathbb{R}^3$ is given by the following well-defined quantity:

$$p_\nu\left(\Omega\right) := \frac{1}{c_0} \sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{-\frac{1}{2},\frac{1}{2}\right\}^n} \int_{\bigcup\limits_{\substack{I_\nu\subset[\![1,n]\!]\\ \text{card } I_\nu=\nu}} \Omega_{I_\nu}} \left| \Psi\left[\begin{pmatrix}\mathbf{x}_1\\ \sigma_1\end{pmatrix},\ldots,\begin{pmatrix}\mathbf{x}_n\\ \sigma_n\end{pmatrix}\right]\right|^2 d\mathbf{x}_1\ldots d\mathbf{x}_n. \tag{14}$$

Then, we observe that such a finite reunion is disjoint i.e. $\Omega_{I_\nu}\cap\Omega_{J_\nu} = \emptyset$ if $I_\nu \neq J_\nu$ so we have:

$$p_\nu\left(\Omega\right) = \frac{1}{c_0} \sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{-\frac{1}{2},\frac{1}{2}\right\}^n} \left(\sum_{\substack{I_\nu\subset[\![1,n]\!]\\ \text{card } I_\nu=\nu}} \int_{\Omega_{I_\nu}} \left| \Psi\left[\begin{pmatrix}\mathbf{x}_1\\ \sigma_1\end{pmatrix},\ldots,\begin{pmatrix}\mathbf{x}_n\\ \sigma_n\end{pmatrix}\right]\right|^2 d\mathbf{x}_1\ldots d\mathbf{x}_n \right).$$

Since (9) is satisfied by Ψ, we get $\int_{\Omega_{I_\nu}} |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2 = \int_{\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} |\Psi^{(\sigma_{p_{I_\nu}(1)},\ldots,\sigma_{p_{I_\nu}(n)})}|^2$, where $p_{I_\nu} : [\![1,n]\!] \to [\![1,n]\!]$ is a bijective map satisfying $p_{I_\nu}([\![1,\nu]\!]) = I_\nu$. A new summation on the spin variables $\tilde{\sigma}_i := \sigma_{p_{I_\nu}(i)}$ yields to $\sum_{\sigma_1,\ldots,\sigma_n} \int_{\Omega_{I_\nu}} |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2 = \sum_{\tilde{\sigma}_1,\ldots,\tilde{\sigma}_n} \int_{\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} |\Psi^{(\tilde{\sigma}_1,\ldots,\tilde{\sigma}_n)}|^2$, which does not depend on I_ν any longer. It can thus be removed from the corresponding sum for which we know that card$\{I_\nu \subset [\![1,n]\!],\ \text{card } I_\nu = \nu\} = \frac{n!}{\nu!(n-\nu)!} := \binom{n}{\nu}$. We deduce that:

$$p_\nu\left(\Omega\right) = \frac{1}{c_0}\binom{n}{\nu} \sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{-\frac{1}{2},\frac{1}{2}\right\}^n} \int_{\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} \left| \Psi\left[\begin{pmatrix}\mathbf{x}_1\\ \sigma_1\end{pmatrix},\ldots,\begin{pmatrix}\mathbf{x}_n\\ \sigma_n\end{pmatrix}\right]\right|^2 d\mathbf{x}_1\ldots d\mathbf{x}_n. \tag{15}$$

Although (14) should be the original definition for p_ν in the sense that it is clear with (14) that $p_\nu \in [0,1]$ as it is the case for (12) and (13), we will however use the more practical formula (15) for p_ν in the remaining part of the article. In other words, we are now in position to properly define the shape functional in which we will be interested throughout the article.

Definition 2.2. *Assume that the wave function Ψ given in (8) satisfies Assumption 2.1. Let $\mathcal{M}$ be the set of all (Lebesgue) measurable subsets of $\mathbb{R}^3$ and $c_0 > 0$ as in (11). Then, for any $\nu \in [\![0,n]\!]$, the following shape functional is a well-defined map:*

$$\begin{array}{rccl} p_\nu: & \mathcal{M} & \longrightarrow & [0,1] \\ & \Omega & \longmapsto & p_\nu\left(\Omega\right), \end{array}$$

where the probability $p_\nu(\Omega)$ to find exactly ν electrons in the domain Ω is well defined by (15) if $\nu \in [\![1,n-1]\!]$, by (12) if $\nu = n$, and by (13) if $\nu = 0$.

Remark 2.3. *From the convention $A^0 \times B = B \times A^0 = B$ for any sets A and B, we can deduce (12)–(13) from (15) by setting $\nu = 0$ or $\nu = n$ in (15). We will adopt this convention in the article, in order to simplify the proofs and not to have to treat specifically the cases $\nu = 0$ and $\nu = n$.*

Finally, we can state a first result concerning the symmetry property of the probability.

Lemma 2.4. *Let $\mathcal{M}$ be the class of all (Lebesgue) measurable subsets of $\mathbb{R}^3$. We assume that the wave function Ψ given in (8) satisfies Assumption 2.1. Then, the map $p_\nu : \Omega \in \mathcal{M} \mapsto p_\nu(\Omega) \in [0,1]$ of Definition 2.2 is well defined and we have:*

$$p_n\left(\mathbb{R}^3\right) = p_0\left(\emptyset\right) = 1 \qquad \text{and} \qquad \forall\Omega\in\mathcal{M},\quad p_\nu\left(\Omega\right) = p_{n-\nu}\left(\mathbb{R}^3\backslash\Omega\right).$$

In particular, the whole space $\mathbb{R}^3$ (respectively the empty set $\emptyset$) is optimal for p_n (resp. for p_0). Moreover, if Ω^* is optimal for p_ν, then $\mathbb{R}^3\backslash\Omega^*$ is optimal for $p_{n-\nu}$ i.e.

$$\exists\Omega^* \in \mathcal{M}, \quad p_\nu\left(\Omega^*\right) = \max_{\Omega\in\mathcal{M}} p_\nu\left(\Omega\right) \quad \Longrightarrow \quad p_{n-\nu}\left(\mathbb{R}^3\backslash\Omega^*\right) = \max_{\Omega\in\mathcal{M}} p_{n-\nu}\left(\Omega\right).$$

In other words, the shape optimization problem (1) *only needs to be studied for integers $\nu \leqslant \frac{n+1}{2}$ and it has an obvious global maximizer if $\nu = 0$ or if $\nu = n$.*

Proof. Let $\mathcal{M}$ contain all the measurable subsets of $\mathbb{R}^3$. We assume that the wave function Ψ given in (8) satisfies Assumption 2.1. Hence, from the foregoing, the map $p_\nu : \Omega \in \mathcal{M} \mapsto p_\nu(\Omega) \in [0,1]$ introduced in Definition 2.2 is well defined. First, we get $p_n(\mathbb{R}^3) = p_0(\emptyset) = 1$ if we consider (12)–(13) with $\Omega = \mathbb{R}^3$ and $\Omega = \emptyset$. Then, let $\Omega \in \mathcal{M}$. From (15), we get:

$$p_\nu\left(\Omega\right) = \frac{1}{c_0}\binom{n}{\nu} \sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{-\frac{1}{2},\frac{1}{2}\right\}^n} \int_{\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2,$$

where $\Psi^{(\sigma_1,\ldots,\sigma_n)}$ and $c_0 > 0$ are respectively defined by (10) and (11). Using the property (9) of the wave function, we deduce that $\int_{\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2 = \int_{(\mathbb{R}^3\backslash\Omega)^{n-\nu}\times\Omega^\nu} |\Psi^{(\sigma_{\nu+1},\ldots,\sigma_n,\sigma_1,\ldots,\sigma_\nu)}|^2$. Observing that $\binom{n}{\nu} := \frac{n!}{\nu!(n-\nu)!} = \binom{n}{n-\nu}$ and re-indexing the summation on the spin variables $\tilde{\sigma}_i := \sigma_{\nu+i}$ for any $i \in [\![1, n-\nu]\!]$ and $\tilde{\sigma}_i := \sigma_{i-n+\nu}$ for any $i \in [\![n-\nu+1, n]\!]$, we obtain:

$$p_\nu\left(\Omega\right) = \frac{1}{c_0}\binom{n}{n-\nu} \sum_{(\tilde{\sigma}_1,\ldots,\tilde{\sigma}_n)\in\left\{-\frac{1}{2},\frac{1}{2}\right\}^n} \int_{(\mathbb{R}^3\backslash\Omega)^{n-\nu}\times\Omega^\nu} |\Psi^{(\tilde{\sigma}_1,\ldots,\tilde{\sigma}_n)}|^2 = p_{n-\nu}\left(\mathbb{R}^3\backslash\Omega\right).$$

Finally, if we assume that there exists $\Omega^* \in \mathcal{M}$ such that $p_\nu(\Omega^*) = \max_{\Omega\in\mathcal{M}} p_\nu(\Omega)$, then for any $\Omega \in \mathcal{M}$, we deduce from the previous symmetry property:

$$p_{n-\nu}\left(\Omega\right) = p_\nu\left(\mathbb{R}^3\backslash\Omega\right) \leqslant \max_{A\in\mathcal{M}} p_\nu(A) = p_\nu\left(\Omega^*\right) = p_{n-\nu}\left(\mathbb{R}^3\backslash\Omega^*\right).$$

Hence, we get $p_{n-\nu}(\mathbb{R}^3\backslash\Omega^*) = \max_{\Omega\in\mathcal{M}} p_{n-\nu}(\Omega)$, concluding the proof of Lemma 2.4. □

2.2 On the shape derivatives of the probability for measurable domains

First, we recall some terminology about shape differentiability. We refer to Section 1 for notation.

Definition 2.5. *Assume that the following shape functional is a well-defined map for a certain class of admissible shapes:*

$$F : \Omega \longmapsto F\left(\Omega\right).$$

By abuse of terminology, we say that F is shape differentiable at Ω if the following associated functional is well defined around the origin and Fréchet differentiable at the origin:

$$F_\Omega : \theta \longmapsto F_\Omega\left(\theta\right) := F\left[\left(I+\theta\right)\left(\Omega\right)\right].$$

If it is the case, then the differential $D_{\mathbf{0}}F_\Omega$ of the map F_Ω at the origin is called the (first-order) shape derivative of F at Ω. Similarly, for any integer $k \geqslant 2$, if F_Ω is $(k-1)$ times differentiable around the origin and k times differentiable at the origin, then we say that F is k times shape differentiable at Ω, and the k-th-order differential $D^k_{\mathbf{0}}F_\Omega$ of the map F_Ω at the origin is called the k-th-order shape derivative of F at Ω. Moreover, by analogy with the finite-dimensional case, assume that there exists a unique well-defined function $f_\Omega : \partial\Omega \to \mathbb{R}$ such that:

$$D_{\mathbf{0}}F_\Omega\left(\theta\right) = \int_{\partial\Omega} f_\Omega \theta_{\mathbf{n}} dA.$$

Then, the map f_Ω, eventually depending on Ω (but not on θ), is denoted by abuse of notation $\frac{\partial F}{\partial\Omega}$ and called the shape gradient of F at Ω. Similarly, assume that in addition to the existence of a shape gradient, there exists a unique well-defined function $\tilde{f}_\Omega : \partial\Omega \to \mathbb{R}$ such that:

$$D^2_{\mathbf{0}}F_\Omega(\theta,\tilde{\theta}) \quad = \quad \int_{\partial\Omega} \tilde{f}_\Omega \theta_{\mathbf{n}}\tilde{\theta}_{\mathbf{n}} dA \quad - \quad \int_{\partial\Omega} \frac{\partial F}{\partial\Omega} Z[\theta,\tilde{\theta}] dA,$$

where $Z[\theta,\tilde{\theta}]$ is defined by (4). The map $\tilde{f}_\Omega$, eventually depending on Ω (but not on $(\theta,\tilde{\theta})$), is denoted by abuse of notation $\frac{\partial^2 F}{\partial\Omega^2}$ and called the shape Hessian of F at Ω.

The shape gradient and Hessian form are expected from shape derivatives [28] [22, Section 5.9] [6] but note that in Definition 2.5, we did not clearly specify on which spaces are defined F and F_Ω because such a structure depends on the required regularity for the domain Ω and the vector field θ. We also recall that $Z[\theta,\tilde{\theta}]$ defined by (4) represents the contribution of the tangential components. In particular, $Z[\theta,\tilde{\theta}] \equiv 0$ if θ and $\tilde{\theta}$ are orthogonal to the boundary $\partial\Omega$ i.e. if $\theta_{\partial\Omega} = \tilde{\theta}_{\partial\Omega} = 0$.

Before stating our main result concerning the shape differentiability of $p_\nu : \Omega \mapsto p_\nu(\Omega)$ i.e. the differentials at the origin of the associated map $p_{\nu,\Omega} : \theta \mapsto p_\nu[(I+\theta)(\Omega)]$, we study the continuity properties of $p_{\nu,\Omega}$. We recall that $\mathcal{M}$ refers to the class of measurable subset of $\mathbb{R}^3$, that $C^{0,1}$ denotes the set of Lipschitz continuous vector fields $\theta : \mathbb{R}^3 \to \mathbb{R}^3$, that $W^{1,\infty} := L^\infty \cap C^{0,1}$ is the set of Lipschitz continuous bounded vector fields, and that $\mathbb{B}^{0,1} := \{\theta \in C^{0,1}, \|\theta\|_{C^{0,1}} < 1\}$ is the open unit ball of $C^{0,1}$ centred at the origin i.e. the space of Lipschitz contractions.

Lemma 2.6. *Let $n \geqslant 2$ and $\nu \in [\![0,n]\!]$. Assume that the wave function Ψ given by (8) satisfies Assumption 2.1. Then, the shape functional $p_\nu : \Omega \in \mathcal{M} \mapsto p_\nu(\Omega)$ of Definition 2.2 is well defined, and for any $\Omega \in \mathcal{M}$, the associated map $p_{\nu,\Omega} : \theta \in C^{0,1} \mapsto p_\nu[(I+\theta)(\Omega)]$ is well defined on $\mathbb{B}^{0,1}$. Moreover, for any $\Omega \in \mathcal{M}$, the map $p_{\nu,\Omega} : \theta \in W^{1,\infty} \mapsto p_\nu[(I+\theta)(\Omega)]$ is continuous on $\mathbb{B}^{0,1} \cap W^{1,\infty}$.*

Proof. Let $n \geqslant 2$ and $\nu \in [\![0,n]\!]$. We aim to consider the probability as a volume integral on an higher-dimensional space. For this purpose, we need to keep track of the dimension of the space in which we are working. Hence, the notation are modified in this direction. For example, $\mathcal{M}_3$ now refers to the set of $\Omega \subseteq \mathbb{R}^3$ measurable, $\mathbb{B}^{0,1}_3$ to the set of Lipschitz contraction $\theta : \mathbb{R}^3 \to \mathbb{R}^3$, etc. Let $\theta \in \mathbb{B}^{0,1}_3$. From Proposition 4.1, the Lipschitz continuous map $I_3 + \theta : \mathbf{x} \in \mathbb{R}^3 \mapsto \mathbf{x} + \theta(\mathbf{x}) \in \mathbb{R}^3$ is bijective and its inverse $(I_3+\theta)^{-1}$ is also Lipschitz continuous. In particular, $(I_3+\theta)^{-1}$ is a measurable map and for any $\Omega \in \mathcal{M}_3$, we get $(I_3+\theta)(\Omega) \in \mathcal{M}_3$. Hence, for any $\Omega \in \mathcal{M}_3$, the map $p_{\nu,\Omega} : \theta \in C^{0,1}_3 \mapsto p_\nu[(I_3+\theta)(\Omega)]$ is well defined on $\mathbb{B}^{0,1}_3$. We now study its continuity by introducing the following higher-dimensional version of p_ν:

$$\begin{array}{rccl} \tilde{p}_\nu : & \mathcal{M}_{3n} & \longrightarrow & \mathbb{R} \\ & \widetilde{\Omega} & \longmapsto & \tilde{p}_\nu(\widetilde{\Omega}) := \dfrac{1}{c_0}\dbinom{n}{\nu} \displaystyle\sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{-\frac{1}{2},\frac{1}{2}\right\}^n} \int_{\widetilde{\Omega}} |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2, \end{array} \tag{16}$$

where (10) defines $\Psi^{(\sigma_1,\ldots,\sigma_n)}$. Since $\Psi^{(\sigma_1,\ldots,\sigma_n)}$ and $\widetilde{\Omega}$ are measurable, the integral is well defined and it is finite since $\Psi^{(\sigma_1,\ldots,\sigma_n)}$ is square integrable. Hence, the map $\tilde{p}_\nu$ is well defined by (16) and we can thus apply Lemma 3.1 to $\tilde{p}_\nu$. For any $\widetilde{\Omega} \in \mathcal{M}_{3n}$, the map $\tilde{p}_{\nu,\widetilde{\Omega}} : \tilde{\theta} \in C^{0,1}_{3n} \mapsto \tilde{p}_\nu[(I_{3n}+\tilde{\theta})(\widetilde{\Omega})]$ is well defined on $\mathbb{B}^{0,1}_{3n}$ and moreover, the following map is continuous on $\mathbb{B}^{0,1}_{3n} \cap W^{1,\infty}_{3n}$:

$$\begin{array}{rccl} \tilde{p}_{\nu,\widetilde{\Omega}} : & W^{1,\infty}_{3n} & \longrightarrow & \mathbb{R} \\ & \tilde{\theta} & \longmapsto & \tilde{p}_{\nu,\widetilde{\Omega}}(\tilde{\theta}) := \tilde{p}_\nu\left[\left(I_{3n}+\tilde{\theta}\right)(\widetilde{\Omega})\right]. \end{array} \tag{17}$$

Then, we want to relate $\tilde{p}_\nu$ and p_ν. For this purpose, we consider the following map:

$$\begin{array}{rccl} f : & W^{1,\infty}(\mathbb{R}^3,\mathbb{R}^3) & \longrightarrow & W^{1,\infty}\left((\mathbb{R}^3)^n,(\mathbb{R}^3)^n\right) \\ & (\theta : \mathbf{x} \mapsto \theta(\mathbf{x})) & \longmapsto & f(\theta) := (\mathbf{x}_1,\ldots,\mathbf{x}_n) \mapsto (\theta(\mathbf{x}_1),\ldots,\theta(\mathbf{x}_n)), \end{array} \tag{18}$$

which is well defined and linear. It is also continuous since one can check by direct calculations:

$$\forall \theta \in W^{1,\infty}_3, \quad \|f(\theta)\|_{W^{1,\infty}_{3n}} \leqslant \sqrt{n}\|\theta\|_{W^{1,\infty}_3} \qquad \text{and} \qquad \|f(\theta)\|_{C^{0,1}_{3n}} = \|\theta\|_{C^{0,1}_3}. \tag{19}$$

Moreover, let $\Omega \in \mathcal{M}_3$. Since the set $\Omega^\nu \times (\mathbb{R}^3\backslash\Omega)^{n-\nu}$ belongs to $\mathcal{M}_{3n}$, we get:

$$p_\nu(\Omega) = \tilde{p}_\nu[\Omega^\nu \times (\mathbb{R}^3\backslash\Omega)^{n-\nu}] \qquad \text{and} \qquad p_{\nu,\Omega} = \tilde{p}_{\nu,\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} \circ f. \tag{20}$$

Since f is continuous and $\tilde{p}_{\nu,\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}}$ is continuous on $\mathbb{B}^{0,1}_{3n} \cap W^{1,\infty}_{3n}$, we deduce from (19)–(20) that $p_{\nu,\Omega}$ is continuous on $\mathbb{B}^{0,1}_3 \cap W^{1,\infty}_3$, concluding the proof of Lemma 2.6. $\square$

We are now in position to prove our main shape differentiability result concerning the shape functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$ of Definition 2.2. A striking feature is that we are able to get an explicit formula (21) for the shape derivative of p_ν at any order. As for Lemma 2.6, the proof completely relies on the shape differentiability results of Section 3 for a volume integral. We refer to Section 1 for the notation and we recall that H^k denotes the usual Sobolev space of L^2-maps whose partial derivatives (in the weak distributional sense) are also L^2-functions up to the order k.

Theorem 2.7. *Let $n \geqslant 2$, $\nu \in [\![0,n]\!]$, and $k_0 \geqslant 1$ be three integers. First, we assume that the wave function Ψ given by (8) satisfies Assumption 2.1. In particular, the shape functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$ of Definition 2.2 is well defined. Moreover, we assume that the map $\Psi^{(\sigma_1,\dots,\sigma_n)}$ defined by (10) belongs to $H^{k_0}((\mathbb{R}^3)^n,\mathbb{C})$ for any $(\sigma_1,\dots,\sigma_n) \in \{-\frac{1}{2},\frac{1}{2}\}^n$. Then, for any $\Omega \in \mathcal{M}$, the associated map $p_{\nu,\Omega} : \theta \in W^{1,\infty} \mapsto p_\nu[(I+\theta)(\Omega)]$ is k_0 times Fréchet differentiable at the origin and for any $k \in [\![1,k_0]\!]$, its differential of order k at the origin is given by the following continuous symmetric k-linear form defined for any $(\theta_1,\dots,\theta_k) \in W^{1,\infty} \times \dots \times W^{1,\infty}$ by:*

$$
\begin{aligned}
D^k_{\mathbf{0}} p_{\nu,\Omega}(\theta_1,\dots,\theta_k) := \frac{1}{c_0}\binom{n}{\nu} \sum_{(\sigma_1,\dots,\sigma_n)\in\{-\frac{1}{2},\frac{1}{2}\}^n} \sum_{i_1,\dots,i_k=1}^{n} \sum_{m_1,\dots,m_k=1}^{3} \sum_{l=0}^{k} \sum_{\substack{I_l \subseteq [\![1,k]\!] \\ \mathrm{card}\ I_l = l}} \sum_{p\in\mathcal{S}_{I_l}} s(p) \\
\int_{\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} \frac{\partial^{k-l}\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)}{\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_l}} \partial\left(\mathbf{x}_{i_j}\right)_{m_j}} (\mathbf{x}_1,\dots,\mathbf{x}_n) \left(\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_l}} \left[\theta_j\left(\mathbf{x}_{i_j}\right)\right]_{m_j} \right) \\
\left(\prod_{j\in I_l} I_{i_j i_{p(j)}} \left[D_{\mathbf{x}_{i_j}}\theta_j\right]_{m_j m_{p(j)}} \right) d\mathbf{x}_1\dots d\mathbf{x}_n,
\end{aligned}
\tag{21}
$$

where $I_{i_j i_{p(j)}} = 1$ if $i_j = i_{p(j)}$ otherwise zero. In other words, the functional p_ν of Definition 2.2 is k_0 times shape differentiable at any measurable subset of $\mathbb{R}^n$, and its shape derivative of order k is given by (21) for any $k \in [\![1,k_0]\!]$. Moreover, the associated map $p_{\nu,\Omega} : \theta \in W^{1,\infty} \mapsto p_\nu[(I+\theta)(\Omega)]$ is k_0 times continuously differentiable at any point of $W^{1,\infty}\cap\mathbb{B}^{0,1}$ and for any $k \in [\![1,k_0]\!]$, its k-th-order Fréchet differential is well defined by the following continuous map:

$$
\begin{array}{rcl}
D^k_{\bullet} p_{\nu,\Omega} : W^{1,\infty}\cap\mathbb{B}^{0,1} & \longrightarrow & \mathcal{L}^k_c\left(\left(W^{1,\infty}\right)^k,\mathbb{R}\right) \\
\theta_0 & \longmapsto & (\theta_1,\dots,\theta_k) \mapsto D^k_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}\left[\theta_1\circ(I+\theta_0)^{-1},\dots,\theta_k\circ(I+\theta_0)^{-1}\right],
\end{array}
\tag{22}
$$

where $D^k_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}$ is the k-th-order shape derivative of p_ν at $(I+\theta_0)(\Omega)$ given by (21), and where $\mathcal{L}^k_c$ refers to the class of continuous k-linear maps.

Proof. We use the notation of Lemma 2.6. We aim to relate (17) with p_ν in order to use the results of Section 3 available for volume integrals. Let $n \geqslant 2$, $\nu \in [\![0,n]\!]$, and $k_0 \geqslant 1$ be three integers. We assume that the wave function Ψ given by (8) satisfies Assumption 2.1. In particular, the shape functional $p_\nu : \Omega \in \mathcal{M}_3 \mapsto p_\nu(\Omega)$ of Definition 2.2 is well defined. Moreover, we assume that the map $\Psi^{(\sigma_1,\dots,\sigma_n)}$ in (10) belongs to $H^{k_0}((\mathbb{R}^3)^n,\mathbb{C})$ for any $(\sigma_1,\dots,\sigma_n) \in \{-\frac{1}{2},\frac{1}{2}\}^n$. Note that H^{k_0}-regularity is required on Ψ to get the k_0-th-order shape differentiability. First, let $\Omega \in \mathcal{M}_3$. From Lemma 2.6, the map $p_{\nu,\Omega} : \theta \in W^{1,\infty}_3 \cap \mathbb{B}^{0,1}_3 \mapsto p_\nu[(I_3+\theta)(\Omega)]$ is well defined and continuous. We now show that it is k_0 times differentiable at the origin. In the proof of Lemma 2.6, we also established that the map $\tilde{p}_\nu : \widetilde{\Omega} \in \mathcal{M}_{3n} \mapsto \tilde{p}_\nu(\widetilde{\Omega})$ is well defined by (16). Since we have $|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2 \in W^{k_0,1}$, we can apply Theorem 3.2 to the map $\tilde{p}_\nu$, from which we deduce that $\tilde{p}_{\nu,\widetilde{\Omega}} : \tilde{\theta} \in W^{1,\infty}_{3n} \mapsto \tilde{p}_\nu[(I_{3n}+\tilde{\theta})(\widetilde{\Omega})]$ is well defined and k_0 times differentiable at the origin. Moreover, for any $k \in [\![1,k_0]\!]$, its k-th-order differential at the origin is given by the following continuous symmetric k-linear form:

$$
\begin{aligned}
\forall(\tilde{\theta}_1,\dots,\tilde{\theta}_k) \in \left(W^{1,\infty}\right)^k,\ \ D^k_{\mathbf{0}} \tilde{p}_{\nu,\widetilde{\Omega}}(\tilde{\theta}_1,\dots,\tilde{\theta}_k) \ := \ \frac{1}{c_0}\binom{n}{\nu} \sum_{i_1,\dots,i_k=1}^{n} \sum_{m_1,\dots,m_k=1}^{3} \sum_{l=0}^{k} \sum_{\substack{I_l \subseteq [\![1,k]\!] \\ \mathrm{card}\ I_l = l}} \\
\sum_{(\sigma_1,\dots,\sigma_n)\in\{-\frac{1}{2},\frac{1}{2}\}^n} \int_{\widetilde{\Omega}} \frac{\partial^{k-l}\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)}{\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_l}} \partial\left(\mathbf{x}_{i_j}\right)_{m_j}} (\mathbf{x}_1,\dots,\mathbf{x}_n) \left(\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_l}} \left[\tilde{\theta}_j\left(\mathbf{x}_1,\dots,\mathbf{x}_n\right)\right]_{3(i_j-1)+m_j} \right) \\
\left(\sum_{p\in\mathcal{S}_{I_l}} s(p) \prod_{j\in I_l} \left[\frac{\partial(\tilde{\theta}_j)}{\partial\left(\mathbf{x}_{i_{p(j)}}\right)_{m_{p(j)}}} (\mathbf{x}_1,\dots,\mathbf{x}_n) \right]_{3(i_j-1)+m_j} \right) d\mathbf{x}_1\dots d\mathbf{x}_n.
\end{aligned}
\tag{23}
$$

Then, we want to relate the k-th-order shape derivative of $\tilde{p}_\nu$ with the one of p_ν. Let $\Omega \in \mathcal{M}_3$. We thus have $\Omega^\nu \times (\mathbb{R}^3 \backslash \Omega)^{n-\nu} \in \mathcal{M}_{3n}$. Considering the continuous linear map f given in (18), we deduce from (19)–(20) that the map $p_{\nu,\Omega} = \tilde{p}_{\nu,\Omega^\nu \times (\mathbb{R}^3\backslash\Omega)^{n-\nu}} \circ f$ is k_0 times differentiable at the origin and for any $k \in [\![1, k_0]\!]$, its k-th-order differential at the origin is given by the following continuous symmetric k-linear form:

$$\begin{aligned}
\forall(\theta_1,\ldots,\theta_k) \in \left(W_3^{1,\infty}\right)^k, \; D^k_{\mathbf{0}} p_{\nu,\Omega}(\theta_1,\ldots,\theta_k) &= D^k_{\mathbf{0}}\left(\tilde{p}_{\nu,\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} \circ f\right)(\theta_1,\ldots,\theta_k) \\
&= D^k_{f(\mathbf{0})}\tilde{p}_{\nu,\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}}\left[D_{\mathbf{0}} f(\theta_1),\ldots,D_{\mathbf{0}} f(\theta_k)\right] \\
&= D^k_{\mathbf{0}}\tilde{p}_{\nu,\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}}\left[f(\theta_1),\ldots,f(\theta_k)\right].
\end{aligned}$$

Since $[f(\theta_j)(\mathbf{x}_1,\ldots,\mathbf{x}_n)]_{3(i_j-1)+m_j} = [\theta_j(\mathbf{x}_{i_j})]_{m_j}$, we deduce that $[\partial_{(\mathbf{x}_{i_{p(j)}})_{m_{p(j)}}} f(\theta_j)]_{3(i_j-1)+m_j}$ is equal to zero if $i_{p(j)} \neq i_j$ otherwise it is equal to $[\partial_{m_{p(j)}}\theta_j(\mathbf{x}_{i_j})]_{m_j}$. Using this observation in (23), we conclude that relation (21) holds true. Let us now consider the second part of Theorem 3.2. For any set $\widetilde{\Omega} \in \mathcal{M}_{3n}$, the map $\tilde{p}_{\nu,\widetilde{\Omega}} : \tilde{\theta} \in W^{1,\infty}_{3n} \mapsto \tilde{p}_\nu[(I_{3n} + \tilde{\theta})(\widetilde{\Omega})]$ is well defined and k_0 times continuously differentiable at any point of $W^{1,\infty}_{3n} \cap \mathbb{B}^{0,1}_{3n}$. Moreover, for any $k \in [\![1, k_0]\!]$, its k-th-order differential is well defined by the following continuous map:

$$\begin{aligned}
D^k_{\bullet}\tilde{p}_{\nu,\widetilde{\Omega}} : W^{1,\infty}_{3n} \cap \mathbb{B}^{0,1}_{3n} &\longrightarrow \mathcal{L}^k_c\left(\left(W^{1,\infty}_{3n}\right)^k, \mathbb{R}\right) \\
\tilde{\theta}_0 &\longmapsto D^k_{\tilde{\theta}_0}\tilde{p}_{\nu,\widetilde{\Omega}} := (\tilde{\theta}_1,\ldots,\tilde{\theta}_k) \mapsto D^k_{\mathbf{0}}\tilde{p}_{\nu,(I_{3n}+\tilde{\theta}_0)(\widetilde{\Omega})}\Big[\tilde{\theta}_1\circ(I_{3n}+\tilde{\theta}_0)^{-1},\ldots \\
&\qquad\qquad ,\tilde{\theta}_k\circ(I_{3n}+\tilde{\theta}_0)^{-1}\Big],
\end{aligned} \tag{24}$$

where $D^k_{\mathbf{0}}\tilde{p}_{\nu,(I_{3n}+\tilde{\theta}_0)(\widetilde{\Omega})}$ is the k-th-order shape derivative of $\tilde{p}_\nu$ at $(I_{3n}+\tilde{\theta}_0)(\widetilde{\Omega})$ given by (23). Then, as before, we can relate the k-th-order differential of $\tilde{p}_{\nu,\widetilde{\Omega}}$ with the one of $p_{\nu,\Omega}$. Let $\Omega \in \mathcal{M}_3$ so we have $\Omega^\nu \times (\mathbb{R}^3\backslash\Omega)^{n-\nu} \in \mathcal{M}_{3n}$. Considering the continuous linear map f given in (18), we deduce from (19)–(20) that the map $p_{\nu,\Omega} = \tilde{p}_{\nu,\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} \circ f$ is k_0 times continuously differentiable at any point $\theta_0 \in W^{1,\infty}_3 \cap \mathbb{B}^{0,1}_3$ and we have for any $k \in [\![1, k_0]\!]$ and for any $(\theta_1,\ldots,\theta_k) \in W^{1,\infty}\times\ldots\times W^{1,\infty}$:

$$\begin{aligned}
D^k_{\theta_0} p_{\nu,\Omega}(\theta_1,\ldots\theta_k) &= D^k_{\theta_0}\left(\tilde{p}_{\nu,\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}}\circ f\right)(\theta_1,\ldots,\theta_k) \\
&= D^k_{f(\theta_0)}\tilde{p}_{\nu,\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}}\left[D_{\theta_0} f(\theta_1),\ldots,D_{\theta_0} f(\theta_k)\right] \\
&= D^k_{f(\theta_0)}\tilde{p}_{\nu,\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}}\left[f(\theta_1),\ldots,f(\theta_k)\right] \\
&= D^k_{\mathbf{0}}\tilde{p}_{\nu,[I_{3n}+f(\theta_0)](\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu})}\Big[f(\theta_1)\circ(I_{3n}+f(\theta_0))^{-1},\ldots \\
&\qquad ,f(\theta_k)\circ(I_{3n}+f(\theta_0))^{-1}\Big],
\end{aligned}$$

where we have used (24) to obtain the last equality. Note also that using Proposition 4.1, we have $[I_{3n}+f(\theta_0)](\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}) = [(I_3+\theta_0)(\Omega)]^\nu \times [\mathbb{R}^3\backslash(I_3+\theta_0)(\Omega)]^{n-\nu}$. We can also check that $f(\theta_i)\circ[I_{3n}+f(\theta_0)]^{-1} = f[\theta_i\circ(I_3+\theta_0)^{-1}]$ for any $i \in [\![1,k]\!]$ so we deduce that:

$$\begin{aligned}
D^k_{\theta_0} p_{\nu,\Omega}(\theta_1,\ldots,\theta_k) &= D^k_{\mathbf{0}}\tilde{p}_{\nu,[(I_3+\theta_0)(\Omega)]^\nu\times[\mathbb{R}^3\backslash(I_3+\theta_0)(\Omega)]^{n-\nu}}\Big[f\left(\theta_1\circ(I_3+\theta_0)^{-1}\right),\ldots \\
&\qquad ,f\left(\theta_k\circ(I_3+\theta_0)^{-1}\right)\Big] \\
&= D^k_{f(\mathbf{0})}\tilde{p}_{\nu,[(I_3+\theta_0)(\Omega)]^\nu\times[\mathbb{R}^3\backslash(I_3+\theta_0)(\Omega)]^{n-\nu}}\Big(D_{\mathbf{0}} f\left[\theta_1\circ(I_3+\theta_0)^{-1}\right],\ldots \\
&\qquad ,D_{\mathbf{0}} f\left[\theta_k\circ(I_3+\theta_0)^{-1}\right]\Big) \\
&= D^k_{\mathbf{0}}\left[\tilde{p}_{\nu,[(I_3+\theta_0)(\Omega)]^\nu\times[\mathbb{R}^3\backslash(I_3+\theta_0)(\Omega)]^{n-\nu}}\circ f\right]\Big[\theta_1\circ(I_3+\theta_0)^{-1},\ldots \\
&\qquad ,\theta_k\circ(I_3+\theta_0)^{-1}\Big] \\
&= D^k_{\mathbf{0}} p_{\nu,(I_3+\theta_0)(\Omega)}\left[\theta_1\circ(I_3+\theta_0)^{-1},\ldots,\theta_k\circ(I_3+\theta_0)^{-1}\right].
\end{aligned}$$

Hence, we have proved that the k-th-order differential of $p_{\nu,\Omega}$ is well defined by the continuous map (22) for any $k \in [\![1, k_0]\!]$, concluding the proof of Theorem 2.7. $\square$

2.3 On the first-order shape derivative of the probability

We refer to Sections 1 and 2.1–2.2 for notation, especially Definition 2.5 for explanations about the notion of shape differentiability. Theorem 2.7 is stated in the specific $k_0 = 1$ and we show that we can recover the shape gradient structure (2) by assuming the Lipschitz boundary of the domain.

Theorem 2.8. *Let us consider the assumptions of Theorem 2.7 in the specific case $k_0 = 1$. Then, the following map is well defined and integrable:*

$$\begin{array}{rccl} P: & \mathbb{R}^3 \times \ldots \times \mathbb{R}^3 & \longrightarrow & \mathbb{R} \\ & (\mathbf{x}_1, \ldots, \mathbf{x}_n) & \longmapsto & P(\mathbf{x}_1, \ldots, \mathbf{x}_n) := \left\langle \nabla_{\mathbf{x}_1} \left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2 \right)(\mathbf{x}_1, \ldots, \mathbf{x}_n) \ \middle| \ \theta(\mathbf{x}_1) \right\rangle \\ & & & \qquad + \ |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2 (\mathbf{x}_1, \ldots, \mathbf{x}_n) \ \operatorname{div} \theta(\mathbf{x}_1). \end{array}$$

Moreover, the map $p_{\nu,\Omega} : \theta \in W^{1,\infty} \mapsto p_\nu[(I+\theta)(\Omega)]$ is Fréchet differentiable at the origin and its differential is given by the following continuous linear form defined for any $\theta \in W^{1,\infty}$ by:

$$\begin{aligned} D_{\mathbf{0}} p_{\nu,\Omega}(\theta) = \frac{1}{c_0}\binom{n}{\nu} \sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{\frac{1}{2},\frac{1}{2}\right\}^n} & \nu \int_\Omega \left(\int_{\Omega^{\nu-1}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} P(\mathbf{x}_1,\ldots,\mathbf{x}_n)\, d\mathbf{x}_2 \ldots d\mathbf{x}_n \right) d\mathbf{x}_1 \\ & + \ (n-\nu) \int_{\mathbb{R}^3\backslash\Omega} \left(\int_{\Omega^{\nu}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu-1}} P(\mathbf{x}_1,\ldots,\mathbf{x}_n)\, d\mathbf{x}_2 \ldots d\mathbf{x}_n \right) d\mathbf{x}_1. \end{aligned} \tag{25}$$

In other words, the functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$ of Definition 2.2 is shape differentiable at any measurable subset of $\mathbb{R}^3$. If in addition, we now assume that Ω is an open bounded subset of $\mathbb{R}^3$ with a Lipschitz boundary, then the shape derivative of p_ν at Ω takes the form given in (2), where the shape gradient is uniquely determined up to a set of zero $A(\bullet \cap \partial\Omega)$-measure, and defined for any point $\mathbf{x} \in \partial\Omega$ by:

$$\begin{aligned} \frac{\partial p_\nu}{\partial \Omega}(\mathbf{x}) := \frac{1}{c_0}\binom{n}{\nu} \sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{\frac{1}{2},\frac{1}{2}\right\}^n} & \nu \int_{\Omega^{\nu-1}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_n) d\mathbf{x}_2 \ldots d\mathbf{x}_n \\ & - \ (n-\nu) \int_{\Omega^{\nu}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu-1}} |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_n)\, d\mathbf{x}_2 \ldots d\mathbf{x}_n. \end{aligned} \tag{26}$$

In (26), the boundary values of $\Psi^{(\sigma_1,\ldots,\sigma_n)} \in H^1((\mathbb{R}^3)^n, \mathbb{C})$ are understood in the sense of trace. Finally, the conventions $A^0 \times B = B \times A^0 = A$, $A^{-1} \times B = B \times A^{-1} = \emptyset$, and $\int_\emptyset f(x,y)dy = f(x)$ are used to interpret (2) and (25)–(26) if $\nu \in \{0, 1, n-1, n\}$.

Proof. First, the map P of the statement is well defined and integrable because $\theta \in W^{1,\infty}$, $\Psi \in H^1$, and $\nabla(|\Psi|^2) = 2\mathrm{Real}(\overline{\Psi}\nabla\Psi)$. Then, we can apply Theorem 2.7 with $k_0 = k = 1$. The functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$ of Definition 2.2 is thus shape differentiable at Ω and its shape derivative $D_{\mathbf{0}} p_{\nu,\Omega}(\theta)$ is defined for any $\theta \in W^{1,\infty}$ by the following quantity:

$$\begin{aligned} \frac{1}{c_0}\binom{n}{\nu} \sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{-\frac{1}{2},\frac{1}{2}\right\}^n} \int_{\Omega^{\nu}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} \sum_{i=1}^n \Bigg[& \left\langle \nabla_{\mathbf{x}_i} \left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2 \right)(\mathbf{x}_1,\ldots,\mathbf{x}_n) \ \middle| \ \theta(\mathbf{x}_i) \right\rangle \\ & + |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2 (\mathbf{x}_1,\ldots,\mathbf{x}_n) \operatorname{div} \theta(\mathbf{x}_i) \Bigg] d\mathbf{x}_1 \ldots d\mathbf{x}_n. \end{aligned} \tag{27}$$

Finally, we can use the alternating property (9) satisfied by the wave function Ψ in order to get for any $i \in [\![1,n]\!]$, for any $(\mathbf{x}_1,\ldots,\mathbf{x}_n) \in \mathbb{R}^3 \times \ldots \times \mathbb{R}^3$, and for any $(\sigma_1,\ldots,\sigma_n) \in \{-\frac{1}{2},\frac{1}{2}\}^n$:

$$\nabla_{\mathbf{x}_i} \left(|\Psi^{(\sigma_1,\ldots,\sigma_i,\ldots,\sigma_n)}|^2 \right)(\mathbf{x}_1,\ldots,\mathbf{x}_i,\ldots,\mathbf{x}_n) = \nabla_{\mathbf{x}_1} \left(|\Psi^{(\sigma_i,\ldots,\sigma_1,\ldots,\sigma_n)}|^2 \right)(\mathbf{x}_i,\ldots,\mathbf{x}_1,\ldots,\mathbf{x}_n). \tag{28}$$

Inserting (28) in (27) and rearranging the summation on the spins variables in (27) by setting $\tilde{\sigma}_i = \sigma_1$, $\tilde{\sigma}_1 = \sigma_i$, and $\tilde{\sigma}_j = \sigma_j$ for any $j \in [\![1,n]\!]\backslash\{1,i\}$, we obtain that (25) holds true. It remains to study the Lipschitz case. Hence, we now assume that Ω is an open bounded subset of $\mathbb{R}^3$ with a Lipschitz boundary. First, we recall that for any measurable subset A of $(\mathbb{R}^3)^{n-1}$ and for any $g \in W^{1,1}((\mathbb{R}^3)^n, \mathbb{C})$, we have in the sense of distributions thus for almost every $\mathbf{x} \in \mathbb{R}^3$:

$$\int_A \nabla_{\mathbf{x}_1}(g)(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_n) d\mathbf{x}_2 \ldots d\mathbf{x}_n = \nabla_{\mathbf{x}_1} \left[\int_A g(\bullet,\mathbf{x}_2,\ldots,\mathbf{x}_n)\, d\mathbf{x}_2 \ldots d\mathbf{x}_n \right](\mathbf{x}). \tag{29}$$

Then, we can apply the Trace Theorem [17, Section 4.3] in (25) for any $\theta \in W^{1,\infty} \cap C^1$. Observing that the unit outer normal to the boundary $\partial\Omega = \partial(\mathbb{R}^3\backslash\Omega)$ satisfies $\mathbf{n}_{\mathbb{R}^3\backslash\Omega} = -\mathbf{n}_\Omega$, we deduce that (2) holds true for any $\theta \in W^{1,\infty} \cap C^1$. Finally, we can extend the result to any $\theta \in W^{1,\infty}$ from standard approximating arguments. Indeed, for any $\theta \in W^{1,\infty}$, there exists a sequence $(\theta_i)_{i\in\mathbb{N}} \subset W^{1,\infty} \cap C^1$ converging to θ strongly in L^∞, weakly-star in $W^{1,\infty}$, and uniformly on compact sets (consider the usual mollifier [17, Section 4.2.1 Theorem 1]). Note also that in (26) the boundary values of $\Psi^{(\sigma_1,\ldots,\sigma_n)} \in H^1((\mathbb{R}^3)^n, \mathbb{C})$ are understood in the sense of trace. In particular, they are uniquely determined up to a set of zero $A(\bullet \cap \partial\Omega)$-measure. It implies that the shape gradient of p_ν is unique and well defined by (26), concluding the proof of Theorem 2.8. $\square$

We conclude this section by specifying the Fréchet differentiability property of the associated map $p_{\nu,\Omega}$ in the specific case $k_0 = k = 1$ of Theorem 2.7.

Corollary 2.9. *Let us consider the assumptions of Theorem 2.7 in the specific case $k_0 = 1$. Then, the map $p_{\nu,\Omega} : \theta \in W^{1,\infty} \mapsto p_\nu[(I+\theta)(\Omega)]$ is well defined and continuously differentiable at any point of $W^{1,\infty} \cap \mathbb{B}^{0,1}$. Moreover, its (first-order) differential is well defined by the following continuous map:*

$$\begin{array}{rccl} D_\bullet p_{\nu,\Omega} : & W^{1,\infty} \cap \mathbb{B}^{0,1} & \longrightarrow & \mathcal{L}_c\left(W^{1,\infty}, \mathbb{R}\right) \\ & \theta_0 & \longmapsto & D_{\theta_0} p_{\nu,\Omega} := \theta \mapsto D_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)} \left[\theta \circ (I+\theta_0)^{-1}\right], \end{array} \tag{30}$$

where $D_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}$ is the shape derivative of p_ν at $(I+\theta_0)(\Omega)$ defined by (25). If in addition, we assume that Ω is an open bounded subset of $\mathbb{R}^3$ with a Lipschitz boundary, then the same result still holds true but we can now use the expression (2) to define $D_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}$ in (30).

Proof. First, for measurable $\Omega \subseteq \mathbb{R}^3$, the above statement is precisely the content of Theorem 2.7 with $k_0 = k = 1$. If in addition, Ω is an open bounded subset of $\mathbb{R}^3$ with a Lipschitz boundary, then $(I+\theta_0)(\Omega)$ is also a open bounded Lipschitz domain satisfying $\partial[(I+\theta_0)(\Omega)] = (I+\theta_0)(\partial\Omega)$. Moreover, $\theta \circ (I+\theta_0)^{-1} \in W^{1,\infty}$ for any $\theta \in W^{1,\infty}$ and any $\theta_0 \in W^{1,\infty} \cap \mathbb{B}^{0,1}$ so we deduce that the expression (2) defines well $D_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}$ in (30), concluding the proof of Corollary 2.9. $\square$

2.4 On the second-order shape derivative of the probability

We refer to Sections 1 and 2.1–2.2 for notation, especially Definition 2.5 for explanations about the notion of shape differentiability. Theorem 2.7 is stated in the specific $k_0 = 2$ and we show that we can recover the shape Hessian structure (3) by assuming the $C^{1,1}$-regularity of the domain.

Theorem 2.10. *Let us consider the assumptions of Theorem 2.7 in the specific case $k_0 = 2$. First, the two following maps are well defined and integrable:*

$$\begin{array}{rll} Q: \ \mathbb{R}^3 \times \ldots \times \mathbb{R}^3 & \longrightarrow & \mathbb{R} \\ (\mathbf{x}_1, \ldots, \mathbf{x}_n) & \longmapsto & Q(\mathbf{x}_1, \ldots, \mathbf{x}_n) := \left\langle \mathrm{Hess}_{\mathbf{x}_1}\left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\right)(\mathbf{x}_1, \ldots, \mathbf{x}_n)\,\theta(\mathbf{x}_1) \ \middle|\ \tilde{\theta}(\mathbf{x}_1)\right\rangle \\ & & + \left\langle \nabla_{\mathbf{x}_1}\left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\right)(\mathbf{x}_1, \ldots, \mathbf{x}_n) \ \middle|\ \theta(\mathbf{x}_1)\,\mathrm{div}\,\tilde{\theta}(\mathbf{x}_1) + \tilde{\theta}(\mathbf{x}_1)\,\mathrm{div}\,\theta(\mathbf{x}_1)\right\rangle \\ & & + |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2(\mathbf{x}_1, \ldots, \mathbf{x}_n)\left[\mathrm{div}\,\theta(\mathbf{x}_1)\,\mathrm{div}\,\tilde{\theta}(\mathbf{x}_1) - \mathrm{trace}\left(D_{\mathbf{x}_1}\theta D_{\mathbf{x}_1}\tilde{\theta}\right)\right] \end{array}$$

$$\begin{array}{rll} R: \ \mathbb{R}^3 \times \ldots \times \mathbb{R}^3 & \longrightarrow & \mathbb{R} \\ (\mathbf{x}_1, \ldots, \mathbf{x}_n) & \longmapsto & R(\mathbf{x}_1, \ldots, \mathbf{x}_n) := |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2(\mathbf{x}_1, \ldots, \mathbf{x}_n)\,\mathrm{div}\,\theta(\mathbf{x}_1)\,\mathrm{div}\,\tilde{\theta}(\mathbf{x}_2) \\ & & + \left\langle \nabla_{\mathbf{x}_1}\left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\right)(\mathbf{x}_1, \ldots, \mathbf{x}_n) \ \middle|\ \theta(\mathbf{x}_1)\right\rangle \mathrm{div}\,\tilde{\theta}(\mathbf{x}_2) \\ & & + \left\langle \nabla_{\mathbf{x}_2}\left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\right)(\mathbf{x}_1, \ldots, \mathbf{x}_n) \ \middle|\ \tilde{\theta}(\mathbf{x}_2)\right\rangle \mathrm{div}\,\theta(\mathbf{x}_1) \\ & & + \ \sum_{k,l=1}^3 \partial^2_{(\mathbf{x}_1)_k,(\mathbf{x}_2)_l}\left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\right)(\mathbf{x}_1, \ldots, \mathbf{x}_n)\,\theta_k(\mathbf{x}_1)\,\tilde{\theta}_l(\mathbf{x}_2). \end{array}$$

We also introduce the following map, which is well defined and integrable if Ω is an open bounded subset of $\mathbb{R}^3$ with a Lipschitz boundary and if $\theta \in W^{1,\infty} \cap C^1$:

$$\begin{array}{rl} S: \ \partial\Omega \times \mathbb{R}^3 \times \ldots \times \mathbb{R}^3 \longrightarrow & \mathbb{R} \\ (\mathbf{x}_1, \ldots, \mathbf{x}_n) \longmapsto & S(\mathbf{x}_1, \ldots, \mathbf{x}_n) := \left\langle \nabla_{\mathbf{x}_1}\left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\right)(\mathbf{x}_1, \ldots, \mathbf{x}_n) \ \middle|\ \theta(\mathbf{x}_1)\right\rangle \tilde{\theta}_{\mathbf{n}}(\mathbf{x}_1) \\ & + |\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2(\mathbf{x}_1, \ldots, \mathbf{x}_n)\left\langle \mathrm{div}\,\theta(\mathbf{x}_1)\,\tilde{\theta}(\mathbf{x}_1) - D_{\mathbf{x}_1}\theta\left[\tilde{\theta}(\mathbf{x}_1)\right] \ \middle|\ \mathbf{n}_\Omega(\mathbf{x}_1)\right\rangle. \end{array} \tag{31}$$

Then, the map (30) is Fréchet differentiable at the origin i.e. $p_{\nu,\Omega}:\theta\in W^{1,\infty}\mapsto p_\nu[(I+\theta)(\Omega)]$ is twice differentiable at the origin and its second-order differential is given by the following continuous symmetric bilinear form defined for any $(\theta,\tilde{\theta})\in W^{1,\infty}\times W^{1,\infty}$ by:

$$\begin{aligned}
D^2_{\mathbf{0}}p_{\nu,\Omega}(\theta,\tilde{\theta}) = \frac{1}{c_0}\binom{n}{\nu} \sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{\frac{1}{2},\frac{1}{2}\right\}^n} & \nu\int_{\Omega}\left(\int_{\Omega^{\nu-1}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} Q\left(\mathbf{x}_1,\ldots,\mathbf{x}_n\right)d\mathbf{x}_2\ldots d\mathbf{x}_n\right)d\mathbf{x}_1\\
&+\ (n-\nu)\int_{\mathbb{R}^3\backslash\Omega}\left(\int_{\Omega^{\nu}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu-1}} Q\left(\mathbf{x}_1,\ldots,\mathbf{x}_n\right)d\mathbf{x}_2\ldots d\mathbf{x}_n\right)d\mathbf{x}_1\\
&+\nu\left(\nu-1\right)\int_{\Omega\times\Omega}\left(\int_{\Omega^{\nu-2}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} R\left(\mathbf{x}_1,\ldots,\mathbf{x}_n\right)d\mathbf{x}_3\ldots d\mathbf{x}_n\right)d\mathbf{x}_1 d\mathbf{x}_2\\
&+2\nu\left(n-\nu\right)\int_{\Omega\times(\mathbb{R}^3\backslash\Omega)}\left(\int_{\Omega^{\nu-1}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu-1}} R\left(\mathbf{x}_1,\ldots,\mathbf{x}_n\right)d\mathbf{x}_3\ldots d\mathbf{x}_n\right)d\mathbf{x}_1 d\mathbf{x}_2\\
&+\ (n-\nu)\left(n-\nu-1\right)\int_{(\mathbb{R}^3\backslash\Omega)\times(\mathbb{R}^3\backslash\Omega)}\left(\int_{\Omega^{\nu}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu-2}} R\left(\mathbf{x}_1,\ldots,\mathbf{x}_n\right)d\mathbf{x}_3\ldots d\mathbf{x}_n\right)d\mathbf{x}_1 d\mathbf{x}_2.
\end{aligned} \tag{32}$$

In other words, the functional $p_\nu:\Omega\mapsto p_\nu(\Omega)$ of Definition 2.2 is twice shape differentiable at any measurable subset of $\mathbb{R}^3$. If in addition, we now assume that Ω is an open bounded subset Ω of $\mathbb{R}^3$ with a Lipschitz boundary, then the restriction $D_{\bullet}p_{\nu,\Omega}:W^{1,\infty}\cap C^1\cap\mathbb{B}^{0,1}\to\mathcal{L}_c(W^{1,\infty}\cap C^1,\mathbb{R})$ remains differentiable at the origin i.e. $p_{\nu,\Omega}:\theta\in W^{1,\infty}\cap C^1\mapsto p_\nu[(I+\theta)(\Omega)]$ is twice differentiable at the origin but its second-order differential can now be defined for any $(\theta,\tilde{\theta})\in(W^{1,\infty}\cap C^1)^2$ by:

$$\begin{aligned}
D^2_{\mathbf{0}}p_{\nu,\Omega}(\theta,\tilde{\theta}) \ =\ & \int_{\partial\Omega\times\partial\Omega} K_\Omega\left(\mathbf{x},\mathbf{y}\right)\theta_{\mathbf{n}}\left(\mathbf{x}\right)\tilde{\theta}_{\mathbf{n}}\left(\mathbf{y}\right)dA\left(\mathbf{x}\right)dA\left(\mathbf{y}\right)\\
&+\frac{1}{c_0}\binom{n}{\nu}\sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{\frac{1}{2},\frac{1}{2}\right\}^n}\int_{\partial\Omega}\left(\nu\int_{\Omega^{\nu-1}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} S\left(\mathbf{x}_1,\ldots,\mathbf{x}_n\right)d\mathbf{x}_2\ldots d\mathbf{x}_n\right.\\
&\qquad\left.-\ (n-\nu)\int_{\Omega^{\nu}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu-1}} S\left(\mathbf{x}_1,\ldots,\mathbf{x}_n\right)d\mathbf{x}_2\ldots d\mathbf{x}_n\right)dA\left(\mathbf{x}_1\right),
\end{aligned} \tag{33}$$

where the kernel $K_\Omega:\partial\Omega\times\partial\Omega\to\mathbb{R}$ is given for any $(\mathbf{x},\mathbf{y})\in\partial\Omega\times\partial\Omega$ by the following formula:

$$\begin{aligned}
K_\Omega\left(\mathbf{x},\mathbf{y}\right)=\frac{1}{c_0}\binom{n}{\nu}\sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{\frac{1}{2},\frac{1}{2}\right\}^n} & \nu\left(\nu-1\right)\int_{\Omega^{\nu-2}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}}|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\left(\mathbf{x},\mathbf{y},\mathbf{x}_3,\ldots,\mathbf{x}_n\right)d\mathbf{x}_3\ldots d\mathbf{x}_n\\
&-2\nu\left(n-\nu\right)\int_{\Omega^{\nu-1}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu-1}}|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\left(\mathbf{x},\mathbf{y},\mathbf{x}_3,\ldots,\mathbf{x}_n\right)d\mathbf{x}_3\ldots d\mathbf{x}_n\\
&+\left(n-\nu\right)\left(n-\nu-1\right)\int_{\Omega^{\nu}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu-2}}|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\left(\mathbf{x},\mathbf{y},\mathbf{x}_3,\ldots,\mathbf{x}_n\right)d\mathbf{x}_3\ldots d\mathbf{x}_n.
\end{aligned} \tag{34}$$

Finally, if we now assume that Ω is an open bounded subset of $\mathbb{R}^3$ with a boundary of class $C^{1,1}$, then the second-order shape derivative of p_ν at Ω can take the form given by (3), where the shape Hessian is uniquely determined up to a set of zero $A(\bullet\cap\partial\Omega)$-measure, and defined for any $\mathbf{x}\in\partial\Omega$ by:

$$\begin{aligned}
\frac{\partial^2 p_\nu}{\partial\Omega^2}\left(\mathbf{x}\right)=\frac{1}{c_0}\binom{n}{\nu}\sum_{(\sigma_1,\ldots,\sigma_n)\in\left\{\frac{1}{2},\frac{1}{2}\right\}^n} & \nu\int_{\Omega^{\nu-1}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} H_\Omega\left(\mathbf{x}\right)|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\left(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_n\right)\\
&\qquad+\left\langle\nabla_{\mathbf{x}_1}\left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\right)\left(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_n\right)\ \middle|\ \mathbf{n}_\Omega\left(\mathbf{x}\right)\right\rangle d\mathbf{x}_2\ldots d\mathbf{x}_n\\
&-\left(n-\nu\right)\int_{\Omega^{\nu}\times(\mathbb{R}^3\backslash\Omega)^{n-\nu-1}} H_\Omega\left(\mathbf{x}\right)|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\left(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_n\right)\\
&\qquad+\left\langle\nabla_{\mathbf{x}_1}\left(|\Psi^{(\sigma_1,\ldots,\sigma_n)}|^2\right)\left(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_n\right)\ \middle|\ \mathbf{n}_\Omega\left(\mathbf{x}\right)\right\rangle d\mathbf{x}_2\ldots d\mathbf{x}_n.
\end{aligned} \tag{35}$$

In (31) and (34)–(35), the boundary values of $\Psi^{(\sigma_1,\ldots,\sigma_n)}\in H^2((\mathbb{R}^3)^n,\mathbb{C})$ and $\nabla_{\mathbf{x}_1}\Psi^{(\sigma_1,\ldots,\sigma_n)}$ are understood in the sense of trace. The conventions $A^0\times B=B\times A^0=A$, $A^{-1}\times B=B\times A^{-1}=\emptyset$, $A^{-2}\times B=B\times A^{-2}=\emptyset$, and $\int_\emptyset f(x,y)dy=f(x)$ are used to interpret (3) and (32)–(35) if $n\in\{2,3\}$ and $\nu\in\{0,1,2,n-1,n-2,n\}$.

Proof. First, the maps Q and R of the statement are well defined and integrable because we have $\theta, \tilde{\theta} \in W^{1,\infty}$, $\Psi \in H^2$, $\nabla(|\Psi|^2) = 2\mathrm{Real}(\overline{\Psi}\nabla\Psi)$, and $\mathrm{Hess}(|\Psi|^2) = 2\mathrm{Real}(\overline{\Psi}\mathrm{Hess}\Psi + \nabla\overline{\Psi}[\nabla\Psi]^T)$. The map S is also well defined and integrable but we have to assume the Lipschitz regularity of the domain Ω to get the existence almost everywhere of the unit normal field $\mathbf{n}_\Omega$, and also impose that $\theta \in W^{1,\infty} \cap C^1$ since we need to compute the boundary values of $D_\bullet\theta$ and div θ. Then, we can apply Theorem 2.7 with $k_0 = k = 2$. The functional $p_\nu : \Omega \mapsto p_\nu(\Omega)$ of Definition 2.2 is thus twice shape differentiable at Ω and its second-order shape derivative $D^2_{\mathbf{0}} p_{\nu,\Omega}(\theta, \tilde{\theta})$ is defined for any $(\theta, \tilde{\theta}) \in W^{1,\infty} \times W^{1,\infty}$ by the following quantity:

$$\frac{1}{c_0}\binom{n}{\nu} \sum_{(\sigma_1,\dots,\sigma_n)\in\left\{-\frac{1}{2},\frac{1}{2}\right\}^n} \sum_{i,j=1}^{n}\sum_{k,l=1}^{3} \int_{\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} \frac{\partial^2\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)}{\partial(\mathbf{x}_i)_k\partial(\mathbf{x}_j)_l}(\mathbf{x}_1,\dots,\mathbf{x}_n)\left[\theta(\mathbf{x}_i)\right]_k[\tilde{\theta}(\mathbf{x}_j)]_l$$
$$+ \frac{\partial\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)}{\partial(\mathbf{x}_i)_k}(\mathbf{x}_1,\dots,\mathbf{x}_n)\left[\theta(\mathbf{x}_i)\right]_k[D_{\mathbf{x}_j}\tilde{\theta}]_{ll}$$
$$+ \frac{\partial\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)}{\partial(\mathbf{x}_j)_l}(\mathbf{x}_1,\dots,\mathbf{x}_n)[\tilde{\theta}(\mathbf{x}_j)]_l\,[D_{\mathbf{x}_i}\theta]_{kk}$$
$$+ |\Psi^{(\sigma_1,\dots,\sigma_n)}|^2(\mathbf{x}_1,\dots,\mathbf{x}_n)\left([D_{\mathbf{x}_i}\theta]_{kk}[D_{\mathbf{x}_j}\tilde{\theta}]_{ll} - I_{ij}[D_{\mathbf{x}_i}\theta]_{kl}[D_{\mathbf{x}_j}\tilde{\theta}]_{lk}\right).$$

Distinguishing the two cases $i = j$ and $i \neq j$, we deduce that $D^2_{\mathbf{0}} p_{\nu,\Omega}(\theta, \tilde{\theta})$ is equal to:

$$\frac{1}{c_0}\binom{n}{\nu} \sum_{(\sigma_1,\dots,\sigma_n)\in\left\{-\frac{1}{2},\frac{1}{2}\right\}^n} \sum_{i=1}^{n} \int_{\Omega^\nu\times(\mathbb{R}^3\backslash\Omega)^{n-\nu}} \Bigg[\left\langle \mathrm{Hess}_{\mathbf{x}_i}\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)(\mathbf{x}_1,\dots,\mathbf{x}_n)\theta(\mathbf{x}_i)\ \middle|\ \tilde{\theta}(\mathbf{x}_i)\right\rangle$$
$$+ \left\langle \nabla_{\mathbf{x}_i}\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)(\mathbf{x}_1,\dots\mathbf{x}_n)\ \middle|\ \theta(\mathbf{x}_i)\,\mathrm{div}\,\tilde{\theta}(\mathbf{x}_i) + \tilde{\theta}(\mathbf{x}_i)\,\mathrm{div}\,\theta(\mathbf{x}_i)\right\rangle$$
$$+ |\Psi^{(\sigma_1,\dots,\sigma_n)}|^2(\mathbf{x}_1,\dots\mathbf{x}_n)\left[\mathrm{div}\,\theta(\mathbf{x}_i)\,\mathrm{div}\,\tilde{\theta}(\mathbf{x}_i) - \mathrm{trace}\left(D_{\mathbf{x}_i}\theta D_{\mathbf{x}_i}\tilde{\theta}\right)\right]$$
$$+ \sum_{\substack{j\in[\![1,n]\!]\\ j\neq i}}\sum_{k,l=1}^{3} \frac{\partial^2\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)}{\partial(\mathbf{x}_i)_k\partial(\mathbf{x}_j)_l}(\mathbf{x}_1,\dots,\mathbf{x}_n)\left[\theta(\mathbf{x}_i)\right]_k[\tilde{\theta}(\mathbf{x}_j)]_l$$
$$+ \left\langle \nabla_{\mathbf{x}_i}\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)(\mathbf{x}_1,\dots\mathbf{x}_n)\ \middle|\ \theta(\mathbf{x}_i)\right\rangle \mathrm{div}\,\tilde{\theta}(\mathbf{x}_j)$$
$$+ \left\langle \nabla_{\mathbf{x}_j}\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)(\mathbf{x}_1,\dots\mathbf{x}_n)\ \middle|\ \tilde{\theta}(\mathbf{x}_j)\right\rangle \mathrm{div}\,\theta(\mathbf{x}_i)$$
$$+ |\Psi^{(\sigma_1,\dots,\sigma_n)}|^2(\mathbf{x}_1,\dots\mathbf{x}_n)\,\mathrm{div}\,\theta(\mathbf{x}_i)\,\mathrm{div}\,\tilde{\theta}(\mathbf{x}_j)\Bigg]\, d\mathbf{x}_1\dots d\mathbf{x}_n. \tag{36}$$

We now proceed as in the proof of Theorem 2.8. We use the alternating property (9) of the wave function Ψ in order to get:

$$\mathrm{Hess}_{\mathbf{x}_i}\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)(\mathbf{x}_1,\dots,\mathbf{x}_n) = \mathrm{Hess}_{\mathbf{x}_1}\left(|\Psi^{(\sigma_i,\dots,\sigma_1,\dots,\sigma_n)}|^2\right)(\mathbf{x}_i,\dots,\mathbf{x}_1,\dots,\mathbf{x}_n)$$

and

$$\frac{\partial^2\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)}{\partial(\mathbf{x}_i)_k\partial(\mathbf{x}_j)_l}(\mathbf{x}_1,\dots,\mathbf{x}_n) = \frac{\partial^2\left(|\Psi^{(\sigma_i,\sigma_j,\dots,\sigma_1,\dots,\sigma_2,\dots,\sigma_n)}|^2\right)}{\partial(\mathbf{x}_1)_k\partial(\mathbf{x}_2)_l}(\mathbf{x}_i,\mathbf{x}_j,\dots,\mathbf{x}_1,\dots,\mathbf{x}_2,\dots,\mathbf{x}_n).$$

Combining these observations and (28), we can now rearrange the summation on the spin variables in (36). We deduce that relation (32) holds true by distinguishing the cases $(\mathbf{x}_i, \mathbf{x}_j) \in \Omega\times\Omega$, $(\mathbf{x}_i,\mathbf{x}_j) \in (\mathbb{R}^3\backslash\Omega)\times(\mathbb{R}^3\backslash\Omega)$, $(\mathbf{x}_i,\mathbf{x}_j) \in \Omega\times(\mathbb{R}^3\backslash\Omega)$, and $(\mathbf{x}_i,\mathbf{x}_j) \in (\mathbb{R}^3\backslash\Omega)\times\Omega$, where the two last cases lead to the same expression by exchanging the role of i and j with (9) and relabelling again the spin variables.

Let us now study the Lipschitz case so we assume that $\Omega \subset \mathbb{R}^3$ is an open bounded set with a Lipschitz boundary and we consider the restriction map $p_{\nu,\Omega} : \theta \in W^{1,\infty}\cap C^1 \mapsto p_\nu[(I+\theta)(\Omega)]$. Since $W^{1,\infty}\cap C^1$ is also equipped with the $W^{1,\infty}$-norm, we deduce from Corollary 2.9 that $p_{\nu,\Omega}$ is continuously differentiable on $W^{1,\infty}\cap C^1\cap\mathbb{B}^{0,1}$, its differential being well defined by:

$$\begin{array}{rccl} D_\bullet p_{\nu,\Omega}: & W^{1,\infty}\cap C^1\cap\mathbb{B}^{0,1} & \longrightarrow & \mathcal{L}_c\left(W^{1,\infty}\cap C^1,\mathbb{R}\right) \\ & \theta_0 & \longmapsto & D_{\theta_0}p_{\nu,\Omega} : \theta \mapsto D_{\mathbf{0}}p_{\nu,(I+\theta_0)(\Omega)}\left[\theta\circ(I+\theta_0)^{-1}\right]. \end{array} \tag{37}$$

Moreover, we obtain from the foregoing that the map (37) is differentiable at the origin i.e. $p_{\nu,\Omega}$ is twice differentiable at the origin and its second-order differential is well defined by (32) for any $(\theta,\tilde{\theta}) \in (W^{1,\infty}\cap C^1)\times(W^{1,\infty}\cap C^1)$. Let us now use the additional regularity of Ω, θ, and $\tilde{\theta}$ in order to improve the expression (32). On the one hand, one can observe that the map R of the statement can be expressed into a divergence form:

$$\begin{aligned} R(\mathbf{x}_1,\dots,\mathbf{x}_n) &= \operatorname{div}\Big[\theta\Big(\Big\langle\nabla_{\mathbf{x}_2}\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)(\bullet,\mathbf{x}_2,\dots,\mathbf{x}_n)\ \big|\ \tilde{\theta}(\mathbf{x}_2)\Big\rangle \\ &\qquad +|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2(\bullet,\mathbf{x}_2,\dots,\mathbf{x}_n)\operatorname{div}\tilde{\theta}(\mathbf{x}_2)\Big)\Big](\mathbf{x}_1). \end{aligned}$$

Arguing as in (29), we can thus apply the Trace Theorem [17, Section 4.3] to the integrals involving R in (32). A similar argument with the variable $\mathbf{x}_2$ yields to transform the integrals involving R in (32) into the one involving the kernel K_Ω in (33). The sign obtained depends on the outer normal $\mathbf{n}_{\mathbb{R}^3\backslash\Omega}=-\mathbf{n}_\Omega$ of the boundary $\partial\Omega=\partial(\mathbb{R}^3\backslash\Omega)$. On the other hand, we can treat the integrals involving Q in (32) as follows. First, we assume that $(\theta,\tilde{\theta})\in W^{2,\infty}\times W^{2,\infty}$ so we can write:

$$\begin{aligned} Q(\mathbf{x}_1,\dots,\mathbf{x}_n) &= \operatorname{div}\Big[\operatorname{div}\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2(\bullet,\mathbf{x}_2,\dots,\mathbf{x}_n)\,\theta\right)\tilde{\theta}-D_\bullet\theta(\tilde{\theta})\Big](\mathbf{x}_1) \\ &= \operatorname{div}\Big[\operatorname{div}\Big(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2(\bullet,\mathbf{x}_2,\dots,\mathbf{x}_n)\,\tilde{\theta}\Big)\theta-D_\bullet\tilde{\theta}(\theta)\Big](\mathbf{x}_1). \end{aligned}$$

We emphasize that fact that the above equalities only hold true because we have assumed that $(\theta,\tilde{\theta})\in W^{2,\infty}\times W^{2,\infty}$. Then, arguing as in (29), we apply the Trace Theorem [17, Section 4.3] for the integrals involving Q in (32), from which we deduce the expressions involving S in (33). More precisely, we need here to use the Trace Theorem for $W^{1,\infty}$-fields, which can be obtained from usual density arguments (see below (29)). Consequently, using again the fact that the unit outer normal to the boundary $\partial\Omega=\partial(\mathbb{R}^3\backslash\Omega)$ satisfies $\mathbf{n}_{\mathbb{R}^3\backslash\Omega}=-\mathbf{n}_\Omega$, we have proved that (33) holds true for any $(\theta,\tilde{\theta})\in W^{2,\infty}\times W^{2,\infty}$. Note also that even if (33) is not symmetric in θ and $\tilde{\theta}$, the symmetry can be obtained from the above equalities. Finally, we get that (33) holds true for any $(\theta,\tilde{\theta})\in(W^{1,\infty}\cap C^1)\times(W^{1,\infty}\cap C^1)$ by standard approximating arguments. Indeed, for any $\theta\in W^{1,\infty}\cap C^1$, there exists a sequence $(\theta_k)_{k\in\mathbb{N}}$ of elements in $W^{2,\infty}$ such that θ_k and $[D_\bullet\theta_k]_{ij}$ respectively converges to θ and $[D_\bullet\theta]_{ij}$ uniformly on any compact subset of $\mathbb{R}^n$ as $k\to+\infty$ and for any $(i,j)\in[\![1,n]\!]^2$ (consider again the usual mollifier [17, Section 4.2.1 Theorem 1]).

It remains to treat the $C^{1,1}$-regularity. First, we decompose the operators in S and the vector fields into a tangential and normal components. We thus have:

$$\begin{aligned} S(\mathbf{x}_1,\dots,\mathbf{x}_n) &= \operatorname{div}_{\partial\Omega}\left[\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)(\bullet,\mathbf{x}_2,\dots,\mathbf{x}_n)\,\theta\right](\mathbf{x}_1)\,\tilde{\theta}_{\mathbf{n}}(\mathbf{x}_1) \\ &\quad+\left\langle\nabla_{\mathbf{x}_1}\left(|\Psi^{(\mathbf{x}_1,\dots,\mathbf{x}_n)}|^2\right)(\mathbf{x}_1,\dots,\mathbf{x}_n)\ \big|\ \mathbf{n}_\Omega(\mathbf{x}_1)\right\rangle\theta_{\mathbf{n}}(\mathbf{x}_1)\,\tilde{\theta}_{\mathbf{n}}(\mathbf{x}_1) \\ &\quad-|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2(\mathbf{x}_1,\dots,\mathbf{x}_n)\Big\langle D_{\partial\Omega}\theta(\tilde{\theta}_{\partial\Omega})\ \big|\ \mathbf{n}_\Omega\Big\rangle(\mathbf{x}_1). \end{aligned}$$

Then, we assume that Ω is an open bounded subset of $\mathbb{R}^3$ with a boundary of class $C^{1,1}$. Since the outer normal field $\mathbf{n}_\Omega$ is now Lipschitz continuous, we deduce from Rademacher's Theorem [17, Section 3.1.2] that it is differentiable almost everywhere. Hence, we can write:

$$\begin{aligned} S(\mathbf{x}_1,\dots,\mathbf{x}_n) &= \operatorname{div}_{\partial\Omega}\Big[\left(|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2\right)(\bullet,\mathbf{x}_2,\dots,\mathbf{x}_n)\,\tilde{\theta}_{\mathbf{n}}\theta\Big](\mathbf{x}_1) \\ &\quad+\left\langle\nabla_{\mathbf{x}_1}\left(|\Psi^{(\mathbf{x}_1,\dots,\mathbf{x}_n)}|^2\right)(\mathbf{x}_1,\dots,\mathbf{x}_n)\ \big|\ \mathbf{n}_\Omega(\mathbf{x}_1)\right\rangle\theta_{\mathbf{n}}(\mathbf{x}_1)\,\tilde{\theta}_{\mathbf{n}}(\mathbf{x}_1) \\ &\quad-|\Psi^{(\sigma_1,\dots,\sigma_n)}|^2(\mathbf{x}_1,\dots,\mathbf{x}_n)\,Z[\theta,\tilde{\theta}](\mathbf{x}_1), \end{aligned}$$

where we recall that $Z[\theta,\tilde{\theta}]$ is defined by (4). Finally, arguing as in (29) with the above expression of S, we can apply the Divergence Theorem for surfaces [27, Theorem 6.10] in (33), which is valid with $C^{1,1}$-regularity (adapt for example the proofs of [22, Proposition 5.4.9]). We deduce that the second-order shape derivative of p_ν at Ω can take the form given in (3). We emphasize the fact that in (31) and (34)–(35), the boundary values of $\Psi^{(\sigma_1,\dots,\sigma_n)}\in H^2((\mathbb{R}^3)^n,\mathbb{C})$ and $\nabla_{\mathbf{x}_1}\Psi^{(\sigma_1,\dots,\sigma_n)}$ have to be understood in the sense of trace. In particular, the shape Hessian (35) is uniquely determined up to a set of zero $A(\bullet\cap\partial\Omega)$-measure and the same holds true for the kernel (34), concluding the proof of Theorem 2.10. □

We conclude this section by specifying the Fréchet differentiability of the associated map $p_{\nu,\Omega}$ in the specific case $k_0=k=2$ of Theorem 2.7.

Corollary 2.11. *Let us consider the assumptions of Theorem 2.7 in the specific case $k_0 = 2$. Then, the map $p_{\nu,\Omega} : \theta \in W^{1,\infty} \mapsto p_\nu[(I+\theta)(\Omega)]$ is well defined and twice continuously differentiable at any point of $W^{1,\infty} \cap \mathbb{B}^{0,1}$. Moreover, its second-order differential is well defined by the following continuous map:*

$$\begin{array}{rccl} D^2_{\bullet} p_{\nu,\Omega} : & W^{1,\infty} \cap \mathbb{B}^{0,1} & \longrightarrow & \mathcal{L}^2_c\left(W^{1,\infty} \times W^{1,\infty}, \mathbb{R}\right) \\ & \theta_0 & \longmapsto & (\theta_1,\theta_2) \mapsto D^2_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)} \left[\theta_1 \circ (I+\theta_0)^{-1}, \theta_2 \circ (I+\theta_0)^{-1}\right], \end{array} \tag{38}$$

where $D^2_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}$ is the second-order shape derivative of p_ν at $(I+\theta_0)(\Omega)$ defined by (32). If in addition, we now assume that Ω is an open bounded subset of $\mathbb{R}^3$ with a Lipschitz boundary, then the restriction map $p_{\nu,\Omega} : \theta \in W^{1,\infty} \cap C^1 \mapsto p_\nu[(I+\theta)(\Omega)]$ is still twice continuously differentiable at any point of $W^{1,\infty} \cap C^1 \cap \mathbb{B}^{0,1}$ and its second-order differential is well defined by the following continuous map:

$$\begin{array}{rccl} D^2_{\bullet} p_{\nu,\Omega} : & W^{1,\infty} \cap C^1 \cap \mathbb{B}^{0,1} & \longrightarrow & \mathcal{L}^2_c\left(\left(W^{1,\infty} \cap C^1\right) \times \left(W^{1,\infty} \cap C^1\right), \mathbb{R}\right) \\ & \theta_0 & \longmapsto & (\theta_1,\theta_2) \mapsto D^2_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)} \left[\theta_1 \circ (I+\theta_0)^{-1}, \theta_2 \circ (I+\theta_0)^{-1}\right], \end{array} \tag{39}$$

where $D^2_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}$ can now be defined by (33). Finally, if we assume that Ω is an open bounded subset of $\mathbb{R}^3$ with a boundary of class $C^{1,1}$, then the last result still holds true but we can now use the expression (3) to define $D^2_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}$ in (39).

Proof. First, for a measurable $\Omega \subseteq \mathbb{R}^3$, the statement (38) is precisely the content of Theorem 2.7 with $k_0 = k = 2$. If in addition, Ω is an open bounded subset of $\mathbb{R}^3$ with a Lipschitz boundary, then $(I_3+\theta_0)(\Omega)$ is also a open bounded Lipschitz domain satisfying $\partial[(I_3+\theta_0)(\Omega)] = (I_3+\theta_0)(\partial\Omega)$. Moreover, we have $\theta\circ(I_3+\theta_0)^{-1} \in W^{1,\infty}\cap C^1$ for any $\theta \in W^{1,\infty}\cap C^1$ and any $\theta_0 \in W^{1,\infty}\cap C^1 \cap \mathbb{B}^{0,1}$. We deduce that the expression (33) defines well $D^2_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}$ in (39). Finally, if Ω is now an open bounded subset of $\mathbb{R}^3$ with a $C^{1,1}$-boundary, then $(I+\theta_0)(\Omega)$ is also a $C^{1,1}$-domain and we can use the expression (3) to define $D^2_{\mathbf{0}} p_{\nu,(I+\theta_0)(\Omega)}$ in (39), concluding the proof of Corollary 2.11. ☐

3 About the shape derivatives of a volume integral

In this section, the integer $n \geqslant 2$ is still fixed but now refers to the dimension of the real space $\mathbb{R}^n$ in which we are working (and *not* to the number of electrons as it was the case in Sections 1–2). In particular, Ω now denotes a subset of $\mathbb{R}^n$ and $\theta : \mathbb{R}^n \to \mathbb{R}^n$ is a well-defined vector field on $\mathbb{R}^n$. Our goal here is to study the shape differentiability properties of the following map:

$$\begin{array}{rccl} F : & \mathcal{M} & \longrightarrow & \mathbb{R} \\ & \Omega & \longmapsto & F(\Omega) := \displaystyle\int_\Omega f(\mathbf{x})\, d\mathbf{x}, \end{array} \tag{40}$$

where the integration is done with respect to the n-dimensional Lebesgue measure, and where $\mathcal{M}$ now refers to the class of (Lebesgue) measurable subset of $\mathbb{R}^n$. We refer to Sections 1 and 2.1–2.2 for notation, especially Definition 2.5 for explanations about the notion of shape differentiability. First, note that if $f \in L^1(\mathbb{R}^n,\mathbb{R})$, the map $F : \Omega \mapsto F(\Omega)$ is well defined by (40).

Then, we aim to establish precise shape differentiability results concerning (40) since the proofs of Section 2 were all relying on the shape derivatives of a volume integral. We distinguish three cases according to the regularity of the given domain. We also mention that from our statements, we can recover the standard formulas for the first- and second-order shape derivatives of a volume integral [16, Chapter 9] [22, Chapter 5] [40, Chapter 2].

3.1 The general case of a measurable domain

For any integer $k \geqslant 1$, we define $W^{k,1}$ as the standard Sobolev space of L^1-maps from $\mathbb{R}^n$ into $\mathbb{R}$ whose partial derivatives (in the weak distributional sense) are also L^1-functions up to the order k. In this section, we prove that if $f \in W^{k,1}$ and $\Omega \in \mathcal{M}$, then the map $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I+\theta)(\Omega)]$ associated with (40) is of class C^k around the origin. In particular, we get an explicit formula (43) for the shape derivative of a volume integral at any order. The proof is made by induction on k so we first need to initialize the process by studying the continuity properties of F_Ω.

Lemma 3.1. *Let $n \geqslant 2$, $f \in L^1(\mathbb{R}^n, \mathbb{R})$, and $\Omega \in \mathcal{M}$. Then, the map $F_\Omega : \theta \in C^{0,1} \mapsto F[(I+\theta)(\Omega)]$ is well defined on $\mathbb{B}^{0,1}$. Moreover, $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I+\theta)(\Omega)]$ is continuous on $\mathbb{B}^{0,1} \cap W^{1,\infty}$.*

Proof. Let $n \geqslant 2$, $f \in L^1(\mathbb{R}^n, \mathbb{R})$, and $\Omega \in \mathcal{M}$. First, applying Proposition 4.1, the map $I+\theta$ has a Lipschitz continuous inverse for any $\theta \in \mathbb{B}^{0,1}$, from which we deduce that $(I+\theta)(\Omega)$ is measurable. Hence, the map $F_\Omega : \theta \in C^{0,1} \mapsto F[(I+\theta)(\Omega)]$ is well defined on $\mathbb{B}^{0,1}$. Then, let $\theta \in W^{1,\infty} \cap C^{0,1}$. We use the change of variables formula valid for any Lipschitz continuous map [17, Section 3.3.3] and the (reverse) triangle inequality in order to get:

$$\left| \int_{(I+\theta)(\Omega)} f - \int_\Omega f \right| \leqslant \left| \int_\Omega [f \circ (I+\theta) - f] \left| \det \left[D_\bullet (I+\theta) \right] \right| \right| + \left| \int_\Omega f \left(\left| \det \left[D_\bullet (I+\theta) \right] \right| - 1 \right) \right|$$

$$\leqslant \| \det \left[D_\bullet (I+\theta) \right] \|_{L^\infty} \| f \circ (I+\theta) - f \|_{L^1} + \| \det \left[D_\bullet (I+\theta) \right] - 1 \|_{L^\infty} \| f \|_{L^1}.$$

Combining (63) and the continuity at the origin of the Jacobian determinant of $(I+\theta)$ ensured by Proposition 4.4 with the one of $\theta \in W^{1,\infty} \mapsto f \circ (I+\theta) \in L^1(\mathbb{R}^n, \mathbb{R})$ ensured by Proposition 4.6, we can let $\|\theta\|_{W^{1,\infty}} \to 0$ in the above inequality. Hence, the map $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I+\theta)(\Omega)]$ is continuous at the origin. Finally, let $\theta \in W^{1,\infty} \cap \mathbb{B}^{0,1}$. We recall that $(I+\theta)(\Omega)$ is measurable and moreover, note that for any $h \in W^{1,\infty}$ such that $\|h\|_{W^{1,\infty}} < 1 - \|\theta\|_{C^{0,1}}$, we have $\|\theta + h\|_{C^{0,1}} < 1$ so we can write:

$$\int_{(I+\theta+h)(\Omega)} f - \int_{(I+\theta)(\Omega)} f = \int_{(I+h_\theta)(\Omega_\theta)} f - \int_{\Omega_\theta} f, \tag{41}$$

where we have set $\Omega_\theta := (I+\theta)(\Omega)$ and $h_\theta := h \circ (I+\theta)^{-1}$. One can check that $\|h_\theta\|_{L^\infty} \leqslant \|h\|_{L^\infty}$ and $\|h_\theta\|_{C^{0,1}} \leqslant \|h\|_{C^{0,1}} \|(I+\theta)^{-1}\|_{C^{0,1}} \leqslant \|h\|_{C^{0,1}} (1 - \|\theta\|_{C^{0,1}})^{-1}$ by Proposition 4.1 so we deduce that:

$$\|h_\theta\|_{W^{1,\infty}} \leqslant \|h\|_{L^\infty} + \frac{\|h\|_{C^{0,1}}}{1 - \|\theta\|_{C^{0,1}}} = \frac{\|h\|_{W^{1,\infty}} - \|h\|_{L^\infty} \|\theta\|_{C^{0,1}}}{1 - \|\theta\|_{C^{0,1}}} \leqslant \frac{\|h\|_{W^{1,\infty}}}{1 - \|\theta\|_{C^{0,1}}}. \tag{42}$$

In particular, we have $\|h_\theta\|_{W^{1,\infty}} \to 0$ as $\|h\|_{W^{1,\infty}} \to 0$. Considering the continuity at the origin of $h_\theta \in W^{1,\infty} \mapsto F[(I+h_\theta)(\Omega_\theta)]$, we can let $\|h\|_{W^{1,\infty}} \to 0$ in (41). We have obtained the continuity of $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I+\theta)(\Omega)]$ on $W^{1,\infty} \cap \mathbb{B}^{0,1}$, concluding the proof of Lemma 3.1. $\square$

Theorem 3.2. *Let $n \geqslant 2$ and $k_0 \geqslant 1$ be two integers. We consider $f \in W^{k_0,1}(\mathbb{R}^n, \mathbb{R})$ and $\Omega \in \mathcal{M}$. Then, the map $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I+\theta)(\Omega)]$ is k_0 times Fréchet differentiable at the origin and for any $k \in [\![1, k_0]\!]$, its differential of order k at the origin is given by the following continuous symmetric k-linear form defined for any $(\theta_1, \ldots, \theta_k) \in W^{1,\infty} \times \ldots \times W^{1,\infty}$ by:*

$$\begin{aligned} D^k_{\mathbf{0}} F_\Omega (\theta_1, \ldots, \theta_k) \quad = \\ \sum_{i_1,\ldots,i_k=1}^{n} \sum_{l=0}^{k} \sum_{\substack{I_l \subseteq [\![1,k]\!] \\ \text{card } I_l = l}} \sum_{p \in \mathcal{S}_{I_l}} s(p) \int_\Omega \frac{\partial^{k-l} f}{\prod\limits_{\substack{j \in [\![1,k]\!] \\ j \notin I_l}} \partial \mathbf{x}_{i_j}} (\mathbf{x}) \prod_{\substack{j \in [\![1,k]\!] \\ j \notin I_l}} [\theta_j(\mathbf{x})]_{i_j} \prod_{j \in I_l} [D_\mathbf{x} \theta_j]_{i_j i_{p(j)}} d\mathbf{x}. \end{aligned} \tag{43}$$

In other words, the functional (40) *is k_0 times shape differentiable at any measurable subset of $\mathbb{R}^n$ and its k-th-order shape derivative is well defined by* (43) *for any $k \in [\![1, k_0]\!]$. Moreover, the map $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I+\theta)(\Omega)]$ is k_0 times continuously differentiable at any point of $W^{1,\infty} \cap \mathbb{B}^{0,1}$ and for any $k \in [\![1, k_0]\!]$, its k-th-order differential is well defined by the following continuous map:*

$$\begin{array}{rccl} D^k_\bullet F_\Omega : & W^{1,\infty} \cap \mathbb{B}^{0,1} & \longrightarrow & \mathcal{L}^k_c \left(\left(W^{1,\infty} \right)^k, \mathbb{R} \right) \\ & \theta_0 & \longmapsto & (\theta_1, \ldots, \theta_k) \mapsto D^k_{\mathbf{0}} F_{(I+\theta_0)(\Omega)} \left[\theta_1 \circ (I+\theta_0)^{-1}, \ldots, \theta_k \circ (I+\theta_0)^{-1} \right], \end{array} \tag{44}$$

where $D^k_{\mathbf{0}} F_{(I+\theta_0)(\Omega)}$ is the k-th-order shape derivative of F at $(I+\theta_0)(\Omega)$ given by (43).

Proof. We are going to prove this result by induction on the integer $k \in \mathbb{N}$. First, recalling the usual conventions $\partial^0 f = f$, $\sum_{i \in \emptyset} = 0$, $\prod_{i \in \emptyset} = 1$, and $D^{\mathbf{0}}_{\theta_0} F_\Omega = F_\Omega(\theta_0) = F_{(I+\theta_0)(\Omega)}(\mathbf{0})$, we deduce from Lemma 3.1 that Theorem 3.2 holds true for $k = 0$. Let us assume that it is also true for some integer $k \geqslant 0$. Let $n \geqslant 2$ be an integer, $f \in W^{k+1,1}$, and $\Omega \in \mathcal{M}$. The induction hypothesis ensures that the map $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I+\theta)(\Omega)]$ is k times continuously differentiable at any point of $W^{1,\infty} \cap \mathbb{B}^{0,1}$. We now show that the additional regularity assumption we made on f allows the function (44) to be differentiable at the origin. Let $(\theta_0, \theta_1, \ldots, \theta_k) \in (W^{1,\infty})^{k+1}$ be such that

$\|\theta_0\|_{C^{0,1}} < 1$. First, we express the k-th-order differential in a simpler form, using the change of variables formula valid for Lipschitz continuous maps [17, Section 3.3.3]:

$$\begin{aligned} D^k_{\theta_0} F_\Omega(\theta_1,\dots,\theta_k) \quad := & \quad \sum_{i_1,\dots,i_k=1}^{n} \sum_{l=0}^{k} \sum_{\substack{I_l \subseteq [\![1,k]\!] \\ \text{card } I_l = l}} \sum_{p\in\mathcal{S}_{I_l}} s(p) \int_{(I+\theta_0)(\Omega)} \frac{\partial^{k-l} f}{\prod\limits_{\substack{j\in[\![1,k]\!] \\ j\notin I_l}} \partial \mathbf{x}_{i_j}} \\ & \prod_{\substack{j\in[\![1,k]\!] \\ j\notin I_l}} \left[\theta_j \circ (I+\theta_0)^{-1}\right]_{i_j} \prod_{j\in I_l} D_\bullet \left[\theta_j \circ (I+\theta_0)^{-1}\right]_{i_j i_{p(j)}} \\ = & \quad \sum_{i_1,\dots,i_k=1}^{n} \sum_{l=0}^{k} \sum_{\substack{I_l \subseteq [\![1,k]\!] \\ \text{card} I_l = l}} \sum_{p\in\mathcal{S}_{I_l}} s(p) \int_{\Omega} \frac{\partial^{k-l} f}{\prod\limits_{\substack{j\in[\![1,k]\!] \\ j\notin I_l}} \partial \mathbf{x}_{i_j}} \circ (I+\theta_0) \prod_{\substack{j\in[\![1,k]\!] \\ j\notin I_l}} [\theta_j]_{i_j} \\ & \prod_{j\in I_l} D_{(I+\theta_0)(\bullet)} \left[\theta_j \circ (I+\theta_0)^{-1}\right]_{i_j i_{p(j)}} |\det[D_\bullet(I+\theta_0)]|. \end{aligned}$$

For any $\theta \in W^{1,\infty}$, we define $Def(\theta)$ as the set of points in $\mathbb{R}^n$ at which θ is differentiable. Note that from Rademacher's Theorem [17, Section 3.1.2], $\mathbb{R}^n \backslash \mathrm{Def}(\theta)$ has a zero n-dimensional Lebesgue measure. We can now introduce the set $A := Def(\theta) \cap Def(\theta_0) \cap (I+\theta_0)^{-1}[Def(\theta \circ (I+\theta_0)^{-1})]$. From Lemma 4.2, we get for almost every point $\mathbf{x} \in \mathbb{R}^n$ (more precisely for any $\mathbf{x} \in A$ since $\mathbb{R}^n \backslash A$ has a zero n-dimensional Lebesgue measure):

$$D_{\mathbf{x}}\theta\,(I + D_{\mathbf{x}}\theta_0)^{-1} = D_{(I+\theta_0)(\mathbf{x})} \left[\theta \circ (I+\theta_0)^{-1}\right].$$

Furthermore, we get from Proposition 4.4 that $\det[D_\bullet(I+\theta)] \to 1$ for the L^∞-norm as $\|\theta\|_{W^{1,\infty}} \to 0$. Hence, there exists $\delta \in]0,1[$ such that for any $\|\theta_0\|_{W^{1,\infty}} < \delta$, the Jacobian determinant of $(I+\theta_0)$ is positive. Combining these two observations, we obtain from the foregoing that for any $\theta_0 \in W^{1,\infty}$ such that $\|\theta_0\|_{W^{1,\infty}} < \delta$:

$$\begin{aligned} D^k_{\theta_0} F_\Omega(\theta_1,\dots,\theta_k) \quad = & \quad \sum_{i_1,\dots,i_k=1}^{n} \sum_{l=0}^{k} \sum_{\substack{I_l \subseteq [\![1,k]\!] \\ \text{card } I_l = l}} \sum_{p\in\mathcal{S}_{I_l}} s(p) \int_{\Omega} \frac{\partial^{k-l} f}{\prod\limits_{\substack{j\in[\![1,k]\!] \\ j\notin I_l}} \partial \mathbf{x}_{i_j}} \circ (I+\theta_0) \prod_{\substack{j\in[\![1,k]\!] \\ j\notin I_l}} [\theta_j]_{i_j} \\ & \prod_{j\in I_l} \left[D_\bullet\theta_j\,(I + D_\bullet\theta_0)^{-1}\right]_{i_j i_{p(j)}} \det\left[D_\bullet(I+\theta_0)\right]. \end{aligned} \tag{45}$$

Then, we introduce the continuous $(k+1)$-linear form (43), which is symmetric i.e. for any $p \in \mathsf{S}_{k+1}$ and any $(\theta_1,\dots,\theta_{k+1}) \in (W^{1,\infty})^{k+1}$, we have $D^{k+1}_{\mathbf{0}} F_\Omega(\theta_{p(1)},\dots,\theta_{p(k+1)}) = D^{k+1}_{\mathbf{0}} F_\Omega(\theta_1,\dots,\theta_{k+1})$. We now prove that this good candidate is the $(k+1)$-th order differential of F_Ω at the origin. For this purpose, we express it differently. We emphasize the fact that we have not (yet) proved that (43) is the $(k+1)$-th order differential of F_Ω but we use its notation for convenience. We set $\theta_{k+1} := \theta_0$ to keep this in mind. We thus have:

$$\begin{aligned} & D^{k+1}_{\mathbf{0}} F_\Omega\left(\theta_1,\dots,\theta_k,\theta_0\right) := \\ & \sum_{i_1,\dots,i_k,i_{k+1}=1}^{n} \sum_{l=0}^{k+1} \sum_{\substack{I_l \subseteq [\![1,k+1]\!] \\ \text{card } I_l = l}} \sum_{p\in\mathcal{S}_{I_l}} s(p) \int_{\Omega} \frac{\partial^{k+1-l} f}{\prod\limits_{\substack{j\in[\![1,k+1]\!] \\ j\notin I_l}} \partial \mathbf{x}_{i_j}} \prod_{\substack{j\in[\![1,k+1]\!] \\ j\notin I_l}} [\theta_j]_{i_j} \prod_{j\in I_l} [D_\bullet\theta_j]_{i_j i_{p(j)}}. \end{aligned}$$

We split the above expression into two disjoint situations, the last one being itself splitted into two subcases. In the first situation, we assume $k+1 \notin I_l$. In this particular case, the sum on l can stop at k since we are assuming that I_l has at most k elements. Moreover, we can explicit the indice i_{k+1} and the subset I_l is included in $[\![1,k]\!]$. In the second situation, we assume $k+1 \in I_l$. Similarly, the sum on l can start from one since we are assuming that I_l is not empty. Then, two subcases follow. On the one hand, we assume $p(k+1) = k+1$. In this case, this is equivalent to search only for subsets $I_{l-1} \subseteq [\![1,k]\!]$ of $l-1$ pairwise distinct elements, and also bijective maps $q : I_{l-1} \to I_{l-1}$, then set $I_l := I_{l-1} \cup \{k+1\}$ and $p := q$ on I_{l-1} with $p(k+1) := k+1$. On the other hand, we assume $p(k+1) \neq k+1$ so we can make a partition on the bijections $p : I_l \to I_l$ by fixing the element $k+1$. We thus have:

$$D_{\mathbf{0}}^{k+1}F_\Omega(\theta_1,\ldots,\theta_k,\theta_0) = \sum_{i_1,\ldots,i_k=1}^{n}\sum_{l=0}^{k}\sum_{\substack{I_l\subseteq[\![1,k]\!]\\ \mathrm{card}\ I_l=l}}\sum_{p\in\mathcal{S}_{I_l}} s(p)\int_\Omega \sum_{i_{k+1}=1}^{n}\frac{\partial}{\partial \mathbf{x}_{i_{k+1}}}\left(\frac{\partial^{k-l}f}{\prod\limits_{\substack{j\in[\![1,k]\!]\\ j\notin I_l}}\partial\mathbf{x}_{i_j}}\right)$$
$$[\theta_0]_{i_{k+1}}\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_l}}[\theta_j]_{i_j}\prod_{j\in I_l}[D_\bullet\theta_j]_{i_j i_{p(j)}}$$

$$+\sum_{i_1,\ldots,i_k=1}^{n}\sum_{l=1}^{k+1}\sum_{\substack{I_{l-1}\subseteq[\![1,k]\!]\\ \mathrm{card}\ I_{l-1}=l-1\\ I_l:=I_{l-1}\cup\{k+1\}}}\sum_{\substack{q\in\mathcal{S}_{I_{l-1}}\\ p:=q\ \mathrm{on}\ I_{l-1}\\ p(k+1):=k+1}} s(p)\int_\Omega\frac{\partial^{k-(l-1)}f}{\prod\limits_{\substack{j\in[\![1,k]\!]\\ j\notin I_{l-1}}}\partial\mathbf{x}_{i_j}}\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_{l-1}}}[\theta_j]_{i_j}\prod_{j\in I_{l-1}}[D_\bullet\theta_j]_{i_j i_{q(j)}}$$
$$\sum_{i_{k+1}=1}^{n}[D_\bullet\theta_0]_{i_{k+1}i_{k+1}}$$

$$+\sum_{i_1,\ldots,i_k=1}^{n}\sum_{l=1}^{k+1}\sum_{\substack{I_{l-1}\subseteq[\![1,k]\!]\\ \mathrm{card}\ I_{l-1}=l-1\\ I_l:=I_{l-1}\cup\{k+1\}}}\sum_{j_0\in I_{l-1}}\sum_{\substack{p\in\mathcal{S}_{I_l}\\ p(k+1)\neq k+1\\ p(j_0)=k+1}} s(p)\int_\Omega\frac{\partial^{k-(l-1)}f}{\prod\limits_{\substack{j\in[\![1,k]\!]\\ j\notin I_{l-1}}}\partial\mathbf{x}_{i_j}}\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_{l-1}}}[\theta_j]_{i_j}\prod_{\substack{j\in I_{l-1}\\ j\neq j_0}}[D_\bullet\theta_j]_{i_j i_{p(j)}}$$
$$\sum_{i_{k+1}=1}^{n}[D_\bullet\theta_{j_0}]_{i_{j_0}i_{k+1}}[D_\bullet\theta_0]_{i_{k+1}i_{p(k+1)}}.$$

In the second integral above, $p(k+1)=k+1$ so the number of transpositions needed to decompose $p_{I_l}^{-1}\circ p\circ p_{I_l}$ is the same than for $p_{I_{l-1}}^{-1}\circ q\circ p_{I_{l-1}}$, from which we deduce that $s(p)=s(q)$. Moreover, in the last integral above, we make a change of indices $r:=p\circ t$, where t is only exchanging $k+1$ and j_0. Since the signature is a morphism of group, we have $s(r)=s(p\circ t)=s(p)s(t)=-s(p)$. Indeed, t permutes two indices of I_l thus $p_{I_l}^{-1}\circ t\circ p_{I_l}\in\mathcal{S}_l$ is a transposition, whose signature is -1. We are then back to a summation on r for which $r(k+1)=k+1$ i.e. in the previous situation of the second integral above. We can thus do the same foregoing procedure. We obtain:

$$D_{\mathbf{0}}^{k+1}F_\Omega(\theta_1,\ldots,\theta_k,\theta_0) = \sum_{i_1,\ldots,i_k=1}^{n}\sum_{l=0}^{k}\sum_{\substack{I_l\subseteq[\![1,k]\!]\\ \mathrm{card}\ I_l=l}}\sum_{p\in\mathcal{S}_{I_l}} s(p)\int_\Omega\left\langle\nabla\frac{\partial^{k-l}f}{\prod\limits_{\substack{j\in[\![1,k]\!]\\ j\notin I_l}}\partial\mathbf{x}_{i_j}}\mid\theta_0\right\rangle$$
$$\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_l}}[\theta_j]_{i_j}\prod_{j\in I_l}[D_\bullet\theta_j]_{i_j i_{p(j)}}$$

$$+\sum_{i_1,\ldots,i_k=1}^{n}\sum_{l=1}^{k+1}\sum_{\substack{I_{l-1}\subseteq[\![1,k]\!]\\ \mathrm{card}\ I_{l-1}=l-1\\ I_l:=I_{l-1}\cup\{k+1\}}}\sum_{\substack{q\in\mathcal{S}_{I_{l-1}}\\ p:=q\ \mathrm{on}\ I_{l-1}\\ p(k+1):=k+1}} s(q)\int_\Omega\frac{\partial^{k-(l-1)}f}{\prod\limits_{\substack{j\in[\![1,k]\!]\\ j\notin I_{l-1}}}\partial\mathbf{x}_{i_j}}\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_{l-1}}}[\theta_j]_{i_j}$$
$$\prod_{j\in I_{l-1}}[D_\bullet\theta_j]_{i_j i_{q(j)}}\,\mathrm{div}(\theta_0)$$

$$+\sum_{i_1,\ldots,i_k=1}^{n}\sum_{l=1}^{k+1}\sum_{\substack{I_{l-1}\subseteq[\![1,k]\!]\\ \mathrm{card}\ I_{l-1}=l-1\\ I_l:=I_{l-1}\cup\{k+1\}}}\sum_{j_0\in I_{l-1}}\sum_{\substack{q\in\mathcal{S}_{I_{l-1}}\\ r:=q\ \mathrm{on}\ I_{l-1}\\ r(k+1)=k+1}} s(q)\int_\Omega\frac{\partial^{k-(l-1)}f}{\prod\limits_{\substack{j\in[\![1,k]\!]\\ j\notin I_{l-1}}}\partial\mathbf{x}_{i_j}}\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_{l-1}}}[\theta_j]_{i_j}$$
$$[-D_\bullet\theta_{j_0}D_\bullet\theta_0]_{i_{j_0}i_{q(j_0)}}\prod_{\substack{j\in I_{l-1}\\ j\neq j_0}}[D_\bullet\theta_j]_{i_j i_{q(j)}}.$$

Note that in the last product, we have replaced $i_{r[t(j)]}$ by $i_{q(j)}$ since they coincide on $I_{l-1}\backslash\{j_0\}$. Finally, we can notice that in the two last integrals, we have expressed everything in terms of I_{l-1} and q and so we can drop the notation I_l, p, and r. Re-indexing the summation on l in the two last integrals by $m = l-1$, we get from all these observations:

$$D_{\mathbf{0}}^{k+1}F_\Omega(\theta_1,\dots,\theta_k,\theta_0) = \sum_{i_1,\dots,i_k=1}^{n}\sum_{m=0}^{k}\sum_{\substack{I_m\subseteq[\![1,k]\!]\\ \mathrm{card}\ I_m=m}}\sum_{q\in\mathcal{S}_{I_m}} s(q)\int_\Omega \prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_m}}[\theta_j]_{i_j}\Bigg[\left\langle \nabla\frac{\partial^{k-m}f}{\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_m}}\partial\mathbf{x}_{i_j}} \mid \theta_0\right\rangle \prod_{j\in I_m}[D_\bullet\theta_j]_{i_j i_{q(j)}} + \frac{\partial^{k-m}f}{\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_m}}\partial\mathbf{x}_{i_j}}\prod_{j\in I_m}[D_\bullet\theta_j]_{i_j i_{q(j)}}\,\mathrm{div}\,(\theta_0)$$
$$+\sum_{j_0\in I_m}\frac{\partial^{k-m}f}{\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_m}}\partial\mathbf{x}_{i_j}}\prod_{\substack{j\in I_m\\ j\neq j_0}}[D_\bullet\theta_j]_{i_j i_{q(j)}}\left[-D_\bullet\theta_{j_0}D_\bullet\theta_0\right]_{i_{j_0} i_{q(j_0)}}\Bigg]. \tag{46}$$

We now introduce some more notation in order to handle the quantities (43)–(46) we want to estimate. For this purpose, we set:

$$a_0 := \frac{\partial^{k-m}f}{\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_m}}\partial\mathbf{x}_{i_j}}\circ(I+\theta_0),\qquad b_0 := \frac{\partial^{k-m}f}{\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_m}}\partial\mathbf{x}_{i_j}},\qquad c_0 := \left\langle\nabla\frac{\partial^{k-m}f}{\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_m}}\partial\mathbf{x}_{i_j}}\mid\theta_0\right\rangle,$$

and for any $j\in[\![1,m]\!]$:

$$\begin{cases} a_j := \left[D_\bullet\theta_{p_{I_m}(j)}(I+D_\bullet\theta_0)^{-1}\right]_{i_{p_{I_m}(j)}i_{q[p_{I_m}(j)]}}\\ b_j := [D_\bullet\theta_{p_{I_m}(j)}]_{i_{p_{I_m}(j)}i_{q[p_{I_m}(j)]}}\\ c_j := -[D_\bullet\theta_{p_{I_m}(j)}D_\bullet\theta_0]_{i_{p_{I_m}(j)}i_{q[p_{I_m}(j)]}}.\end{cases}$$

We also set $a_{m+1} := \det[D_\bullet(I+\theta_0)]$, $b_{m+1} := 1$, and $c_{m+1} := \mathrm{div}(\theta_0)$. Then, we introduce the following map:

$$R_k(\theta_0,\dots,\theta_k) := D_{\theta_0}^k F_\Omega(\theta_1,\dots,\theta_k) - D_{\mathbf{0}}^k F_\Omega(\theta_1,\dots,\theta_k) - D_{\mathbf{0}}^{k+1}F_\Omega(\theta_1,\dots,\theta_k,\theta_0).$$

Considering the expressions (43) and the ones (45)–(46) we have established, in each product/sum concerning $j\in I_m$, we make a change of indices $u := p_{I_m}^{-1}(j)$ so as to order the product/sum from $u=1$ to $u=m$. We obtain with our notation:

$$R_k(\theta_0,\dots,\theta_k) = \sum_{i_1,\dots,i_k=1}^{n}\sum_{m=0}^{k}\sum_{\substack{I_m\subseteq[\![1,k]\!]\\ \mathrm{card}\ I_m=m}}\sum_{q\in\mathcal{S}_{I_m}} s(q)\int_\Omega\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_m}}[\theta_j]_{i_j}\left[\prod_{u=0}^{m+1}a_u - \prod_{u=0}^{m+1}b_u - \sum_{u_0=0}^{m+1}c_{u_0}\prod_{\substack{u\in[\![0,m+1]\!]\\ u\neq u_0}}b_u\right].$$

$$= \sum_{i_1,\dots,i_k=1}^{n}\sum_{m=0}^{k}\sum_{\substack{I_m\subseteq[\![1,k]\!]\\ \mathrm{card}\ I_m=m}}\sum_{q\in\mathcal{S}_{I_m}} s(q)\int_\Omega\prod_{\substack{j\in[\![1,k]\!]\\ j\notin I_m}}[\theta_j]_{i_j}$$
$$\sum_{u_0=0}^{m+1}\left(\prod_{u=0}^{u_0-1}b_u\right)\left[(a_{u_0}-b_{u_0}-c_{u_0})\prod_{u=u_0+1}^{m+1}a_u + c_{u_0}\sum_{l=u_0+1}^{m+1}\left(\prod_{u=u_0+1}^{l-1}a_u\right)(a_l-b_l)\left(\prod_{u=l+1}^{m+1}b_u\right)\right].$$

Therefore, we can now estimate each term in the last equality in order to obtain the required relation $|R_k(\theta_0,\dots,\theta_k)|\leqslant R(n,f,k,\theta_0)\prod_{j=0}^{k}\|\theta_j\|_{W^{1,\infty}}$ with $|R(n,f,k,\theta_0)|\to 0$ as $\|\theta_0\|_{W^{1,\infty}}\to 0$. Let us detail this procedure. First, we can apply Proposition 4.6 to the maps $\partial^{k-m}f\in W^{1,1}$, $m\in[\![0,k]\!]$, then use the Cauchy-Schwarz inequality with (61), and combine the relations (62)–(63) with the fact that $\|\theta_0\|_{W^{1,\infty}}<\delta<1$. We deduce that:

$$\left\|(a_0-b_0-c_0)\left(\prod_{u=1}^{m}a_u\right)a_{m+1}\right\|_{L^1}\leqslant(n-1)!\left(\frac{n}{1-\delta}\right)^{m+1}\|\theta_0\|_{W^{1,\infty}}R(\theta_0)\prod_{j\in I_m}\|\theta_j\|_{C^{0,1}},$$

where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{W^{1,\infty}} \to 0$. Hence, we have estimated the first term of the first sum. We can proceed similarly for the other ones. Using the L^1-norm for the maps $\partial^{k-m} f \in W^{1,1}$, $m \in [\![0,k]\!]$, and the L^∞-norm for the remaining terms, we get from the Cauchy-Schwarz inequality with (61), relations (62)–(63) with $\|\theta_0\|_{W^{1,\infty}} < \delta < 1$, and Proposition 4.3:

$$\left\| \sum_{u_0=1}^{m} b_0 \left(\prod_{u=1}^{u_0-1} b_u \right) (a_{u_0} - b_{u_0} - c_{u_0}) \left(\prod_{u=u_0+1}^{m} a_u \right) a_{m+1} \right\|_{L^1} \leqslant m\sqrt{n}(n-1)! \left(\frac{n}{1-\delta} \right)^m \|f\|_{W^{k,1}} \|\theta_0\|_{C^{0,1}} R(\theta_0) \prod_{j \in I_m} \|\theta_j\|_{C^{0,1}},$$

where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{C^{0,1}} \to 0$. The same arguments and Proposition 4.4 also yield to:

$$\left\| b_0 \left(\prod_{u=1}^{m} b_u \right) (a_{m+1} - b_{m+1} - c_{m+1}) \right\|_{L^1} \leqslant \|f\|_{W^{k,1}} \|\theta_0\|_{C^{0,1}} R(\theta_0) \prod_{j \in I_m} \|\theta_j\|_{C^{0,1}},$$

where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{C^{0,1}} \to 0$. We next observe that $m \leqslant k$ and δ only depends on n (in fact one can prove that $\delta = \frac{1}{1+n!}$), where we recall that $\delta \in]0,1[$ is such that the Jacobian determinant of $(I+\theta)$ is positive for any $\|\theta\|_{W^{1,\infty}} < \delta$. Gathering the three last estimations and these observations, we thus have obtained:

$$\left\| \sum_{u_0=0}^{m+1} \left(\prod_{u=0}^{u_0-1} b_u \right) (a_{u_0} - b_{u_0} - c_{u_0}) \left(\prod_{u=u_0+1}^{m+1} a_u \right) \right\|_{L^1} \leqslant C(n,k,f) \|\theta_0\|_{W^{1,\infty}} R(\theta_0) \prod_{j \in I_m} \|\theta_j\|_{W^{1,\infty}}, \tag{47}$$

where $C(n,k,f) > 0$ is a fixed constant depending only on n, k, and $\|f\|_{W^{k,1}}$, and where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{W^{1,\infty}} \to 0$. We continue our estimations. Arguing as in (70) with θ_0 and $\partial^{k-m} f \in W^{1,1}$, $m \in [\![0,k]\!]$, we use the Cauchy-Schwarz inequality with (61), relation (62) with $\|\theta_0\|_{W^{1,\infty}} < \delta < 1$, and Proposition 4.3 in order to get:

$$\left\| c_0 \sum_{l=1}^{m} \left(\prod_{u=1}^{l-1} a_u \right) (a_l - b_l) \left(\prod_{u=l+1}^{m} b_u \right) b_{m+1} \right\|_{L^1} \leqslant m\sqrt{n} \left(\frac{n}{1-\delta} \right)^{m-1} \|f\|_{W^{k+1,1}} \|\theta_0\|_{L^\infty} R(\theta_0) \prod_{j \in I_m} \|\theta_j\|_{C^{0,1}},$$

where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{C^{0,1}} \to 0$. The same arguments combined with Proposition 4.4 give:

$$\left\| c_0 \left(\prod_{u=1}^{m} a_u \right) (a_{m+1} - b_{m+1}) \right\|_{L^1} \leqslant \left(\frac{n}{1-\delta} \right)^m \|f\|_{W^{k+1,1}} \|\theta_0\|_{L^\infty} R(\theta_0) \prod_{j \in I_m} \|\theta_j\|_{C^{0,1}},$$

where $|R(\theta_0)| \to 0$ as $\|\theta\|_{C^{0,1}} \to 0$. Similarly, we get from Proposition 4.3:

$$\left\| \sum_{u_0=1}^{m} b_0 \left(\prod_{u=1}^{u_0-1} b_u \right) c_{u_0} \sum_{l=u_0+1}^{m} \left(\prod_{u=u_0+1}^{l-1} a_u \right) (a_l - b_l) \left(\prod_{u=l+1}^{m} b_u \right) b_{m+1} \right\|_{L^1} \leqslant n\sqrt{n} \left(\frac{n}{1-\delta} \right)^{m-2} m(m-1) \|f\|_{W^{k,1}} \|\theta_0\|_{C^{0,1}} R(\theta_0) \prod_{j \in I_m} \|\theta_j\|_{C^{0,1}},$$

where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{C^{0,1}} \to 0$, and also from Proposition 4.4:

$$\left\| \sum_{u_0=1}^{m} b_0 \left(\prod_{u=1}^{u_0-1} b_u \right) c_{u_0} \left(\prod_{u=u_0+1}^{m} a_u \right) (a_{m+1} - b_{m+1}) \right\|_{L^1} \leqslant nm \left(\frac{n}{1-\delta} \right)^{m-1} \|f\|_{W^{k,1}} \|\theta_0\|_{C^{0,1}} R(\theta_0) \prod_{j \in I_m} \|\theta_j\|_{C^{0,1}},$$

where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{C^{0,1}} \to 0$. Gathering the four last estimations and observing again that $m \leqslant k$ and $\delta < 1$ only depends on n, we obtain:

$$\left\| \sum_{u_0=0}^{m+1} \left(\prod_{u=0}^{u_0-1} b_u \right) c_{u_0} \sum_{l=u_0+1}^{m+1} \left(\prod_{u=u_0+1}^{l-1} a_u \right) (a_l - b_l) \left(\prod_{u=l+1}^{m+1} b_u \right) \right\|_{L^1} \leqslant C(n,k,\|f\|_{W^{k+1,1}}) \|\theta_0\|_{W^{1,\infty}} R(\theta_0) \prod_{j \in I_m} \|\theta_j\|_{W^{1,\infty}}, \tag{48}$$

where $C(n,k,\|f\|_{W^{k+1,1}})>0$ is a fixed constant depending only on n, k, and $\|f\|_{W^{k+1,1}}$, and where $|R(\theta_0)|\to 0$ as $\|\theta\|_{C^{0,1}}\to 0$. Finally, we use (47)–(48) to estimate the last expression obtained for $R_k(\theta_0,\theta_1,\ldots,\theta_k)$. We deduce that:

$$\begin{aligned}
|||R_k(\theta_0,\bullet,\ldots,\bullet)||| &:= \sup_{\substack{(\theta_1,\ldots,\theta_k)\in(W^{1,\infty})^k\\ \theta_1,\ldots,\theta_k\neq\mathbf{0}}} \frac{|R_k\left(\theta_0,\theta_1,\ldots,\theta_k\right)|}{\|\theta_1\|_{W^{1,\infty}}\ldots\|\theta_k\|_{W^{1,\infty}}}\\
&\leqslant \widetilde{C}\left(n,k,\|f\|_{W^{k+1,1}}\right)\|\theta_0\|_{W^{1,\infty}}\sum_{i_1,\ldots,i_k=1}^{k}\sum_{m=0}^{k}\sum_{\substack{I_m\subseteq[\![1,k]\!]\\ \mathrm{card}I_m=m}}\sum_{q\in\mathcal{S}_{I_m}}|R(\theta_0)|.
\end{aligned}$$

We emphasize the fact that even if the notation omitted it, the $R(\theta_0)$ in (47)–(48) depends on n, k, and f, but also on $i_1,\ldots,i_k$, m, I_m, and q. Since all the sums are finite, we can take the maximum of these $R(\theta_0)$ for example, and we end up with $|||R_k(\theta_0,\bullet,\ldots,\bullet)|||\leqslant\|\theta_0\|_{W^{1,\infty}}R(n,k,f,\theta_0)$, where $|R(n,k,f,\theta_0)|\to 0$ as $\|\theta_0\|_{W^{1,\infty}}\to 0$ with $R(n,k,f,\theta)$ depending only on n, k, f and θ_0. We have thus established that the map (44) is differentiable at the origin i.e. $F_\Omega:\theta\in W^{1,\infty}\to F[(I+\theta)(\Omega)]$ is $k+1$ times differentiable at the origin for any measurable subset Ω of $\mathbb{R}^n$.

We now show that F_Ω is $k+1$ times differentiable at any point of $\mathbb{B}^{0,1}\cap W^{1,\infty}$. Let $\theta_0\in W^{1,\infty}$ be such that $\|\theta_0\|_{C^{0,1}}<1$. From Proposition 4.1, the map $I+\theta_0$ has a Lipschitz continuous inverse. In particular, we deduce that $\Omega_0:=(I+\theta_0)(\Omega)$ is measurable. Consequently, from the foregoing, the function $F_{\Omega_0}:\theta\in W^{1,\infty}\mapsto F[(I+\theta)(\Omega_0)]$ is $k+1$ times differentiable at the origin. Let $\varepsilon>0$ and we set $\epsilon:=\varepsilon(1-\|\theta_0\|_{C^{0,1}})^{k+1}>0$. There exists $\delta\in]0,1[$ such that for any $\theta\in W^{1,\infty}$ such that $\|\theta\|_{W^{1,\infty}}<\delta$, we have:

$$|||D^k_\theta F_{\Omega_0}-D^k_{\mathbf{0}}F_{\Omega_0}-D^{k+1}_{\mathbf{0}}F_{\Omega_0}(\bullet,\ldots,\bullet,\theta)|||\leqslant\epsilon\|\theta\|_{W^{1,\infty}}.$$

Proceeding as in (41), we observe that for any $h\in W^{1,\infty}$ such that $\|h\|_{W^{1,\infty}}<\delta(1-\|\theta_0\|_{C^{0,1}})$, we have $\|\theta_0+h\|_{C^{0,1}}<1$ so we can write for any $(\theta_1,\ldots,\theta_k)\in W^{1,\infty}\times\ldots\times W^{1,\infty}$:

$$\begin{aligned}
&\left[D^k_{\theta_0+h}F_\Omega-D^k_{\theta_0}F_\Omega\right](\theta_1,\ldots,\theta_k)\\
&\qquad\qquad -D^{k+1}_{\mathbf{0}}F_{\Omega_0}\left[\theta_1\circ(I+\theta_0)^{-1},\ldots,\theta_k\circ(I+\theta_0)^{-1},h\circ(I+\theta_0)^{-1}\right]\\
&= \left[D^k_\theta F_{\Omega_0}-D^k_{\mathbf{0}}F_{\Omega_0}\right]\left[\theta_1\circ(I+\theta_0)^{-1},\ldots,\theta_k\circ(I+\theta_0)^{-1}\right]\\
&\qquad\qquad -D^{k+1}_{\mathbf{0}}F_{\Omega_0}\left[\theta_1\circ(I+\theta_0)^{-1},\ldots,\theta_k\circ(I+\theta_0)^{-1},\theta\right],
\end{aligned}$$

where we have set $\theta:=h\circ(I+\theta_0)^{-1}$. As in (42), we have $\|\theta\|_{W^{1,\infty}}\leqslant\frac{\|h\|_{W^{1,\infty}}}{1-\|\theta_0\|_{C^{0,1}}}<\delta$ so we get:

$$\begin{aligned}
&|[D^k_{\theta_0+h}F_\Omega-D^k_{\theta_0}F_\Omega](\theta_1,\ldots,\theta_k)-D^{k+1}_{\mathbf{0}}F_{\Omega_0}[\theta_1\circ(I+\theta_0)^{-1},\ldots,\theta_k\circ(I+\theta_0)^{-1},h\circ(I+\theta_0)^{-1}]|\\
&\qquad\leqslant |||D^k_\theta F_{\Omega_0}-D^k_{\mathbf{0}}F_{\Omega_0}-D^{k+1}_{\mathbf{0}}F_{\Omega_0}(\bullet,\ldots,\bullet,\theta)|||\prod_{l=1}^{k}\|\theta_l\circ(I+\theta_0)^{-1}\|_{W^{1,\infty}}\\
&\leqslant \epsilon\|h\circ(I+\theta_0)^{-1}\|_{W^{1,\infty}}\prod_{l=1}^{k}\frac{\|\theta_l\|_{W^{1,\infty}}}{1-\|\theta_0\|_{C^{0,1}}}\leqslant\underbrace{\frac{\epsilon}{(1-\|\theta_0\|_{C^{0,1}})^{k+1}}}_{=\varepsilon}\|h\|_{W^{1,\infty}}\prod_{l=1}^{k}\|\theta_l\|_{W^{1,\infty}}.
\end{aligned}$$

Consequently, we obtain for any $h\in W^{1,\infty}$ such that $\|h\|_{W^{1,\infty}}<\delta(1-\|\theta\|_{C^{0,1}})$:

$$|||D^k_{\theta_0+h}F_\Omega-D^k_{\theta_0}F_\Omega-D^{k+1}_{\mathbf{0}}F_{\Omega_0}[(\bullet)\circ(I+\theta_0)^{-1},\ldots,(\bullet)\circ(I+\theta_0)^{-1},h\circ(I+\theta_0)^{-1}]|||\leqslant\varepsilon\|h\|_{W^{1,\infty}}.$$

Since $(\theta_1,\ldots,\theta_k,h)\in(W^{1,\infty})^{k+1}\mapsto D^{k+1}_{\mathbf{0}}F_{\Omega_0}[\theta_1\circ(I+\theta_0)^{-1},\ldots,\theta_k\circ(I+\theta_0)^{-1},h\circ(I+\theta_0)^{-1}]$ is a continuous symmetric $(k+1)$-linear form, we have proved that $F_\Omega:\theta\in W^{1,\infty}\mapsto F[(I+\theta)(\Omega)]$ is $k+1$ times differentiable at any point of $W^{1,\infty}\cap\mathbb{B}^{0,1}$ and its differential is well defined by (44) with $k+1$ instead of k.

Then, we now show that the $(k+1)$-th order differential of F_Ω is continuous at the origin. Let $\theta_0\in W^{1,\infty}$ be such that $\|\theta_0\|_{W^{1,\infty}}<\delta$, where we recall that $\delta>0$ is such that the Jacobian determinant of $I+\theta_0$ is positive. Since we have just proved that (44) holds true for $k+1$, we can rigorously use the same arguments than we used in the beginning of the proof in order to get that

(45) holds true for $k+1$ instead of k. Moreover, considering the expressions (43) and (45) with $k+1$ instead of k, in each product/sum concerning $j \in I_l$, we make a change of indices $u := p_{I_l}^{-1}(j)$ so as to be able to order the product/sum from $u=1$ to $u=l$. Using again the previous notation we introduced below (46), we thus have for any $(\theta_1, \ldots, \theta_{k+1}) \in W^{1,\infty} \times \ldots \times W^{1,\infty}$:

$$\begin{aligned}
&\left[D_{\theta_0}^{k+1} F_\Omega - D_{\mathbf{0}}^{k+1} F_\Omega\right](\theta_1, \ldots, \theta_{k+1}) \\
&\qquad = \sum_{i_1,\ldots,i_{k+1}=1}^{n} \sum_{l=0}^{k+1} \sum_{\substack{I_l \subseteq [\![1,k+1]\!] \\ \text{card } I_l = l}} \sum_{q \in \mathcal{S}_{I_l}} s(q) \int_\Omega \prod_{\substack{j \in [\![1,k+1]\!] \\ j \notin I_l}} [\theta_j]_{i_j} \left[\prod_{u=0}^{l+1} a_u - \prod_{u=0}^{l+1} b_u\right] \\
&= \sum_{i_1,\ldots,i_{k+1}=1}^{n} \sum_{l=0}^{k+1} \sum_{\substack{I_l \subseteq [\![1,k+1]\!] \\ \text{card } I_l = l}} \sum_{q \in \mathcal{S}_{I_l}} s(q) \int_\Omega \prod_{\substack{j \in [\![1,k+1]\!] \\ j \notin I_l}} [\theta_j]_{i_j} \left[\sum_{u_0=0}^{l+1} \left(\prod_{u=0}^{u_0-1} b_u\right)(a_{u_0} - b_{u_0}) \prod_{u=u_0+1}^{l+1} a_u\right],
\end{aligned}$$

where $(a_j, b_j)_{1 \leqslant j \leqslant l+1}$ are defined as before (see below (46) where m has been replaced by l), but where k is replaced by $k+1$ in the definition of (a_0, b_0). Therefore, we can now estimate as before each term in the last equality in order to get $|||D_{\theta_0}^{k+1} F_\Omega - D_{\mathbf{0}}^{k+1} F_\Omega||| \to 0$ as $\|\theta_0\|_{W^{1,\infty}} \to 0$. Let us detail this procedure. First, we can apply Proposition 4.6 to the maps $\partial^{k+1-l} f \in L^1$, $l \in [\![0, k+1]\!]$, use the Cauchy-Schwarz inequality with (61), and combine relations (62)–(63) with $\|\theta_0\|_{W^{1,\infty}} < \delta < 1$. We deduce that:

$$\left\| (a_0 - b_0) \left(\prod_{u=1}^{l} a_u\right) a_{l+1} \right\|_{L^1} \leqslant (n-1)! \left(\frac{n}{1-\delta}\right)^{l+1} R(\theta_0) \prod_{j \in I_l} \|\theta_j\|_{C^{0,1}},$$

where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{W^{1,\infty}} \to 0$. Hence, we have estimated the first term of the first sum. We proceed similarly for the other ones. Using the L^1-norm for the maps $\partial_{\bullet}^{k+1-l} f$, $l \in [\![0, k+1]\!]$, and the L^∞-norm for the remaining terms, we get from the Cauchy-Schwarz inequality with (61), relations (62)–(63) with $\|\theta_0\|_{W^{1,\infty}} < \delta < 1$, and Proposition 4.3:

$$\begin{aligned}
&\left\| \sum_{u_0=1}^{l} b_0 \left(\prod_{u=1}^{u_0-1} b_u\right)(a_{u_0} - b_{u_0}) \left(\prod_{u=u_0+1}^{l} a_u\right) a_{l+1} \right\|_{L^1} \\
&\qquad\qquad \leqslant l\sqrt{n}(n-1)! \left(\frac{n}{1-\delta}\right)^{l} \|f\|_{W^{k+1,1}} R(\theta_0) \prod_{j \in I_l} \|\theta_j\|_{C^{0,1}},
\end{aligned}$$

where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{C^{0,1}} \to 0$. The same arguments combined with Proposition 4.4 lead to:

$$\left\| b_0 \left(\prod_{u=1}^{l} b_u\right)(a_{l+1} - b_{l+1}) \right\|_{L^1} \leqslant \|f\|_{W^{k+1,1}} \left(\prod_{j \in I_l} \|\theta_j\|_{C^{0,1}}\right) R(\theta_0),$$

where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{C^{0,1}} \to 0$. Gathering the three last estimations and observing that $l \leqslant k+1$ with $\delta \in]0,1[$ only depending on n, we obtain:

$$\left\| \sum_{u_0=0}^{l+1} \left(\prod_{u=0}^{u_0-1} b_u\right)(a_{u_0} - b_{u_0}) \left(\prod_{u=u_0+1}^{l+1} a_u\right) \right\|_{L^1} \leqslant C\left(n, k, \|f\|_{W^{k+1,1}}\right) \left(\prod_{j \in I_l} \|\theta_j\|_{W^{1,\infty}}\right) R(\theta_0),$$

where $C(n, k, \|f\|_{W^{k+1,1}}) > 0$ is a fixed constant depending only on n, k, and $\|f\|_{W^{k+1,1}}$, and where $|R(\theta_0)| \to 0$ as $\|\theta_0\|_{W^{1,\infty}} \to 0$. We use this last inequality in order to estimate the last expression obtained for $D_{\theta_0}^{k+1} F_\Omega - D_{\mathbf{0}}^{k+1} F_\Omega$. We deduce that:

$$\begin{aligned}
|||D_{\theta_0}^{k+1} F_\Omega - D_{\mathbf{0}}^{k+1} F_\Omega||| &:= \sup_{\substack{(\theta_1, \ldots \theta_{k+1}) \in (W^{1,\infty})^{k+1} \\ \theta_1, \ldots, \theta_{k+1} \neq \mathbf{0}}} \frac{\left| \left[D_{\theta_0}^{k+1} F_\Omega - D_{\mathbf{0}}^{k+1} F_\Omega\right](\theta_1, \ldots, \theta_{k+1}) \right|}{\|\theta_1\|_{W^{1,\infty}} \ldots \|\theta_{k+1}\|_{W^{1,\infty}}} \\
&\leqslant C\left(n, k, \|f\|_{W^{k+1,1}}\right) \sum_{i_1,\ldots,i_{k+1}=1}^{n} \sum_{l=0}^{k+1} \sum_{\substack{I_l \subseteq [\![1,k+1]\!] \\ \text{card } I_l = l}} \sum_{q \in \mathcal{S}_{I_l}} R(\theta_0).
\end{aligned}$$

As before, even if the notation omitted it, the $R(\theta_0)$ in the previous estimations were depending on n, k, and f, but also on $i_1,\dots,i_k$, l, I_l, and q. Since all the sums are finite, we can take the maximum of these $R(\theta_0)$ and we end up with $|||D^{k+1}_{\theta_0}F_\Omega - D^{k+1}_{\mathbf{0}}F_\Omega||| \leqslant R(n,k,f,\theta_0)$, where $|R(n,k,f,\theta_0)| \to 0$ as $\|\theta_0\|_{W^{1,\infty}} \to 0$ with $R(n,k,f,\theta)$ depending only on n, k, f and θ_0. Therefore, we have established that the map $D^{k+1}_{\bullet}F_\Omega : \theta_0 \in W^{1,\infty} \mapsto D^{k+1}_{\theta_0}F_\Omega \in \mathcal{L}^{k+1}_c((W^{1,\infty})^{k+1},\mathbb{R})$ is continuous at the origin i.e. $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I+\theta)(\Omega)]$ is $k+1$ times continuously differentiable at the origin for any measurable subset Ω of $\mathbb{R}^n$.

Finally, it remains to establish that the map $D^{k+1}_{\bullet}F_\Omega$ is continuous at any point of $\mathbb{B}^{0,1}\cap W^{1,\infty}$. The arguments are the same than those used to obtain the $(k+1)$-th order differentiability at any point of $W^{1,\infty}\cap\mathbb{B}^{0,1}$ from the one at the origin. Let $\theta_0 \in W^{1,\infty}$ be such that $\|\theta_0\|_{C^{0,1}} < 1$. From Proposition 4.1, the map $I+\theta_0$ has a Lipschitz continuous inverse. In particular, we deduce that $\Omega_0 := (I+\theta_0)(\Omega)$ is measurable. From the foregoing, the map $F_{\Omega_0} : \theta \in W^{1,\infty} \mapsto F[(I+\theta)(\Omega_0)]$ is $k+1$ times continuously differentiable at the origin. Let $\varepsilon > 0$ and set $\epsilon := \varepsilon(1-\|\theta_0\|_{C^{0,1}})^{k+1} > 0$. There exists $\delta \in]0,1[$ such that for any $\theta \in W^{1,\infty}$ such that $\|\theta\|_{W^{1,\infty}} < \delta$, we have the inequality $|||D^{k+1}_{\theta}F_{\Omega_0} - D^{k+1}_{\mathbf{0}}F_{\Omega_0}||| \leqslant \epsilon$. Proceeding as in (41), we observe that for any $h \in W^{1,\infty}$ such that $\|h\|_{W^{1,\infty}} < \delta(1-\|\theta_0\|_{C^{0,1}})$, we have the estimation $\|\theta_0+h\|_{C^{0,1}} < 1$ so we can write for any $(\theta_1,\dots,\theta_{k+1}) \in W^{1,\infty}\times\dots\times W^{1,\infty}$:

$$\left[D^{k+1}_{\theta_0+h}F_\Omega - D^{k+1}_{\theta_0}F_\Omega\right](\theta_1,...,\theta_{k+1}) = \left[D^{k+1}_{\theta}F_{\Omega_0} - D^{k+1}_{\mathbf{0}}F_{\Omega_0}\right][\theta_1\circ(I+\theta_0)^{-1},...,\theta_{k+1}\circ(I+\theta_0)^{-1}],$$

where we have set $\theta := h\circ(I+\theta_0)^{-1}$. As in (42), we have $\|\theta\|_{W^{1,\infty}} \leqslant \frac{\|h\|_{W^{1,\infty}}}{1-\|\theta_0\|_{C^{0,1}}} < \delta$ so we get:

$$\begin{aligned} |[D^{k+1}_{\theta_0+h}F_\Omega - D^{k+1}_{\theta_0}F_\Omega](\theta_1,\dots,\theta_{k+1})| &\leqslant |||D^{k+1}_{\theta}F_{\Omega_0} - D^{k+1}_{\mathbf{0}}F_{\Omega_0}|||\prod_{l=1}^{k+1}\|\theta_l\circ(I+\theta_0)^{-1}\|_{W^{1,\infty}} \\ &\leqslant \frac{\epsilon}{(1-\|\theta_0\|_{C^{0,1}})^{k+1}}\prod_{l=1}^{k+1}\|\theta_l\|_{W^{1,\infty}} = \varepsilon\prod_{l=1}^{k+1}\|\theta_l\|_{W^{1,\infty}} . \end{aligned}$$

Hence, we obtain $|||D^{k+1}_{\theta_0+h}F_\Omega - D^{k+1}_{\theta_0}F_\Omega||| \leqslant \varepsilon$ for any $h \in W^{1,\infty}$ such that $\|h\|_{W^{1,\infty}} < \delta(1-\|\theta\|_{C^{0,1}})$ i.e. $D^{k+1}_{\bullet}F_\Omega$ is continuous at any point $W^{1,\infty}\cap\mathbb{B}^{0,1}$. Consequently, we have proved that the statement is true for $k=0$, and that if it is true for an integer $k \geqslant 0$, then it is true for $k+1$ provided $f \in W^{k+1,1}$. Therefore, by induction, for any integer $k_0 \geqslant 1$, if $f \in W^{k_0,1}$, then we obtain recursively that for any $k \in [\![1,k_0]\!]$, the functional (40) is k times shape differentiable at any measurable subset of $\mathbb{R}^n$, its k-th-order shape derivative being well defined by (43). Moreover, $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I+\theta_0)(\Omega)]$ is k times continuously differentiable on $W^{1,\infty}\cap\mathbb{B}^{0,1}$, its k-th-order differential map being well defined by (44), which concludes the proof of Theorem 3.2. □

3.2 The intermediate case of Lipschitz regularity

In this section, we show that further regularity on the boundary and the vector fields yields to express (43) into a divergence form. Applying the Trace Theorem [17, Section 4.3], we obtain a new relation for the shapes derivatives of a volume integral. Moreover, if we assume that one of the vector fields is normal to the boundary, then the expression can be significantly simplified.

Theorem 3.3. *Let $n \geqslant 2$, $k_0 \geqslant 1$, and $f \in W^{k_0,1}(\mathbb{R}^n,\mathbb{R})$. We consider an open bounded subset Ω of $\mathbb{R}^n$ with a Lipschitz boundary. Then, the map $F_\Omega : \theta \in W^{1,\infty}\cap C^1 \mapsto F[(I+\theta)(\Omega)]$ is k_0 times Fréchet differentiable at the origin and for any $k \in [\![1,k_0]\!]$, its differential of order k at the origin is given for any $(\theta_1,\dots,\theta_k) \in (W^{1,\infty}\cap C^1)\times\dots\times(W^{1,\infty}\cap C^1)$ by:*

$$\begin{aligned} D^k_{\mathbf{0}}F_\Omega(\theta_1,\dots,\theta_k) &= \int_{\partial\Omega}\left(\sum_{i_1,\dots,i_{k-1}=1}^{n}\frac{\partial^{k-1}f}{\prod_{j=1}^{k-1}\partial\mathbf{x}_{i_j}}\prod_{j=1}^{k-1}[\theta_j]_{i_j}\right)(\theta_k)_{\mathbf{n}}\,dA \\ &\quad+\sum_{i_1,\dots,i_{k-1}=1}^{n}\sum_{l=1}^{k-1}\sum_{\substack{I_l\subseteq[\![1,k-1]\!]\\ \mathrm{card}\ I_l=l}}\sum_{p\in\mathcal{S}_{I_l}}s(p)\int_{\partial\Omega}\frac{\partial^{k-1-l}f}{\prod_{\substack{j\in[\![1,k-1]\!]\\ j\notin I_l}}\partial\mathbf{x}_{i_j}}\prod_{\substack{j\in[\![1,k-1]\!]\\ j\notin I_l}}[\theta_j]_{i_j} \\ &\quad\left[(\theta_k)_{\mathbf{n}}\prod_{j\in I_l}[D_\bullet\theta_j]_{i_j i_{p(j)}} - \sum_{j_1\in I_l}[D_\bullet\theta_{j_1}(\theta_k)]_{i_{j_1}}[\mathbf{n}_\Omega]_{i_{p(j_1)}}\prod_{\substack{j\in I_l\\ j\neq j_1}}[D_\bullet\theta_j]_{i_j i_{p(j)}}\right]dA. \end{aligned} \tag{49}$$

Moreover, in the case where θ_k is normal to the boundary i.e. if we have $\theta_k(\mathbf{x}) = (\theta_k)_{\mathbf{n}}(\mathbf{x})\mathbf{n}_\Omega(\mathbf{x})$ for any point $\mathbf{x} \in \partial\Omega$, then relation (49) takes the following form:

$$D_{\mathbf{0}}^k F_\Omega(\theta_1, \ldots, \theta_k) =$$

$$\sum_{i_1,\ldots,i_{k-1}=1}^{n} \sum_{l=0}^{k-1} \sum_{\substack{I_l \subseteq [\![1,k-1]\!] \\ \text{card } I_l = l}} \sum_{p \in \mathcal{S}_{I_l}} s(p) \int_{\partial\Omega} \frac{\partial^{k-1-l} f}{\prod\limits_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} \partial \mathbf{x}_{i_j}} \prod_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} [\theta_j]_{i_j} \prod_{j \in I_l} [D_{\partial\Omega}\theta_j]_{i_j i_{p(j)}} (\theta_k)_{\mathbf{n}} \, dA. \tag{50}$$

Finally, the map $F_\Omega : \theta \in W^{1,\infty} \cap C^1 \mapsto F[(I+\theta)(\Omega)]$ is k_0 times continuously differentiable at any point of $W^{1,\infty} \cap C^1 \cap \mathbb{B}^{0,1}$ and for any $k \in [\![1, k_0]\!]$, its k-th-order differential is well defined by the following continuous map:

$$\begin{array}{rcl} D_{\bullet}^k F_\Omega : W^{1,\infty} \cap C^1 \cap \mathbb{B}^{0,1} & \longrightarrow & \mathcal{L}_c^k\left(\left(W^{1,\infty} \cap C^1\right)^k, \mathbb{R}\right) \\ \theta_0 & \longmapsto & (\theta_1, \ldots, \theta_k) \mapsto D_{\mathbf{0}}^k F_{(I+\theta_0)(\Omega)}[\theta_1 \circ (I+\theta_0)^{-1}, \ldots, \theta_k \circ (I+\theta_0)^{-1}] \end{array} \tag{51}$$

where $D_{\mathbf{0}}^k F_{(I+\theta_0)(\Omega)}$ is the k-th-order shape derivative of (40) at $(I+\theta_0)(\Omega)$ given by (49) in general and by (50) if θ_k is normal to the boundary.

Remark 3.4. *We emphasize here the fact that even if the right member of (49) is not symmetric with respect to the vector fields, the shape derivative (43) is a continuous symmetric k-linear form. In fact, the symmetry of a derivative is a consequence of the Fréchet differentiability. Hence, (49) is a symmetric k-linear form and (50) also holds true if any of the vector fields is normal to $\partial\Omega$.*

Proof. Let $n \geqslant 2$, $k_0 \geqslant 1$, $f \in W^{k_0,1}(\mathbb{R}^n, \mathbb{R})$, and consider an open bounded set $\Omega \subset \mathbb{R}^n$ with a Lipschitz boundary. Since $W^{1,\infty} \cap C^1$ is equipped with the $W^{1,\infty}$-norm, we can apply Theorem 3.2 to the restriction map $F_\Omega : \theta \in W^{1,\infty} \cap C^1 \mapsto F[(I+\theta)(\Omega)]$, which is thus k_0 times continuously differentiable on $W^{1,\infty} \cap C^1 \cap \mathbb{B}^{0,1}$. For any $k \in [\![1, k_0]\!]$, its k-th-order differential is well defined by (51), where $D_{\mathbf{0}}^k F_{(I+\theta_0)(\Omega)}$ is the k-th-order shape derivative of (40) at $(I+\theta_0)(\Omega)$ given by (43) for the moment. We now aim to use the additional regularity we made on the boundary and the vector fields in order to improve (43). First, we assume that $(\theta_1, \ldots, \theta_k) \in W^{2,\infty} \times \ldots \times W^{2,\infty}$. The proof consists in establishing that in this case, the right member of (43) can be expressed in the following divergence form:

$$\sum_{i_1,\ldots,i_k=1}^{n} \sum_{l=0}^{k-1} \sum_{\substack{I_l \subseteq [\![1,k-1]\!] \\ \text{card } I_l = l}} \sum_{p \in \mathcal{S}_{I_l}} s(p) \int_\Omega \frac{\partial}{\partial \mathbf{x}_{i_k}} \left[\frac{\partial^{k-1-l} f}{\prod\limits_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} \partial \mathbf{x}_{i_j}} \prod_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} [\theta_j]_{i_j} \prod_{j \in I_l} [D_{\bullet}\theta_j]_{i_j i_{p(j)}} [\theta_k]_{i_k} \right]$$

$$- \sum_{i_1,\ldots,i_k=1}^{n} \sum_{l=1}^{k-1} \sum_{\substack{I_l \subseteq [\![1,k-1]\!] \\ \text{card } I_l = l}} \sum_{j_1 \in I_l} \sum_{p \in \mathcal{S}_{I_l}} s(p) \int_\Omega \frac{\partial}{\partial \mathbf{x}_{i_{p(j_1)}}} \left[\frac{\partial^{k-1-l} f}{\prod\limits_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} \partial \mathbf{x}_{i_j}} \prod_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} [\theta_j]_{i_j} [\theta_k]_{i_k} \right.$$

$$\left. [D_{\bullet}\theta_{j_1}]_{i_{j_1} i_k} \prod_{\substack{j \in I_l \\ j \neq j_1}} [D_{\bullet}\theta_j]_{i_j i_{p(j)}} \right]. \tag{52}$$

We emphasize the fact that (52) is equal to the right member of (43) only for $W^{2,\infty}$-vector fields. Note also that if this last assertion is true, then we obtain that (49) holds true by applying the Trace Theorem [17, Section 4.3] to (52). More precisely, we obtain that (49) holds true for $W^{2,\infty}$-vector fields and we extend the result to the $W^{1,\infty} \cap C^1$-ones from standard approximating arguments. Indeed, for any $\theta \in W^{1,\infty} \cap C^1$, there exists a sequence $(\theta_k)_{k \in \mathbb{N}}$ of elements in $W^{2,\infty}$ such that θ_k and $[D_{\bullet}\theta_k]_{ij}$ respectively converges to θ and $[D_{\bullet}\theta]_{ij}$ uniformly on any compact subset of $\mathbb{R}^n$ as $k \to +\infty$ and for any $(i,j) \in [\![1,n]\!]^2$ (consider the usual mollifier [17, Section 4.2.1 Theorem 1]). Therefore, the main difficulty here is to check by direct calculations that (52) is equal to the right member of (43). Let us now detail the great lines of this (tedious) calculation. On the one hand, we expand the i_k-partial derivative in the first integral of (52), which is composed of a product of four terms. This expansion (from left to right) thus yields to the sum of four terms respectively denoted by A_1, A_2, A_3 and A_4. Similarly, the $i_{p(j_1)}$-partial derivative in the second integral of (52) is expanded and yields to the sum of five terms referred to as B_1, B_2, B_3, B_4, and B_5. Note that the terms A_2, A_3, B_2 and B_5 take a partial derivative with respect to a product (on $j \notin I_l$ or $j \in I_l$). Hence, a new sum appears for the expansion of these terms and the notation j_0 refers to it. On the other hand, the right member of (43) is divided into three situations as in the proof of Theorem 3.2 (see below (45)). We denote by C_1 the case where $k \notin I_l$, by C_2 the case where $k \in I_l$ and $p(k) = k$, and by C_3 the case where $k \in I_l$ and $p(k) \neq k$. With these notation in mind, we get from the foregoing that (49) holds true if we can prove that:

$$A_1 + A_2 + A_3 + A_4 + B_1 + B_2 + B_3 + B_4 + B_5 = C_1 + C_2 + C_3.$$

More precisely, we are going to check that $C_1 = A_1$, $C_2 = A_4$, $C_3 = B_3$, $A_2 + B_2 = -B_1$, $A_3 = -B_4$, and $B_5 = 0$. Since the term C_1 corresponds to the situation where $k \notin I_l$, the sum on l can stop at $k-1$ and the subset I_l is chosen in $[\![1, k-1]\!]$, from which we immediately get $C_1 = A_1$. Concerning the relation involving C_2, we are in the situation where $k \in I_l$ and $p(k) = k$. The sum on l can thus start at one and it is equivalent to search for $I_{l-1} \subseteq [\![1, k-1]\!]$ and $q \in \mathcal{S}_{I_{l-1}}$ by setting $I_l := I_{l-1} \cup \{k\}$ and $p := q$ on I_{l-1} with $p(k) := k$. Note also that $s(q) = s(p)$. Re-indexing the summation on l by setting $m := l - 1$, we deduce that $C_2 = A_4$. Then, C_3 corresponds to the case where $k \in I_l$ and $p(k) \neq k$ so the sum on l can start at two and we can search for $I_{l-1} \subseteq [\![1, k-1]\!]$ by setting $I_l := I_{l-1} \cup \{k\}$. We can also partition the sum on $p \in \mathcal{S}_{I_l}$ such that $p(k) \neq k$ by fixing the element k. In other words, we get a sum on $j_0 \in I_{l-1}$ followed by a sum on $p \in \mathcal{S}_{I_l}$ such that $p(j_0) = k$. We can re-index this last sum by setting $q := p \circ t$, where t only exchanges j_0 and k. We are back to a summation on $q \in \mathcal{S}_{I_l}$ with $q(k) = k$ i.e. to the situation of C_2 but in this case we have $s(q) = s(p \circ t) = s(p)s(t) = -s(p)$. Proceeding as for C_2, we deduce that $C_3 = B_3$. Then, we decompose the term B_1 into two disjoint situations. On the one hand, we impose $p(j_1) = j_1$, which is equivalent to choose $I_{l-1} \subseteq [\![1, k-1]\!]$ and $j_1 \in [\![1, k-1]\!] \backslash I_{l-1}$ then set $I_l := I_{l-1} \cup \{j_1\}$. Similarly, the sum on $p \in \mathcal{S}_{I_l}$ with $p(j_1) = j_1$ is reduced to a sum on $q \in \mathcal{S}_{I_{l-1}}$ by setting $p := q$ on I_{l-1} and $p(j_1) := j_1$. Note also that $s(p) = s(q)$. Re-indexing the summation on l by setting $m := l - 1$, we get that this expression yields to $-A_2$. On the other hand, we have $p(j_1) \neq j_1$ and we can partition this sum by fixing the element $p(j_1)$. More precisely, searching for $I_l \subseteq [\![1, k-1]\!]$ is equivalent to search for $I_{l-1} \subseteq [\![1, k-1]\!]$ and $j_0 \in [\![1, k-1]\!] \backslash I_{l-1}$ by setting $I_l := I_{l-1} \cup \{j_0\}$. Similarly, the sum on $j_1 \in I_l$ followed by the one $p \in \mathcal{S}_{I_l}$ such that $p(j_1) \neq j_1$ is replaced by a sum on $j_1 \in I_{l-1}$ followed by one on $p \in \mathcal{S}_{I_l}$ with $p(j_1) = j_0$. We can next re-arrange the summation of the permutations by setting $q := p \circ t$, where t is only exchanging j_0 and j_1. We are thus back in the previous situation where $q(j_1) = j_1$ but a negative sign now appears since $s(q) = s(p \circ t) = s(p)s(t) = -s(p)$. Proceeding as before, we get that this term is equal to $-B_2$. Hence, we have proved that $B_1 = -A_2 - B_2$. Comparing the two terms A_3 and B_4, we immediately get that $A_3 = -B_4$ by observing that the sum on l in A_3 can start at one since I_l is not empty in this case. Finally, it remains to check that $B_5 = 0$. This is the term with A_3 and B_4 which needs the $W^{2,\infty}$-regularity assumption on the vector fields. Performing a change of variables the permutations by setting $q := p \circ t$ where t exchanges the two different indices appearing in the second-order partial derivatives of f, one can notice that we obtain the same expression, up to a sign since $s(q) = s(p \circ t) = s(p)s(t) = -s(p)$. We deduce that $B_5 = -B_5$ i.e. $B_5 = 0$. Therefore, we have proved that (49) holds true. Moreover, for any $\theta_0 \in W^{1,\infty} \cap C^1 \cap \mathbb{B}^{0,1}$, the domain $(I + \theta_0)(\Omega)$ also has a Lipschitz boundary $\partial[(I + \theta_0)(\Omega)] = (I + \theta_0)(\partial\Omega)$ and $\theta \circ (I + \theta_0)^{-1} \in W^{1,\infty} \cap C^1$ for any $\theta \in W^{1,\infty} \cap C^1$. Hence, we deduce that we can use (49) instead of (43) to define $D^k_{\mathbf{0}} F_{(I+\theta_0)(\Omega)}$ in (51). It remains to study the case where θ_k is normal to the boundary. Again, the calculations are tedious so we only sketch the proof. We assume $\theta_k = (\theta_k)_{\mathbf{n}} \mathbf{n}_\Omega$ on $\partial\Omega$ and we deduce from (49):

$$\begin{aligned} D^k_{\mathbf{0}} F_\Omega(\theta_1, \ldots, \theta_k) = & \int_{\partial\Omega} \left(\sum_{i_1,\ldots,i_{k-1}=1}^{n} \frac{\partial^{k-1} f}{\prod_{j=1}^{k-1} \partial \mathbf{x}_{i_j}} \prod_{j=1}^{k-1} [\theta_j]_{i_j} \right) (\theta_k)_{\mathbf{n}} \, dA \\ & + \sum_{i_1,\ldots,i_{k-1}=1}^{n} \sum_{l=1}^{k-1} \sum_{\substack{I_l \subseteq [\![1,k-1]\!] \\ \text{card } I_l = l}} \sum_{p \in \mathcal{S}_{I_l}} s(p) \int_{\partial\Omega} \frac{\partial^{k-1-l} f}{\prod\limits_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} \partial \mathbf{x}_{i_j}} \prod_{\substack{j \in [\![1,k-1]\!] \\ j \notin I_l}} [\theta_j]_{i_j} (\theta_k)_{\mathbf{n}} \\ & \left[\prod_{j \in I_l} [D_\bullet \theta_j]_{i_j i_{p(j)}} - \sum_{j_1 \in I_l} [D_\bullet \theta_{j_1}(\mathbf{n}_\Omega)]_{i_{j_1}} [\mathbf{n}_\Omega]_{i_{p(j_1)}} \prod_{\substack{j \in I_l \\ j \neq j_1}} [D_\bullet \theta_j]_{i_j i_{p(j)}} \right] dA. \end{aligned} \qquad (53)$$

Let us now distinguish the tangential and normal part of the differential operator. Therefore, we expand the product $j \in I_l$ in (53) as follows:

$$\begin{aligned}\prod_{j\in I_l} [D_\bullet\theta_j]_{i_j i_{p(j)}} &= \prod_{j\in I_l}\left([D_{\partial\Omega}\theta_j]_{i_j i_{p(j)}} + [D_\bullet\theta_j(\mathbf{n}_\Omega)]_{i_j}[\mathbf{n}_\Omega]_{i_{p(j)}}\right)\\ &= \sum_{m=0}^{l}\sum_{\substack{J_m\subseteq I_l\\ \text{card } J_m = m}}\left(\prod_{j\in J_m}[D_\bullet\theta_j(\mathbf{n}_\Omega)]_{i_j}[\mathbf{n}_\Omega]_{i_{p(j)}}\right)\left(\prod_{j\in I_m\setminus J_m}[D_{\partial\Omega}\theta_j]_{i_j i_{p(j)}}\right).\end{aligned}$$

First, note that the first boundary integral in (53) corresponds to the case $l = 0$ in (50). Hence, we have to check that the remaining part of (50) is equal to the second integral in (53). This latter is the difference of two terms denoted by A_1 and A_2. Then, we expand the product $j \in I_m$ in A_1 as above while the same is done for A_2 in the product $j \in I_m\backslash\{j_1\}$. The idea now consists in setting $J_{m+1} := J_m \cup \{j_1\}$ in A_2. In particular, the summation on $j_1 \in I_l$ followed by the one on $J_m \subseteq I_l\backslash\{j_1\}$ is equivalent to search for $J_{m+1} \subseteq I_l$. Re-indexing the summation on m by setting $\tilde{m} = m + 1$, we deduce that A_2 is equal to A_1, apart from the case $m = 0$ which is exactly the the remaining part of (50) we were talking about. Consequently, we have established that (50) holds true, concluding the proof of Theorem 3.3. □

Corollary 3.5. *Consider the assumptions of Theorem 3.3 in the case $k_0 = k = 1$. Then,* (40) *is shape differentiable at Ω and its shape derivative is given by the following continuous linear form:*

$$\forall\theta \in W^{1,\infty}, \qquad D_{\mathbf{0}}F_\Omega(\theta) = \int_{\partial\Omega} f\theta_{\mathbf{n}}dA. \tag{54}$$

Moreover, the map $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I + \theta)(\Omega)]$ is continuously differentiable on $W^{1,\infty} \cap \mathbb{B}^{0,1}$ and its differential is given by the following continuous map:

$$\begin{array}{rccl} D_\bullet F_\Omega : & W^{1,\infty}\cap\mathbb{B}^{0,1} & \longrightarrow & \mathcal{L}_c\left(W^{1,\infty},\mathbb{R}\right)\\ & \theta_0 & \longmapsto & D_{\theta_0}F_\Omega := \theta \mapsto D_{\mathbf{0}}F_{(I+\theta_0)(\Omega)}\left[\theta\circ(I+\theta_0)^{-1}\right], \end{array} \tag{55}$$

where $D_{\mathbf{0}}F_{(I+\theta_0)(\Omega)}$ is the shape derivative of (40) *at $(I + \theta_0)(\Omega)$ given by* (54)*.*

Proof. Applying Theorem 3.2, we get that $F_\Omega : \theta \in W^{1,\infty} \mapsto F[(I + \theta)(\Omega)]$ is continuously differentiable on $W^{1,\infty} \cap \mathbb{B}^{0,1}$ and its differential is well defined by (55) but the shape derivative of (40) is given by:

$$\forall\theta \in W^{1,\infty}, \qquad D_{\mathbf{0}}F_\Omega(\theta) = \int_\Omega \operatorname{div}(f\theta).$$

Applying the Trace Theorem [17, Section 4.3], we get that (54) holds true for $(W^{1,\infty} \cap C^1)$-vector fields. We can extend the result to any $\theta \in W^{1,\infty}$ from standard approximating arguments. Indeed, for any $\theta \in W^{1,\infty}$, there exists a sequence $(\theta_i)_{i\in\mathbb{N}} \subset W^{1,\infty} \cap C^1$ converging to θ L^∞-strongly, $W^{1,\infty}$-weakly-star, and uniformly on compact sets (consider the usual mollifier [17, Section 4.2.1 Theorem 1]). Finally, for any $\theta_0 \in W^{1,\infty} \cap \mathbb{B}^{0,1}$, the domain $(I + \theta_0)(\Omega)$ has a Lipschitz boundary $\partial[(I + \theta_0)(\Omega)] = (I + \theta_0)(\partial\Omega)$ and $\theta \circ (I + \theta_0)^{-1} \in W^{1,\infty}$ for any $\theta \in W^{1,\infty}$. Hence, (54) can be used to define (55), concluding the proof of Corollary 3.5. □

3.3 The specific case of $C^{1,1}$-domains

In this section, we show that the $C^{1,1}$-regularity of the boundary is enough to ensure the notion of partial derivative with respect to the domain at any order higher than two. We emphasize here a technical issue related to the case where the perturbations are normal to the boundary. The results of Theorem 3.6 that follows could have been found by inserting the relation $\theta_j = (\theta_j)_{\mathbf{n}}\mathbf{n}_\Omega$ in (49). However, in order to do so, we have to define $D_\bullet\mathbf{n}_\Omega$ whereas $\mathbf{n}_\Omega$ is *a priori* only defined on the boundary. This can be done be considering an extension $\mathbf{N}_\Omega \in W^{1,\infty} \cap C^1$ of the normal vector but this is possible only if $\partial\Omega$ is a C^2-surface. Therefore, the great advantage of (50), apart from its simplicity, consists in expressing the shape derivatives with the tangential operator $D_{\partial\Omega}$, which an intrinsic notion. In particular, $D_{\partial\Omega}\mathbf{n}_\Omega$ can be defined via the local parametrization of the surface, for which we only need $C^{1,1}$-regularity. This technical detail can be important in the applications since the $C^{1,1}$-regularity has various geometrical characterizations (positive reach [18], uniform ball property [12], oriented distance function [16, Chapter 7]).

Theorem 3.6. *Let $n \geqslant 2$, $k_0 \geqslant 2$, and $f \in W^{k_0,1}(\mathbb{R}^n,\mathbb{R})$. We consider an open bounded set $\Omega \subset \mathbb{R}^n$ with a boundary of class $C^{1,1}$. If we assume that all the vector fields are normal to the boundary i.e. if $\theta_j = (\theta_j)_{\mathbf{n}}\mathbf{n}_\Omega$ on $\partial\Omega$ for any $j \in [\![1,k_0]\!]$, then the results of Theorem 3.3 hold true but (5)–(6) can be used instead of (50) to define $D^k_{\mathbf{0}}F_{(I+\theta_0)(\Omega)}$ in (51).*

Proof. Let $n \geqslant 2$, $k_0 \geqslant 2$, $f \in W^{k_0,1}(\mathbb{R}^n,\mathbb{R})$, and consider a $C^{1,1}$-domain $\Omega \subset \mathbb{R}^n$. First, assuming that the vector fields are normal to the boundary, we can apply Theorem 3.3: for any $k \in [\![1,k_0]\!]$, the k-th-order shape derivative of (40) is well defined by (50). Since $\mathbf{n}_\Omega$ is a Lipschitz continuous map, it is differentiable almost everywhere using Rademacher's Theorem [17, Section 3.1.2]. Consequently, we can correctly insert the expression $(\theta_j)_{\mathbf{n}}\mathbf{n}_\Omega$ in the term $D_{\partial\Omega}\theta_j$ of (50). Then, we expand the corresponding product as follows:

$$\begin{aligned}\prod_{j\in I_l}[D_{\partial\Omega}\theta_j]_{i_j i_{p(j)}} &= \prod_{j\in I_l}\Big([\mathbf{n}_\Omega]_{i_j}[\nabla_{\partial\Omega}(\theta_j)_{\mathbf{n}}]_{i_{p(j)}} + (\theta_j)_{\mathbf{n}}[D_{\partial\Omega}\mathbf{n}_\Omega]_{i_j i_{p(j)}}\Big)\\ &= \sum_{m=0}^{l}\sum_{\substack{J_m\subseteq I_l\\ \mathrm{card}\ J_m=m}}\left(\prod_{j\in J_m}[\mathbf{n}_\Omega]_{i_j}\right)\left(\prod_{j\in J_m}[\nabla_{\partial\Omega}(\theta_j)_{\mathbf{n}}]_{i_{p(j)}}\right)\left(\prod_{j\in I_m\backslash J_m}(\theta_j)_{\mathbf{n}}[D_{\partial\Omega}\mathbf{n}_\Omega]_{i_j i_{p(j)}}\right).\end{aligned}$$

Inserting the above expansion in (50), we now distinguish two cases, the last one being itself splitted into two subcases. First, we assume that there exists $j \in J_m$ such that $p(j) \in J_m$. In this case, we can consider the sum involving the indice $i_{p(j)}$ and we get that the term will involve $\sum_{i_{p(j)}=1}^n [\mathbf{n}_\Omega]_{i_{p(j)}}[\nabla_{\partial\Omega}(\theta_j)_{\mathbf{n}}]_{i_{p(j)}} = \langle \mathbf{n}_\Omega \mid \nabla_{\partial\Omega}(\theta_j)_{\mathbf{n}}\rangle = 0$ so it is equal to zero. Hence, it only remains terms such that $p(J_m) \subseteq I_l\backslash J_m$. Similarly, we can consider two disjoint subcases. If there exists $j \in I_l\backslash J_m$ such that $p(j) \in J_m$, then we get that such terms will involve a sum $\sum_{i_{p(j)}=1}^n [D_{\partial\Omega}\mathbf{n}_\Omega]_{i_j i_{p(j)}}[\mathbf{n}_\Omega]_{i_{p(j)}} = [D_{\partial\Omega}\mathbf{n}_\Omega(\mathbf{n}_\Omega)]_{i_j} = 0$, the last equality coming from the (tangential) differentiation of the relation $|\mathbf{n}_\Omega|^2 = 1$ in the local parametrization, and the fact that $D_{\partial\Omega}\mathbf{n}_\Omega$ is a self-adjoint endomorphism. Therefore, it only remains the terms for which $p(J_m) \subseteq I_l\backslash J_m$ and $p(I_l\backslash J_m) \subseteq I_l\backslash J_m$. We obtain that it remains only the case $p(I_l) = I_l\backslash J_m$ which is possible only if $J_m = \emptyset$ i.e. if $m = 0$. Finally, one can check that this term is precisely the one given in (5)–(6), concluding the proof of Theorem 3.6. □

Corollary 3.7. *Consider the assumptions of Theorem 3.6 in the case $k_0 = k = 2$. Then, the map (40) is twice shape differentiable at Ω and its second-order shape derivative is given by the following continuous bilinear form:*

$$\forall(\theta,\tilde\theta) \in \left(W^{1,\infty}\cap C^1\right)^2,\qquad D^2_{\mathbf{0}}F_\Omega(\theta,\tilde\theta) = \int_{\partial\Omega}\frac{\partial^2 F}{\partial\Omega^2}\theta_{\mathbf{n}}\tilde\theta_{\mathbf{n}}dA - \int_{\partial\Omega}\frac{\partial F}{\partial\Omega}Z[\theta,\tilde\theta]dA, \tag{56}$$

where $\frac{\partial F}{\partial\Omega}$ and $\frac{\partial^2 F}{\partial\Omega^2}$ are given in (7), and where $Z[\theta,\tilde\theta]$ is defined by (4). Moreover, the map $F_\Omega : \theta \in W^{1,\infty}\cap C^1 \mapsto F[(I+\theta)(\Omega)]$ is twice continuously differentiable on $W^{1,\infty}\cap C^1\cap\mathbb{B}^{0,1}$ and its second-order differential is given by the following continuous map:

$$\begin{array}{rccl} D^2_{\bullet}F_\Omega: & W^{1,\infty}\cap C^1\cap\mathbb{B}^{0,1} & \longrightarrow & \mathcal{L}^2_c\left(\left(W^{1,\infty}\cap C^1\right)^2,\mathbb{R}\right)\\ & \theta_0 & \longmapsto & (\theta,\tilde\theta)\mapsto D^2_{\mathbf{0}}F_{(I+\theta_0)(\Omega)}\left[\theta\circ(I+\theta_0)^{-1},\tilde\theta\circ(I+\theta_0)^{-1}\right], \end{array} \tag{57}$$

where $D^2_{\mathbf{0}}F_{(I+\theta_0)(\Omega)}$ is the second-order shape derivative of (40) at $(I+\theta_0)(\Omega)$ given by (56) .

Proof. Applying Theorem 3.3, we get that $F_\Omega : \theta \in W^{1,\infty}\cap C^1 \mapsto F[(I+\theta)(\Omega)]$ is twice continuously differentiable on $W^{1,\infty}\cap C^1\cap\mathbb{B}^{0,1}$ and its second-order differential is well defined by (57) but the second-order shape derivative of (40) is given by:

$$\forall(\theta,\tilde\theta) \in (W^{1,\infty},\cap C^1)^2,\quad D^2_{\mathbf{0}}F_\Omega(\theta,\tilde\theta) = \int_{\partial\Omega}\left[\langle\nabla f \mid \theta\rangle\tilde\theta_{\mathbf{n}} + f\left\langle \mathrm{div}\,(\theta)\,\tilde\theta - D_{\bullet}\theta(\tilde\theta) \mid \mathbf{n}_\Omega\right\rangle\right]dA.$$

We can now distinguishing the tangential and normal parts of the operators and of the vector fields, which is allowed because $\partial\Omega$ has $C^{1,1}$-regularity. Then, we can apply the Divergence Theorem for surfaces [27, Theorem 6.10], which is valid with $C^{1,1}$-regularity (adapt for example the proofs of [22, Proposition 5.4.9]). We deduce that the second-order shape derivative of (40) takes the form given in (56). Finally, for any $\theta_0 \in W^{1,\infty}\cap C^1\cap\mathbb{B}^{0,1}$, the domain $(I+\theta_0)(\Omega)$ also has a $C^{1,1}$-boundary $\partial[(I+\theta_0)(\Omega)] = (I+\theta_0)(\partial\Omega)$ and $\theta\circ(I+\theta_0)^{-1} \in W^{1,\infty}\cap C^1$ for any $\theta \in W^{1,\infty}\cap C^1$. Hence, (56) can be used to define (57), concluding the proof of Corollary 3.7. □

4 Annexes

In this section, we aim to derive all the technical material that was needed throughout the article. The results presented here are standard [16, Chapter 9] [22, Chapter 5] [40, Chapter 2] and they are organized as follows. First, we recall some terminology about differentiability in Banach spaces and we introduce the Sobolev norms in which we are interested. Then, we give some differentiability results related to the inverse, the Jacobian determinant, and the composition operator.

4.1 Some definitions and notation

Let $n \geqslant 2$ be an integer henceforth set. The space $\mathbb{R}^n$ is equipped with its usual Euclidean structure: for any $(\mathbf{x},\mathbf{y}) \in \mathbb{R}^n \times \mathbb{R}^n$, we have set $\langle \mathbf{x} \mid \mathbf{y} \rangle := \sum_{k=1}^n x_k y_k$ and $|\mathbf{x}| := \sqrt{\langle \mathbf{x} \mid \mathbf{x} \rangle} = \sqrt{\sum_{k=1}^n |x_k|^2}$. More generally, any set E here refers to a real vector space provided with a norm $\| \bullet \|_E$. The set $\mathcal{L}_c(E,F)$ of continuous linear maps between two such spaces is endowed with its operator norm:

$$\forall u \in \mathcal{L}_c\left(E,F\right), \quad |||u||| := \sup_{\substack{\mathbf{x}\in E\\ \mathbf{x}\neq \mathbf{0}_E}} \frac{\|u\left(\mathbf{x}\right)\|_F}{\|\mathbf{x}\|_E}.$$

This norm is complete as soon as $\| \bullet \|_F$ is complete, and $\mathcal{L}_c(E,E)$ is a unitary Banach algebra [33, Chapter 18]. We also recall that if E is finite dimensional, then the norms defined on E are equivalent and complete [4, I §2 Section 3]. In this case, E is necessarily a Banach space and any linear map $u : E \to F$ is continuous. Moreover, a well-defined map $g : E \to F$ is said to be Fréchet differentiable at a point $\mathbf{x} \in E$ if there exists a continuous linear map $L_{\mathbf{x}} \in \mathcal{L}_c\left(E,F\right)$ such that:

$$\forall \mathbf{h} \in E, \quad g\left(\mathbf{x}+\mathbf{h}\right) = g\left(\mathbf{x}\right) + L_{\mathbf{x}}\left(\mathbf{h}\right) + \|\mathbf{h}\|_E \; R\left(\mathbf{h}\right),$$

where $\|R(\mathbf{h})\|_F \to 0$ as $\|\mathbf{h}\|_E \to 0$. In this case, the operator $L_{\mathbf{x}}$ is unique, denoted by $D_{\mathbf{x}}g$, and called the differential of g at the point $\mathbf{x}$. If in addition, the map $D_{\bullet}g : \mathbf{y} \in E \to D_{\mathbf{y}}g \in \mathcal{L}_c(E,F)$ is well defined around $\mathbf{x}$ and continuous at $\mathbf{x}$, then we say that g is of class C^1 at $\mathbf{x}$ or continuously differentiable at $\mathbf{x}$. Similarly, we can proceed recursively for any integer $k \geqslant 2$. Hence, if the map $D^{k-1}_{\bullet}g : \mathbf{y} \in E \mapsto D^{k-1}_{\mathbf{y}}g \in \mathcal{L}^{k-1}_c(E^{k-1},F)$ is well defined around $\mathbf{x}$ and differentiable at $\mathbf{x}$, then we say that g is k times (Fréchet) differentiable at $\mathbf{x}$, and the differential of $D^{k-1}_{\bullet}g$ at $\mathbf{x}$ is identified with a continuous k-linear map, denoted by $D^k_{\mathbf{x}}g$ and called the k-th-order differential of g at $\mathbf{x}$, via the following bijective linear isometry:

$$\begin{array}{rcl} \mathcal{L}_c\left(E,\mathcal{L}^{k-1}_c\left(E^{k-1},F\right)\right) & \longrightarrow & \mathcal{L}^k_c\left(E^k,F\right) \\ \mathbf{y}_0 \mapsto \left[u_{\mathbf{y}_0} : \left(\mathbf{y}_1,\dots,\mathbf{y}_{k-1}\right) \mapsto u_{\mathbf{y}_0}\left(\mathbf{y}_1,\dots,\mathbf{y}_{k-1}\right)\right] & \longmapsto & \left(\mathbf{y}_0,\mathbf{y}_1,\dots,\mathbf{y}_{k-1}\right) \mapsto u_{\mathbf{y}_0}\left(\mathbf{y}_1,\dots,\mathbf{y}_{k-1}\right), \end{array}$$

where $\mathcal{L}^k_c(E^k,F)$ is the set of continuous k-linear maps equipped with the norm:

$$\forall u \in \mathcal{L}^k_c\left(E^k,F\right), \quad |||u||| := \sup_{\substack{(\mathbf{x}_1,\dots,\mathbf{x}_k)\in E^k\\ (\mathbf{x}_1,\dots,\mathbf{x}_k)\neq(\mathbf{0}_E,\dots\mathbf{0}_E)}} \frac{\|u\left(\mathbf{x}_1,\dots,\mathbf{x}_k\right)\|_F}{\|\mathbf{x}_1\|_E \dots \|\mathbf{x}_k\|_E}.$$

If in addition, the map $D^k_{\bullet}g : \mathbf{y} \in E \mapsto D^k_{\mathbf{y}} \in \mathcal{L}^k_c(E^k,F)$ is well defined around $\mathbf{x}$ and continuous at the point $\mathbf{x}$, then we say that g is of class C^k at $\mathbf{x}$ or k times continuous differentiable at $\mathbf{x}$. Then, for any real $p \geqslant 1$, we denote by L^p the space of measurable maps from $\mathbb{R}^n$ into $\mathbb{R}^n$ whose p-th power is integrable, and by L^∞ the space of measurable maps from $\mathbb{R}^n$ into $\mathbb{R}^n$ that are essentially bounded. They are respectively endowed with their usual norm:

$$\forall \left(\mathbf{f},\mathbf{g}\right) \in L^p \times L^\infty, \quad \|\mathbf{f}\|_p := \left(\int_{\mathbb{R}^n} |\mathbf{f}\left(\mathbf{x}\right)|^p d\mathbf{x}\right)^{\frac{1}{p}} \qquad \text{and} \qquad \|\mathbf{g}\|_\infty := \operatorname{ess}\sup_{\mathbf{x}\in\mathbb{R}^n} |\mathbf{g}\left(\mathbf{x}\right)|,$$

where the integration is done with respect to the usual n-dimensional Lebesgue measure. We recall that each L^p and L^∞ are Banach spaces [33, §3.11 Theorem]. Moreover, for any measurable map $f : \mathbb{R}^n \to \mathbb{R}$ which is locally integrable, we say that f is weakly differentiable if there exists a measurable map $\mathbf{g} : \mathbb{R}^n \to \mathbb{R}^n$ which is locally integrable, and such that:

$$\forall \varphi \in C^\infty_c, \quad \int_{\mathbb{R}^n} \langle \mathbf{g}\left(\mathbf{x}\right) \mid \varphi\left(\mathbf{x}\right)\rangle \, d\mathbf{x} = -\int_{\mathbb{R}^n} f\left(\mathbf{x}\right) \; \operatorname{div} \varphi\left(\mathbf{x}\right) d\mathbf{x},$$

where C_c^∞ refers to the set of smooth maps from $\mathbb{R}^n$ into $\mathbb{R}^n$ with compact support. In this case, the function $\mathbf{g}$ is unique, denoted by ∇f, and called the weak gradient of f. For any real $p \geqslant 1$, we can now introduce the Sobolev space $W^{1,p}$ as the set of functions $f \in L^p(\mathbb{R}^n, \mathbb{R})$ that are weakly differentiable and whose weak gradients ∇f are functions of L^p. Moreover, any $W^{1,p}$ is a Banach space [5, Chapter 9] endowed with the norm:

$$\forall f \in W^{1,p}, \quad \|f\|_{1,p} := \left(\int_{\mathbb{R}^n} |f(\mathbf{x})|^p d\mathbf{x} \right)^{\frac{1}{p}} + \|\nabla f\|_p.$$

The space $C^{0,1}$ of Lipschitz continuous maps from $\mathbb{R}^n$ into $\mathbb{R}^n$ is equipped with the norm:

$$\forall \theta \in C^{0,1}, \quad \|\theta\|_{0,1} := \sup_{\substack{(\mathbf{x},\tilde{\mathbf{x}}) \in \mathbb{R}^n \times \mathbb{R}^n \\ \mathbf{x} \neq \tilde{\mathbf{x}}}} \frac{|\theta(\mathbf{x}) - \theta(\tilde{\mathbf{x}})|}{|\mathbf{x} - \tilde{\mathbf{x}}|}.$$

We recall that $C^{0,1}$ is *not* a Banach space i.e. the norm $\| \bullet \|_{0,1}$ is *not* complete. We denote by $\mathbb{B}^{0,1} := \{\theta \in C^{0,1}, \ \ \|\theta\|_{0,1} < 1\}$ the open unit ball of $C^{0,1}$ centred at the origin i.e. the set of Lipschitz contractions. We recall that $C^{0,1}$ can be identified with the subspace of continuous maps from $\mathbb{R}^n$ into $\mathbb{R}^n$ whose weak partial derivatives are functions of L^∞ [17, Section 4.2.3]. Moreover, any Lipschitz continuous map is differentiable almost everywhere [17, Section 3.1.2] and we have $\|\theta\|_{0,1} = \operatorname{ess\,sup}_{\mathbf{x} \in \mathbb{R}^n} |||D_{\mathbf{x}}\theta|||$ for any $\theta \in C^{0,1}$. We also introduce the space $W^{1,\infty} = L^\infty \cap C^{0,1}$ of Lipschitz continuous bounded maps from $\mathbb{R}^n$ into $\mathbb{R}^n$, provided with the norm:

$$\forall \theta \in W^{1,\infty}, \qquad \|\theta\|_{1,\infty} := \|\theta\|_\infty + \|\theta\|_{0,1}.$$

In particular, $W^{1,\infty}$ is a Banach space [5, Proposition 9.1] and $I : \mathbf{x} \in \mathbb{R}^n \mapsto \mathbf{x} \in \mathbb{R}^n$ denotes the identity map. Finally, we can define recursively for any integer $k \geqslant 2$ the Sobolev spaces $W^{k,p}$ as the set of all maps $f : \mathbb{R}^n \to \mathbb{R}$ that are in $W^{1,p}$ and such that each component of its weak gradient is a function of $W^{k-1,p}$. It can be endowed with the norm:

$$\forall f \in W^{k,p}, \quad \|f\|_{k,p} := \|f\|_{1,p} + \sum_{i=1}^{n} \|\partial_i f\|_{k-1,p}.$$

Similarly, the space $W^{k,\infty}$ is defined recursively as the set of maps $\theta : \mathbb{R}^n \to \mathbb{R}^n$ that are in $W^{1,\infty}$ such that their partial derivatives are functions of $W^{k-1,\infty}$. It is equipped with the norm:

$$\forall \theta \in W^{k,\infty}, \quad \|\theta\|_{k,\infty} := \|\theta\|_{1,\infty} + \sum_{i=1}^{n} \|\partial_i \theta\|_{k-1,\infty}.$$

To conclude, $W^{k,p}$ and $W^{k,\infty}$ are Banach spaces for any integer $k \geqslant 2$ [5, §above Section 9.2] and we use the specific notation $H^k := W^{k,2}$ because it is an Hilbert space [5, Proposition 9.1].

4.2 About the differentiability related to the inverse operator

Proposition 4.1. *Let $\theta \in \mathbb{B}^{0,1}$. Then, $I + \theta$ is a $(1 + \|\theta\|_{0,1})$-Lipschitz continuous map which is invertible, and its inverse $(I + \theta)^{-1}$ is a $\frac{1}{1 - \|\theta\|_{0,1}}$-Lipschitz continuous map satisfying:*

$$\| (I + \theta)^{-1} - I \|_{0,1} \leqslant \frac{\|\theta\|_{0,1}}{1 - \|\theta\|_{0,1}}. \tag{58}$$

In particular, the map $\theta \in C^{0,1} \mapsto (I + \theta)^{-1} \in C^{0,1}$ is well defined on $\mathbb{B}^{0,1}$ and it is continuous at the origin. If in addition, we assume that θ is bounded, then we have $(I + \theta)^{-1} - I \in W^{1,\infty}$ and the following estimations hold true:

$$\| (I + \theta)^{-1} - I \|_{1,\infty} \leqslant \frac{\|\theta\|_{1,\infty}}{1 - \|\theta\|_{0,1}}, \tag{59}$$

$$\| (I + \theta)^{-1} - I + \theta \|_{\infty} \leqslant \left(\frac{\|\theta\|_{1,\infty}}{2} \right)^2. \tag{60}$$

In particular, the map $\theta \in W^{1,\infty} \mapsto (I + \theta)^{-1} - I \in W^{1,\infty}$ is well defined on $W^{1,\infty} \cap \mathbb{B}^{0,1}$, and it is continuous at the origin. Moreover, the map $\theta \in W^{1,\infty} \mapsto (I + \theta)^{-1} - I \in L^\infty$ is differentiable at the origin, its differential being the opposite of the inclusion map from $W^{1,\infty}$ into L^∞.

Proof. Let $\theta \in \mathbb{B}^{0,1}$. First, from the triangle inequality, we get the $(1+\|\theta\|_{0,1})$-Lipschitz continuity of $I+\theta$. Then, for any $\mathbf{z} \in \mathbb{R}^n$, the map $\mathbf{x} \in \mathbb{R}^n \mapsto \mathbf{z} - \theta(\mathbf{x}) \in \mathbb{R}^n$ is a contraction thus the Banach Fixed-Point Theorem [5, Theorem 5.7] asserts there exists a unique point $\mathbf{x_z} \in \mathbb{R}^n$ such that $\mathbf{z} - \theta(\mathbf{x_z}) = \mathbf{x_z}$ i.e. $I+\theta$ is a bijective map. Moreover, since $(I+\theta)^{-1} = I - \theta \circ (I+\theta)^{-1}$, we obtain $\|(I+\theta)^{-1}\|_{0,1} \leqslant 1 + \|\theta\|_{0,1}\|(I+\theta)^{-1}\|_{0,1}$, from which we deduce that $(I+\theta)^{-1}$ is a $\frac{1}{1-\|\theta\|_{0,1}}$-Lipschitz continuous map. Similarly, we have $\|(I+\theta)^{-1} - I\|_{0,1} = \| - \theta \circ (I+\theta)^{-1}\|_{0,1} \leqslant \|\theta\|_{0,1}\|(I+\theta)^{-1}\|_{0,1}$ so relation (58) holds true. Finally, if we now assume that θ is bounded, then we also get:

$$\left\{ \begin{array}{l} \| (I+\theta)^{-1} - I\|_{1,\infty} \leqslant \|\theta\|_{\infty} + \dfrac{\|\theta\|_{0,1}}{1-\|\theta\|_{0,1}} = \dfrac{\|\theta\|_{1,\infty} - \|\theta\|_{0,1}\|\theta\|_{\infty}}{1-\|\theta\|_{0,1}} \leqslant \dfrac{\|\theta\|_{1,\infty}}{1-\|\theta\|_{0,1}} \\ \\ \| (I+\theta)^{-1} - I + \theta\|_{\infty} = \|\theta - \theta \circ (I+\theta)^{-1}\|_{\infty} \leqslant \|\theta\|_{0,1} \underbrace{\|I - (I+\theta)^{-1}\|_{\infty}}_{\leqslant \|\theta\|_{\infty}} \leqslant \dfrac{\|\theta\|_{1,\infty}^2}{4}. \end{array} \right.$$

To conclude the proof of Proposition 4.1, $(I-\theta)^{-1} - I \in W^{1,\infty}$ and (59)–(60) hold true. ☐

Lemma 4.2. *Let $\theta \in C^{0,1}$. Then, the differential map $D_\bullet\theta : \mathbf{x} \in \mathbb{R}^n \mapsto D_\mathbf{x}\theta \in \mathbb{R}^{n^2}$ is well defined almost everywhere, measurable, and it is essentially bounded by $\sqrt{n}\|\theta\|_{0,1}$ in the matrix space $\mathbb{R}^{n^2}$. In particular, the map $\theta \in C^{0,1} \mapsto D_\bullet\theta \in L^\infty(\mathbb{R}^n, \mathbb{R}^{n^2})$ is well defined, linear, and continuous. Moreover, for almost every point $\mathbf{x} \in \mathbb{R}^n$, we have $D_\mathbf{x}(I+\theta) = I + D_\mathbf{x}\theta$ and if we assume that $\|\theta\|_{0,1} < 1$, then we also have $D_{(I+\theta)(\mathbf{x})}[(I+\theta)^{-1}] = (I + D_\mathbf{x}\theta)^{-1}$ for almost every point $\mathbf{x} \in \mathbb{R}^n$.*

Proof. Let $\theta \in C^{0,1}$. First, we define $Def(\theta)$ as the set of points in $\mathbb{R}^n$ for which θ is differentiable and Rademacher's Theorem [17, Section 3.1.2] ensures that θ is differentiable almost everywhere. Then, the differential $D_\mathbf{x}\theta$ of θ at any $\mathbf{x} \in Def(\theta)$ is a well-defined linear map, thus identified with its $(n\times n)$-matrix representation in the canonic basis of $\mathbb{R}^n$ denoted by $(\mathbf{e}_1, \ldots, \mathbf{e}_n)$. Hence, the map $D_\bullet\theta : \mathbf{x} \in Def(\theta) \mapsto D_\mathbf{x}\theta \in \mathbb{R}^{n^2}$ is measurable if and only if $[D_\bullet\theta]_{ij} : \mathbf{x} \in Def(\theta) \mapsto \partial_j\theta_i(\mathbf{x}) \in \mathbb{R}$ is measurable for any $(i,j) \in [\![1,n]\!]^2$, which is the case since it is respectively the pointwise limits of the continuous maps $(\theta_{ij}^k)_{k\in\mathbb{N}} : \mathbf{x} \in \mathbb{R}^n \mapsto k[\theta_i(\mathbf{x} + \frac{1}{k}\mathbf{e}_j) - \theta_i(\mathbf{x})] \in \mathbb{R}$. Moreover, for any $\mathbf{x} \in Def(\theta)$, we have:

$$\|D_\mathbf{x}\theta\|_{\mathbb{R}^{n^2}} := \sqrt{\sum_{i,j=1}^{n} |\partial_j\theta_i(\mathbf{x})|^2} \leqslant \sqrt{n}\,|D_\mathbf{x}\theta(\mathbf{e}_{j_0})| \leqslant \sqrt{n}\,\underset{\mathbf{x}\in\mathbb{R}^n}{\text{ess sup}}\,|||D_\mathbf{x}\theta||| = \sqrt{n}\,\|\theta\|_{0,1}, \quad (61)$$

where $j_0 \in [\![1,n]\!]$ satisfies $|\partial_{j_0}\theta_i(\mathbf{x})| = \max_{1\leqslant j\leqslant n}|\partial_j\theta_i(\mathbf{x})|$. Hence, $\theta \in C^{0,1} \mapsto D_\bullet\theta \in L^\infty(\mathbb{R}^n, \mathbb{R}^{n^2})$ is a well-defined map, which is also linear (thus continuous by (61)). Indeed, for any $\lambda \in \mathbb{R}$ and any $(\theta_1, \theta_2) \in C^{0,1} \times C^{0,1}$, we have $D_\mathbf{x}\theta_1 + \lambda D_\mathbf{x}\theta_2 = D_\mathbf{x}(\theta_1 + \lambda\theta_2)$ for any $\mathbf{x} \in Def(\theta_1) \cap Def(\theta_2)$ i.e. almost everywhere by Rademacher's Theorem. Hence, we get $D_\bullet(\theta_1 + \lambda\theta_2) = D_\bullet\theta_1 + \lambda D_\bullet\theta_2$. Similarly, we have $Def(\theta) = Def(I+\theta)$ and $I + D_\mathbf{x}\theta = D_\mathbf{x}(I+\theta)$ for any $\mathbf{x} \in Def(\theta)$. Using again Rademacher's Theorem, the last equality holds true almost everywhere. Finally, let $\theta \in \mathbb{B}^{0,1}$. Proposition 4.1 ensures that $(I+\theta)$ has a Lipschitz continuous inverse. Hence, at any point $\mathbf{x} \in A := Def(I+\theta) \cap (I+\theta)^{-1}\langle Def[(I+\theta)^{-1}]\rangle$, we can correctly differentiate the relation $(I+\theta)^{-1} \circ (I+\theta) = I$ and it yields to $D_{(I+\theta)(\mathbf{x})}[(I+\theta)^{-1}](I + D_\mathbf{x}\theta) = I$. Since we have $|||D_\mathbf{x}\theta||| \leqslant \|\theta\|_{0,1} < 1$, the matrix $I + D_\mathbf{x}\theta$ has an inverse [33, §18.3], which is multiplied to the last equality to get $D_{(I+\theta)(\mathbf{x})}[(I+\theta)^{-1}] = (I + D_\mathbf{x}\theta)^{-1}$. Combining [17, Section 2.4.1 Theorem 1] and [17, Section 2.2 Theorem 2] with Rademacher's Theorem, we deduce that $\mathbb{R}^n\backslash A$ has a zero n-dimensional Lebesgue measure i.e. $D_{(I+\theta)(\mathbf{x})}[(I+\theta)^{-1}] = (I + D_\mathbf{x}\theta)^{-1}$ for almost every $\mathbf{x} \in \mathbb{R}^n$, concluding the proof of Lemma 4.2. ☐

Proposition 4.3. *Let $\theta \in \mathbb{B}^{0,1}$. Then, $(I + D_\bullet\theta)^{-1} : \mathbf{x} \in \mathbb{R}^n \mapsto (I + D_\mathbf{x}\theta)^{-1} \in \mathbb{R}^{n^2}$ is well defined almost everywhere and it is a measurable map satisfying for almost every point $\mathbf{x} \in \mathbb{R}^n$:*

$$\|(I + D_\mathbf{x}\theta)^{-1}\|_{\mathbb{R}^{n^2}} \leqslant \frac{\sqrt{n}}{1-\|\theta\|_{0,1}}. \quad (62)$$

In particular, the map $\theta \in C^{0,1} \mapsto (I + D_\bullet\theta)^{-1} \in L^\infty(\mathbb{R}^n, \mathbb{R}^{n^2})$ is well defined on $\mathbb{B}^{0,1}$. Moreover, it is differentiable at the origin and its differential at the origin is given by the continuous linear map $\theta \in C^{0,1} \mapsto -D_\bullet\theta \in L^\infty(\mathbb{R}^n, \mathbb{R}^{n^2})$.

Proof. Let $\theta \in \mathbb{B}^{0,1}$. First, from Lemma 4.2, we deduce that the map $D_\bullet\theta : \mathbf{x} \in \mathbb{R}^n \mapsto D_\mathbf{x}\theta \in \mathbb{R}^{n^2}$ is well defined for almost every point $\mathbf{x} \in \mathbb{R}^n$ and the matrix $I + D_\mathbf{x}\theta$ is invertible since we have $|||D_\mathbf{x}\theta||| \leqslant \|\theta\|_{0,1} < 1$ [33, §18.3]. Hence, the map $(I + D_\bullet\theta)^{-1}$ is well defined almost everywhere. Moreover, it is measurable as the composition between $D_\bullet\theta$, which is measurable by Lemma 4.2, and the map $A \in \{B \in \mathbb{R}^{n^2}, |||B||| < 1\} \mapsto (I + A)^{-1} \in \mathbb{R}^{n^2}$ which is continuous [33, §18.4]. Then, we use successively Lemma 4.2, relation (61) applied to $(I + \theta)^{-1}$, and Proposition 4.1 in order to get for almost every point $\mathbf{x} \in \mathbb{R}^n$:

$$\| (I + D_\mathbf{x}\theta)^{-1} \|_{\mathbb{R}^{n^2}} \leqslant \|D_\bullet[(I + \theta)^{-1}]\|_{L^\infty(\mathbb{R}^n,\mathbb{R}^{n^2})} \leqslant \sqrt{n}\| (I + \theta)^{-1} \|_{0,1} \leqslant \frac{\sqrt{n}}{1 - \|\theta\|_{0,1}}.$$

Hence, $\theta \in C^{0,1} \mapsto (I + D_\bullet\theta)^{-1} \in L^\infty(\mathbb{R}^n, \mathbb{R}^{n^2})$ is well defined on $\mathbb{B}^{0,1}$. It remains to prove that it is differentiable at the origin. From Lemma 4.2, the map $f : \theta \in C^{0,1} \mapsto D_\bullet\theta \in L^\infty(\mathbb{R}^n, \mathbb{R}^{n^2})$ is well defined, linear and continuous. In particular, f is differentiable at any point and its differential at any point is the map f itself. In addition, the map $g : A \in \{B \in \mathbb{R}^{n^2}, |||B||| < 1\} \mapsto (I+A)^{-1} \in \mathbb{R}^{n^2}$ is differentiable at the origin [33, §18.4] and its differential is given by $D_0 g : A \in \mathbb{R}^{n^2} \mapsto -A \in \mathbb{R}^{n^2}$. We deduce that the map $g \circ f : \theta \in C^{0,1} \mapsto (I + D_\bullet\theta)^{-1} \in L^\infty(\mathbb{R}^n, \mathbb{R}^{n^2})$ is differentiable at the origin, and its differential is given by the following continuous linear map:

$$\forall \theta \in C^{0,1}, \quad D_0(g \circ f)(\theta) = D_{f(0)}g[D_0 f(\theta)] = D_0 g[f(\theta)] = -f(\theta) = -D_\bullet\theta,$$

concluding the proof of Proposition 4.3. □

4.3 About the differentiability related to the Jacobian determinant

Proposition 4.4. *Let $\theta \in \mathbb{B}^{0,1}$. Then, the Jacobian determinant of $I + \theta$ i.e. the function $\mathbf{x} \in \mathbb{R}^n \mapsto \det[D_\mathbf{x}(I + \theta)] \in \mathbb{R}$ is well defined almost everywhere. In addition, it is a measurable map which satisfies for almost every point $\mathbf{x} \in \mathbb{R}^n$:*

$$|\det [D_\mathbf{x} (I + \theta)] | \leqslant \frac{n!}{1 - \|\theta\|_{0,1}}, \tag{63}$$

In particular, the map $\theta \in C^{0,1} \mapsto \det[D_\bullet(I + \theta)] \in L^\infty(\mathbb{R}^n, \mathbb{R})$ is well defined on $\mathbb{B}^{0,1}$. Moreover, it is differentiable at the origin and its differential is given by the divergence operator i.e. by the continuous linear map $\theta \in C^{0,1} \mapsto \operatorname{div}(\theta) := \operatorname{trace}(D_\bullet\theta) \in L^\infty(\mathbb{R}^n, \mathbb{R})$.

Proof. Let $\theta \in \mathbb{B}^{0,1}$. From Lemma 4.2, the map $D_\bullet\theta : \mathbf{x} \in \mathbb{R}^n \mapsto D_\mathbf{x}\theta \in \mathbb{R}^{n^2}$ is well defined almost everywhere and measurable. Since the determinant is a continuous map and $D_\bullet(I + \theta) = I + D_\bullet\theta$ by Lemma 4.2, the Jacobian determinant of $I+\theta$ is well defined almost everywhere and measurable. First, we can express the Jacobian determinant of $I + \theta$ by using the set $\mathcal{S}_n$ of permutations of n elements i.e. the set of bijective maps from $[\![1, n]\!]$ into $[\![1, n]\!]$. Introducing the map $s : \mathcal{S}_n \to \{-1, 1\}$ defining the signature a permutation, it follows for almost every point $\mathbf{x} \in \mathbb{R}^n$:

$$\det [D_\mathbf{x} (I + \theta)] \quad = \quad \det (I + D_\mathbf{x}\theta) \quad = \quad \sum_{p\in\mathcal{S}_n} s(p) \prod_{i=1}^{n} [I_{p(i)i} + \partial_i\theta_{p(i)} (\mathbf{x})] \tag{64}$$

Expanding the product and using the fact that $I_{p(j)j} = 1$ if and only if $j = p(j)$, we deduce that:

$$\det [D_\mathbf{x} (I + \theta)] = \sum_{k=0}^{n} \sum_{\substack{I_k\subseteq[\![1,n]\!]\\ \operatorname{card} I_k = k}} \sum_{\substack{p\in\mathcal{S}_n\\ \forall j\notin I_k, p(j)=j}} s(p) \prod_{i\in I_k} \partial_i\theta_{p(i)} (\mathbf{x}) . \tag{65}$$

Then, note that $\partial_i\theta_{p(i)}(\mathbf{x})$ is the $p(i)$-th component of the vector $D_\mathbf{x}\theta(\mathbf{e}_i)$ where $\mathbf{e}_i$ is the unit vector whose components are zero except the i-th one which is equal to one. Therefore, we have:

$$|\partial_i\theta_{p(i)} (\mathbf{x}) | = | [D_\mathbf{x}\theta (\mathbf{e}_i)]_{p(i)} | \leqslant \sqrt{\sum_{j=1}^{n} [D_\mathbf{x}\theta (\mathbf{e}_i)]_j^2} = |D_\mathbf{x}\theta (\mathbf{e}_i) | \leqslant |||D_\mathbf{x}\theta||| \; |\mathbf{e}_i| \leqslant \|\theta\|_{0,1}. \tag{66}$$

Combining (65) and (66), we obtain:

$$|\det\left[D_{\mathbf{x}}\left(I+\theta\right)\right]| \leqslant \sum_{k=0}^{n} \sum_{\substack{I_k\subseteq[\![1,n]\!]\\ \mathrm{card}I_k=k}} \sum_{\substack{p\in\mathcal{S}_n\\ \forall j\notin I_k, p(j)=j}} \underbrace{|s\left(p\right)|}_{=1} \prod_{i\in I_k} \underbrace{|\partial_i\theta_{p(i)}\left(\mathbf{x}\right)|}_{\leqslant\|\theta\|_{0,1}} \leqslant \sum_{k=0}^{n}\left(\prod_{i=0}^{k-1}(n-i)\right)\|\theta\|_{0,1}^{k}.$$

The last inequality comes from the fact that $\prod_{i\in I_k}\|\theta\|_{0,1}=\|\theta\|_{0,1}^k$ does not depend on p and I_k. We can thus remove it from the corresponding sums for which $\mathrm{card}\{p\in\mathcal{S}_n \mid \forall j\notin I_k,\ p(j)=j\}=k!$ and $\mathrm{card}\{I_k\subseteq[\![1,n]\!],\ \mathrm{card}\ I_k=k\}=\binom{n}{k}=\frac{n(n-1)\dots(n-k+1)}{k!}$. Hence, we get:

$$|\det\left[D_{\mathbf{x}}\left(I+\theta\right)\right]| \leqslant \sum_{k=0}^{n} n(n-1)\dots(n-k+1)\|\theta\|_{0,1}^k \leqslant n!\sum_{k=0}^{n}\|\theta\|_{0,1}^k \leqslant n!\sum_{k=0}^{+\infty}\|\theta\|_{0,1}^k = \frac{n!}{1-\|\theta\|_{0,1}}.$$

The last inequality holds true because $\|\theta\|_{0,1}<1$ and the geometric series $\sum_{k\in\mathbb{N}}\|\theta\|_{0,1}^k$ converges. Hence, estimation (63) holds true. Finally, the map $J:\theta\in C^{0,1}\mapsto\det[D_{\bullet}(I+\theta)]\in L^{\infty}(\mathbb{R}^n,\mathbb{R})$ is the composition of the determinant $\det:\mathbb{R}^{n^2}\to\mathbb{R}$ with the affine map $I+f$, where f is its linear part defined as $f:\theta\in C^{0,1}\mapsto D_{\bullet}\theta\in L^{\infty}(\mathbb{R}^n,\mathbb{R}^{n^2})$. Since the determinant is differentiable and since f is linear and continuous by Lemma 4.2, we deduce that J is differentiable at the origin and its differential is given by:

$$\forall\theta\in C^{0,1},\quad D_0J(\theta)=D_0\left[\det\circ\left(I+f\right)\right]\left(\theta\right)=D_I\det[D_0(I+f)(\theta)]=\mathrm{trace}\left[f(\theta)\right]\mathrm{div}\left(\theta\right).$$

To conclude, the divergence operator is the differential of $J=\det\circ\left(I+f\right)$ at the origin. □

Corollary 4.5. *Let $\theta\in\mathbb{B}^{0,1}$. Then, the map $\mathbf{x}\in\mathbb{R}^n\mapsto\det([D_{\mathbf{x}}(I+\theta)]^{-1})\in\mathbb{R}$ is well defined almost everywhere, measurable, and it satisfies for almost every point $\mathbf{x}\in\mathbb{R}^n$:*

$$|\det\left(\left[D_{\mathbf{x}}\left(I+\theta\right)\right]^{-1}\right)| \leqslant \frac{n!}{\left(1-\|\theta\|_{0,1}\right)^n}. \tag{67}$$

In particular, the map $\theta\in C^{0,1}\mapsto\det([D_{\bullet}(I+\theta)]^{-1})\in L^{\infty}(\mathbb{R}^n,\mathbb{R})$ is well defined on $\mathbb{B}^{0,1}$.

Proof. Let $\theta\in\mathbb{B}^{0,1}$. Considering Proposition 4.3 and Lemma 4.2, $(I+D_{\bullet}\theta)^{-1}=[D_{\bullet}(I+\theta)]^{-1}$ is well defined almost everywhere and measurable. Since the determinant is a continuous map, we deduce that $\mathbf{x}\in\mathbb{R}^n\mapsto\det([D_{\mathbf{x}}(I+\theta)]^{-1})\in\mathbb{R}$ is well defined almost everywhere and measurable. Applying relation (64) to $[D_{\bullet}(I+\theta)]^{-1}$, we get for almost every point $\mathbf{x}\in\mathbb{R}^n$:

$$\begin{aligned}|\det\left(\left[D_{\mathbf{x}}\left(I+\theta\right)\right]^{-1}\right)| &= |\det\left[\left(I+D_{\mathbf{x}}\theta\right)^{-1}\right]| \leqslant \sum_{p\in\mathcal{S}_n}\underbrace{|s\left(p\right)|}_{=1}\prod_{i=1}^{n}\underbrace{|\left[\left(I+D_{\mathbf{x}}\theta\right)^{-1}\right]_{p(i)i}|}_{\leqslant|||(I+D_{\mathbf{x}}\theta)^{-1}|||}\\ &\leqslant \sum_{p\in\mathcal{S}_n}\left(\frac{1}{1-|||D_{\mathbf{x}}\theta|||}\right)^n \leqslant \frac{n!}{(1-\|\theta\|_{0,1})^n}.\end{aligned}$$

Hence, relation (67) holds true and the map $\theta\in C^{0,1}\mapsto\det([D_{\bullet}(I+\theta)]^{-1})\in L^{\infty}(\mathbb{R}^n,\mathbb{R})$ is well defined at any point of $\mathbb{B}^{0,1}$, concluding the proof of Corollary 4.5. □

4.4 About the differentiability related to the composition operator

Proposition 4.6. *Let $f\in L^1(\mathbb{R}^n,\mathbb{R})$. Then, the map $\theta\in C^{0,1}\mapsto f\circ(I+\theta)\in L^1(\mathbb{R}^n,\mathbb{R})$ is well defined on $\mathbb{B}^{0,1}$. Moreover, $\theta\in W^{1,\infty}\mapsto f\circ(I+\theta)\in L^1(\mathbb{R}^n,\mathbb{R})$ is continuous at the origin. If in addition, we have $f\in W^{1,1}$, then $\theta\in W^{1,\infty}\mapsto f\circ(I+\theta)\in L^1(\mathbb{R}^n,\mathbb{R})$ is differentiable at the origin and its differential is given by the continuous linear map $\theta\in W^{1,\infty}\mapsto\langle\nabla f\mid\theta\rangle\in L^1(\mathbb{R}^n,\mathbb{R})$.*

Proof. Let $f\in L^1(\mathbb{R}^n,\mathbb{R})$. First, we check that the map $\theta\in C^{0,1}\mapsto f\circ(I+\theta)\in L^1(\mathbb{R}^n,\mathbb{R})$ is well defined around the origin. Let $\theta\in\mathbb{B}^{0,1}$. The function $f\circ(I+\theta)$ is measurable as the composition of the Lipschitz continuous map $(I+\theta)$ with the measurable map f. Proposition 4.1 ensures that the map $(I+\theta)$ has a Lipschitz continuous inverse, from which we deduce for almost every $\mathbf{x}\in\mathbb{R}^n$:

$$1=\det\left(I\right)=\det\left(\left[D_{\mathbf{x}}\left(I+\theta\right)\right]^{-1}\circ D_{\mathbf{x}}\left(I+\theta\right)\right)=\det\left(\left[D_{\mathbf{x}}\left(I+\theta\right)\right]^{-1}\right)\,\det\left[D_{\mathbf{x}}\left(I+\theta\right)\right].$$

Consequently, using this last observation, relation (67), and the change of variables formula valid for any Lipschitz continuous map [17, Section 3.3.3], we get:

$$\begin{aligned} \int_{\mathbb{R}^n} |f[\mathbf{x}+\theta(\mathbf{x})]|d\mathbf{x} &= \int_{\mathbb{R}^n} |f[\mathbf{x}+\theta(\mathbf{x})]\det\left[(I+D_{\mathbf{x}}\theta)^{-1}\right]\ \det[D_{\mathbf{x}}(I+\theta)]|d\mathbf{x} \\ &\leqslant \frac{n!}{(1-\|\theta\|_{0,1})^n}\underbrace{\int_{\mathbb{R}^n}|f[\mathbf{x}+\theta(\mathbf{x})]\det(D_{\mathbf{x}}(I+\theta))|d\mathbf{x}}_{=\int_{\mathbb{R}^n}|f(\mathbf{y})|d\mathbf{y}<+\infty}. \end{aligned} \tag{68}$$

Hence, we obtain $f\circ(I+\theta)\in L^1(\mathbb{R}^n,\mathbb{R})$ for any $f\in L^1(\mathbb{R}^n,\mathbb{R})$ and any $\theta\in\mathbb{B}^{0,1}$. Then, we prove that the map $\theta\in W^{1,\infty}\mapsto f\circ(I+\theta)\in L^1(\mathbb{R}^n,\mathbb{R})$ is continuous at the origin. Let $\theta\in W^{1,\infty}$ be such that $\|\theta\|_{1,\infty}\leqslant\frac{1}{2}$. We proceed by a density argument: there exists a sequence of smooth maps $(f_i)_{i\in\mathbb{N}}:\mathbb{R}^n\to\mathbb{R}$ with compact support converging to f in $L^1(\mathbb{R}^n,\mathbb{R})$ [5, Corollary 4.23]. On the one hand, we have $\|\theta\|_{0,1}\leqslant\frac{1}{2}<1$ so the foregoing holds true. We can apply the arguments of (68) to the map $f-f_i$ in order to get for any $i\in\mathbb{N}$:

$$\|f\circ(I+\theta)-f_i\circ(I+\theta)\|_{L^1(\mathbb{R}^n,\mathbb{R})}\leqslant\frac{n!\|f-f_i\|_{L^1(\mathbb{R}^n,\mathbb{R})}}{(1-\|\theta\|_{0,1})^n}\leqslant n!2^n\|f-f_i\|_{L^1(\mathbb{R}^n,\mathbb{R})}.$$

On the other hand, since the map f_i is smooth with compact support, we have for any $i\in\mathbb{N}$:

$$\|f_i\circ(I+\theta)-f_i\|_{L^1(\mathbb{R}^n,\mathbb{R})}=\int_{\mathbb{R}^n}|f_i[\mathbf{x}+\theta(\mathbf{x})]-f_i(\mathbf{x})|d\mathbf{x}\leqslant\|f_i\|_{C^{0,1}(\mathbb{R}^n,\mathbb{R})}\ \|\theta\|_\infty\ \mathcal{L}^n(\mathrm{supp}\ f_i).$$

Combining the triangle inequality with these two observations, we deduce that for any $i\in\mathbb{N}$:

$$\|f\circ(I+\theta)-f\|_{L^1(\mathbb{R}^n,\mathbb{R})}\ \leqslant\ (1+2^n n!)\|f-f_i\|_{L^1(\mathbb{R}^n,\mathbb{R})}+\|f_i\|_{C^{0,1}(\mathbb{R}^n,\mathbb{R})}\ \|\theta\|_{1,\infty}\ \mathcal{L}^n(\mathrm{supp}\ f_i). \tag{69}$$

Let $\varepsilon>0$. There exists $I\in\mathbb{N}$ such that $\|f_I-f\|_{L^1(\mathbb{R}^n,\mathbb{R})}\leqslant\frac{\varepsilon}{2(1+2^n n!)}$. We set:

$$\delta:=\min\left(\frac{1}{2},\ \frac{\varepsilon}{2\|f_I\|_{C^{0,1}(\mathbb{R}^n,\mathbb{R})}\ \mathcal{L}^n(\mathrm{supp}\ f_I)}\right).$$

For any $\theta\in W^{1,\infty}$ such that $\|\theta\|_{1,\infty}<\delta$, we get from (69) that $\|f\circ(I+\theta)-f\|_{L^1(\mathbb{R}^n,\mathbb{R})}\leqslant\varepsilon$ i.e. the map $\theta\in W^{1,\infty}\mapsto f\circ(I+\theta)\in L^1(\mathbb{R}^n,\mathbb{R})$ is continuous at the origin. We now assume that $f\in W^{1,1}$ and we prove that $\theta\in W^{1,\infty}\mapsto f\circ(I+\theta)\in L^1(\mathbb{R}^n,\mathbb{R})$ is differentiable at the origin. First, note that the linear map $\theta\in W^{1,\infty}\mapsto\langle\nabla f\mid\theta\rangle\in L^1(\mathbb{R}^n,\mathbb{R})$ is well defined and continuous since we get from the Cauchy-Schwarz inequality:

$$\int_{\mathbb{R}^n}|\langle\nabla f(\mathbf{x})\ \mid\theta(\mathbf{x})\rangle|d\mathbf{x}\leqslant\int_{\mathbb{R}^n}|\nabla f(\mathbf{x})|\ \ |\theta(\mathbf{x})|d\mathbf{x}\leqslant\|\theta\|_{1,\infty}\|\nabla f\|_1<+\infty. \tag{70}$$

We want to show it is the differential of $\theta\in W^{1,\infty}\mapsto f\circ(I+\theta)\in L^1(\mathbb{R}^n,\mathbb{R})$ at the origin. For this purpose, we introduce the following map:

$$\begin{array}{rccl} R_f: & W^{1,\infty} & \longrightarrow & L^1(\mathbb{R}^n,\mathbb{R}) \\ & \theta & \longmapsto & R_f(\theta):=f\circ(I+\theta)-f-\langle\nabla f\mid\theta\rangle. \end{array}$$

From the foregoing observations (68) and (70), the map R_f is well defined on the open unit ball of $W^{1,\infty}$ centred at the origin. Therefore, let $\theta\in W^{1,\infty}$ be such that $\|\theta\|_{1,\infty}<1$. Now, let us assume for a moment that f is a smooth map with compact support i.e. $f\in C_c^\infty(\mathbb{R}^n,\mathbb{R})$. We consider $\mathbf{x}\in\mathbb{R}^n$ and introduce the function $\varphi:t\in[0,1]\mapsto f[\mathbf{x}+t\theta(\mathbf{x})]$. Since φ is the composition of the affine map $g_{\mathbf{x}}:t\in[0,1]\mapsto\mathbf{x}+t\theta(\mathbf{x})\in\mathbb{R}^n$ with f, it is differentiable on $[0,1]$ and we have:

$$\forall t\in[0,1],\quad\varphi'(t)=D_t(f\circ g_{\mathbf{x}})=D_{g_{\mathbf{x}}(t)}f\circ D_t g_{\mathbf{x}}=\langle\nabla f[g_{\mathbf{x}}(t)]\mid g'_{\mathbf{x}}(t)\rangle=\langle\nabla f[\mathbf{x}+t\theta(\mathbf{x})]\ \mid\theta(\mathbf{x})\rangle.$$

The Fundamental Theorem of Calculus [33, §7.16] gives $\int_0^1[\varphi'(t)-\varphi'(0)]dt=\varphi(1)-\varphi(0)-\varphi'(0)$ thus for any $\mathbf{x}\in\mathbb{R}^n$, we obtain:

$$\int_0^1\langle\nabla f[\mathbf{x}+t\theta(\mathbf{x})]-\nabla f(\mathbf{x})\ \mid\theta(\mathbf{x})\rangle\,dt=f[\mathbf{x}+\theta(\mathbf{x})]-f(\mathbf{x})-\langle\nabla f(\mathbf{x})\ \mid\theta(\mathbf{x})\rangle.$$

Then, it comes successively:

$$\begin{aligned}\int_{\mathbb{R}^n} |R_f(\theta)| &= \int_{\mathbb{R}^n} \left| \int_0^1 \langle \nabla f\left[\mathbf{x} + t\theta\left(\mathbf{x}\right)\right] - \nabla f\left(\mathbf{x}\right) \mid \theta\left(\mathbf{x}\right)\rangle \, dt \right| d\mathbf{x} \\ &\leqslant \int_{\mathbb{R}^n} |\theta\left(\mathbf{x}\right)| \left(\int_0^1 |\nabla f\left[\mathbf{x} + t\theta\left(\mathbf{x}\right)\right] - \nabla f\left(\mathbf{x}\right)| dt \right) d\mathbf{x}.\end{aligned}$$

Hence, using the Fubini-Tonelli Theorem [33, §8.8 Theorem], we have established that:

$$\forall f \in C_c^\infty(\mathbb{R}^n, \mathbb{R}), \quad \|R_f(\theta)\|_{L^1(\mathbb{R}^n,\mathbb{R})} \leqslant \|\theta\|_{1,\infty} \int_0^1 \left(\int_{\mathbb{R}^n} |\nabla f\left[\mathbf{x} + t\theta\left(\mathbf{x}\right)\right] - \nabla f\left(\mathbf{x}\right)| dt \right) d\mathbf{x}. \quad (71)$$

We now assume that $f \in W^{1,1}$ and we show that (71) still holds true by a density argument. Indeed, there exists a sequence $(f_i)_{i\in\mathbb{N}}$ of smooth maps with compact support converging to f in the $W^{1,1}$-norm [5, Theorem 9.2]. Let $i \in \mathbb{N}$. We get from (71) applied to f_i:

$$\|R_f(\theta)\|_{L^1(\mathbb{R}^n,\mathbb{R})} \leqslant \|R_f(\theta) - R_{f_i}(\theta)\|_{L^1(\mathbb{R}^n,\mathbb{R})} + \|\theta\|_{1,\infty} \underbrace{\int_0^1 \left(\int_{\mathbb{R}^n} |\nabla f_i\left[\mathbf{x} + t\theta\left(\mathbf{x}\right)\right] - \nabla f_i\left(\mathbf{x}\right)| dt \right) d\mathbf{x}}_{:=\widetilde{R}_{f_i}(\theta)}.$$

On the one hand, we combine relation (68) applied to the maps $f_i - f$ and θ, with observation (70) applied to $\nabla(f_i - f)$ in order to obtain:

$$\|R_f(\theta) - R_{f_i}(\theta)\|_{L^1(\mathbb{R}^n,\mathbb{R})} \leqslant \left[1 + \frac{n!}{(1 - \|\theta\|_{0,1})^n}\right] \|f_i - f\|_{L^1(\mathbb{R}^n,\mathbb{R})} + \|\theta\|_\infty \|\nabla f_i - \nabla f\|_1.$$

On the other hand, we combine relation (68) applied to $\nabla(f_i - f)$ and $t\theta$ in order to get:

$$\widetilde{R}_{f_i}(\theta) \leqslant \widetilde{R}_f(\theta) + \left[1 + \int_0^1 \frac{n!}{(1 - \|t\theta\|_{0,1})^n} dt\right] \|\nabla f_i - \nabla f\|_1.$$

Therefore, from these two last inequalities, we deduce that:

$$\|R_f(\theta)\|_{L^1(\mathbb{R}^n,\mathbb{R})} \leqslant \|\theta\|_{1,\infty} \widetilde{R}_f(\theta) + \left[1 + 2\|\theta\|_{1,\infty} + n! \frac{1 + \|\theta\|_{1,\infty}}{(1 - \|\theta\|_{1,\infty})^n}\right] \|f_i - f\|_{1,1}.$$

By letting $i \to +\infty$, we have obtained that relation (71) holds true for any $f \in W^{1,1}$. Finally, it only remains to prove that $|\widetilde{R}_f(\theta)| \to 0$ as $\|\theta\|_{1,\infty} \to 0$ in order to conclude about the differentiability of the map $\theta \in W^{1,\infty} \mapsto f \circ (I + \theta) \in L^1(\mathbb{R}^n, \mathbb{R})$ at the origin. Again, we are using a density argument. Let $f \in W^{1,1}$ and $\theta \in W^{1,\infty}$ be such that $\|\theta\|_{1,\infty} \leqslant \frac{1}{2}$. There exists a sequence $(f_i)_{i\in\mathbb{N}}$ of smooth maps with compact support converging to f in $W^{1,1}$. Let $i \in \mathbb{N}$. As before, we get from the triangle inequality and relation (68) applied to the maps $\nabla(f_i - f)$ and $t\theta$:

$$|\widetilde{R}_f(\theta)| \leqslant \widetilde{R}_{f_i}(\theta) + \left[1 + \frac{n!}{(1 - \|\theta\|_{1,\infty})^n}\right] \|f_i - f\|_{1,1} \leqslant \widetilde{R}_{f_i}(\theta) + (1 + 2^n n!) \|f_i - f\|_{1,1}.$$

Moreover, since f_i is smooth with compact support, we have:

$$\widetilde{R}_{f_i}(\theta) := \int_0^1 \left(\int_{\mathbb{R}^n} |\nabla f_i\left[\mathbf{x} + t\theta\left(\mathbf{x}\right)\right] - \nabla f_i\left(\mathbf{x}\right)| dt \right) d\mathbf{x} \leqslant \mathcal{L}^n\left(\operatorname{supp} f_i\right) \|\theta\|_{1,\infty} \|\nabla f_i\|_{0,1}.$$

Let $\varepsilon > 0$. There exists $I \in \mathbb{N}$ such that $\|f_I - f\|_{1,1} \leqslant \frac{\varepsilon}{2(1+2^n n!)}$. We set:

$$\delta := \min\{\frac{1}{2}, \frac{\varepsilon}{2\mathcal{L}^n\left(\operatorname{supp} f_I\right) \|\nabla f_I\|_{0,1}}\}.$$

Consequently, for any $\theta \in W^{1,\infty}$ such that $\|\theta\|_{1,\infty} < \delta$, we have obtained $|\widetilde{R}_f(\theta)| \leqslant \varepsilon$ as required. To conclude, $|\widetilde{R}_f(\theta)| \to 0$ as $\|\theta\|_{1,\infty} \to 0$ so the map $\theta \in W^{1,\infty} \mapsto f \circ (I + \theta) \in L^1(\mathbb{R}^n, \mathbb{R})$ is differentiable at the origin, and its differential is given by $\theta \in W^{1,\infty} \mapsto \langle \nabla f \mid \theta \rangle \in L^1(\mathbb{R}^n, \mathbb{R})$. $\square$

Conclusion

In this article, we have derived various formulas (43) (49) (50) (54) (5) (56) for the shape derivatives of a volume integral, depending on the regularity of the domain. In particular, we have proved that $C^{1,1}$-regularity is enough to define a notion (6)–(7) of partial derivatives with respect to the domain at any order higher than two, while the Lipschitz regularity is enough to define a shape gradient. Then, we have applied these results in order to obtain the fine shape differentiability properties associated with (1) and sum up in Table 1. These results have important applications in Quantum Chemistry for the model of Maximal Probability domains (MPDs).

Finally, we conclude by giving some numerical considerations associated with the formula (21), which is *a priori* computable by Quantum-Monte-Carlo methods. However, we have seen that it can also involve integrals (2)–(3) on the boundary of a domain, which has zero measure from a probabilistic point of view. However, the shape gradient (26), shape Hessian (35), and the kernel (34) of p_ν are $(n-1)$- or $(n-2)$-dimensional volume integrals. In particular, they can be reasonably computed by Quantum-Monte-Carlo methods. In a future work, we will consider the specific case of wave functions given by a sum of Slater determinants with some numerical applications.

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[1] Institut des Sciences du Calcul et des Données (ISCD), Université Pierre et Marie Curie (UPMC), Tours 33-34, 4 place Jussieu, boîte courrier 380, 75252 Paris Cedex 5, France.

[2] Laboratoire de Chimie Théorique (LCT), Université Pierre et Marie Curie (UPMC), Tours 12-13 4ième étage CC-137, 4 place Jussieu, 75252 Paris Cedex 5, France.

[3] Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique (CERMICS), Ecole Nationale des Ponts et Chaussées (ENPC), Bâtiment Coriolis, 6-8 Avenue Blaise Pascal, Cité Descartes - Champs sur Marne, 77455 Marne la Vallée Cedex 2, France.

[4] Centro de Modelamiento Matemático, Facultad de Ciencas Físicas y Matemáticas (FCFM), UMR 2071 CNRS-Universidad de Chile, Beauchef 851, Santiago, Chile.

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