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ANALYZING SMOOTH AND SINGULAR DOMAIN PERTURBATIONS IN LEVEL SET METHODS*

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Abstract. In the standard level set method, the evolution of the level set function is determined by solving the Hamilton–Jacobi equation, which is derived by considering smooth boundary perturbations of the zero level set. The converse approach is to consider smooth perturbations of the level set function and to find the corresponding perturbations of the zero level set. In this paper, we show how the latter approach allows us to analyze not only smooth perturbations of the level set, but also singular perturbations in the form of topological changes. In particular, it is an appropriate framework for analyzing splitting and merging of components. In this way, we establish a link between the Gâteaux derivative with respect to the level set function and the shape and topological derivatives. In the smooth case, we determine a transformation of the zero level set, defined as the flow of a vector field, which corresponds to the perturbation of the level set function. For topological changes, we study the cases of splitting or merging and creation of an island or a hole, and provide asymptotic expansions of volume and boundary integrals.

Key words. level set method, shape optimization, topological derivative, asymptotic analysis

AMS subject classifications. 49Q10, 49Q12, 65K10

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1. Introduction.

Since its inception, the level set method [25, 27] has proven extremely popular for numerical modeling of complex shape evolutions. The principal reason for its popularity is the ability to perform topological changes such as merging and splitting of two shapes in a simple way, thanks to the implicit representation of the geometry. Indeed, in prior boundary variation-based methods for modeling shape evolution, such as splines or explicit boundary parameterizations, performing topological changes was tedious.

The foundation of the original level set algorithm, as presented in [25, 27], is an *evolution approach*. Given a vector field V perturbing the zero level set $\Omega_{\varphi(\cdot,0)}$ of an initial level set function $\varphi(\cdot,0)$, the evolution of φ is determined by a Hamilton–Jacobi equation

$$\partial_t\varphi(x,t) + V(x)\cdot\nabla\varphi(x,t) = 0, \tag{1}$$

which is obtained by differentiating $\varphi(x(t),t)$ with respect to t, for a particle $x(t)$ on the boundary $\partial\Omega_{\varphi(\cdot,t)}$, moving with speed V. An aspect which is rarely discussed in the literature is that the assumption that the particle $x(t)$ is moving with a regular speed V implies that one is considering a smooth perturbation of the zero level set $\Omega_{\varphi(\cdot,0)}$, in the sense that the corresponding transformation of $\Omega_{\varphi(\cdot,0)}$ is a diffeomorphism; see, for instance, [8, section 9.4.3, p. 29]. Therefore, it seems that topological changes should not occur when solving (1). However, numerical methods for solving (1) are based on a notion of weak solutions, the so-called viscosity solutions, which do not necessarily satisfy (1) everywhere. In particular, (1) is typically not satisfied at a point where a topological change occurs. The drawback for shape optimization

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problems is that, when V is chosen to provide a descent direction for a given cost functional considering smooth boundary perturbations, the viscosity solution will not necessarily lead to a decrease of the cost functional, in particular when a topological change of $\Omega_{\varphi(\cdot,t)}$ occurs. Therefore, there is a gap between the desired update of the level set function and the actual evolution of the shape in the numerical practice, which has rarely been addressed in the literature so far; see, however, [2, 17], which we discuss further.

The converse approach consists in considering perturbations $\phi + th$ of a level set function ϕ, which now depends only on x, and determining the corresponding perturbation $\Omega_{\phi+th}$ of Ω_ϕ. If smooth perturbations of Ω_ϕ are implicitly assumed, then the perturbed level set $\Omega_{\phi+th}$ can be described using the flow of a vector field $V = V(h)$. Thus, for smooth perturbations of Ω_ϕ, this approach is equivalent to the evolution approach. However, it is easily observed that a smooth perturbation $\phi + th$ of ϕ can also lead to a topological change of Ω_ϕ such as merging and splitting. Therefore, this framework is appropriate to analyze topological changes in the level set method. The approach of perturbing ϕ rather than Ω_ϕ is common in the literature on level set methods; its origin can be traced to [31] (see also [7, 9, 26] or [30] for a review). However, it has been used only for analyzing smooth boundary perturbations. Roughly speaking, one usually represents integrals on Ω_ϕ using $H(\phi)$, where H is the Heaviside function, and upon differentiating with respect to ϕ, a Dirac mass $\delta(\phi)$ appears, which yields integrals on the boundary $\partial\Omega_\phi$. Although not explicitly stated, this implies that smooth boundary perturbations of Ω_ϕ are considered. These two approaches have also been studied in the calculus of variations, where both perturbations of the dependent variable and perturbations of the domain via diffeomorphisms are considered; see [15, Chapter 3]. The aim of the present paper is to perform a rigorous mathematical study of the approach based on perturbing ϕ, and to show how it allows one to analyze and model smooth perturbations as well as topological changes of Ω_ϕ.

The analysis of topological changes in the level set method is an important issue for the study of the convergence of the method for shape optimization problems. It is also important for numerical methods; indeed, even if topological changes by merging and splitting occur naturally in the numerics, the variation of the cost functional is not under control if the analysis of the topological change is not performed. In particular, for the task of minimizing some objective functional, the analysis allows one to determine whether or not a specific topological change has the effect of decreasing the functional.

The framework presented in the present paper has several interesting features. First of all, since ϕ is the variable and lives in a vector space, the usual notions of differentiation are available, such as the Fréchet and Gâteaux derivatives of the functional. One of the main features of the present paper is to precisely relate the Gâteaux derivative with respect to ϕ of a general objective functional with the shape and topological derivatives; see [28, 29]. This provides a unified notion of domain derivative, since we show that the Gâteaux derivative for smooth perturbations of ϕ may correspond to the shape derivative or to the topological derivative, depending on the configuration. Also, we relax the standard condition of the level set method, i.e., that ϕ be a distance function in a neighborhood of $\partial\Omega_\phi$, by letting ϕ be any function with a nonvanishing gradient on the boundary. When we want to consider topological changes, we slightly relax this condition by allowing $|\nabla\phi|$ to vanish at isolated points of the boundary. Still, the gradient should not vanish on a set of positive measure intersecting the boundary; otherwise, one could not guarantee the differentiability of the cost functional, and the model would be pointless. When ϕ does not have critical points on $\partial\Omega_\phi$, small perturbations of ϕ lead to smooth perturbations of Ω_ϕ.

Even if this framework allows one to analyze topological changes, the question of the differentiability of a general cost functional $J(\phi)$ with respect to these topological changes remains challenging. The purpose of this paper is to study quantitatively the continuity and differentiability properties of certain cost functionals $J(\phi)$. For topological changes by merging/splitting, we study the two-dimensional case, which is more singular than for higher dimensions, and leads to nondifferentiability of the functional; see [17].

Topological changes for level set methods have been analyzed in [2, 17]. In [17], differentiability properties of the volume of the zero level set Ω_ϕ with respect to perturbations of ϕ are obtained in dimension $d \geq 2$. However, asymptotic expansions of the cost functionals are not computed. In the present paper, we are interested in quantitative results, as we have the application to optimization problems in mind. Thus, we compute the first term of the asymptotic expansion for cost functionals defined as volume or boundary integrals. In [2, 3], a different approach to level set methods is introduced, which does not rely on the Hamilton–Jacobi equations and smooth perturbations of the domain, but is based instead on the *topological derivative* [28]. In these papers, the functional also depends on ϕ, and the authors consider both smooth boundary perturbations resulting from perturbations of the level set function and topological changes in the form of drilling a hole, but topological changes of the type splitting/merging are not studied. To compute asymptotic expansions for shape functionals defined as volume integrals in [2], the author uses the coarea formula. Here we use a different approach, based on the implicit function theorem.

We also mention phase field models, where a diffusive layer with positive thickness models the interface, as an alternative to level set methods. The main advantage is that topological changes occur naturally in this framework, also for multiphase problems, and the sensitivity of the cost functional is easier to compute than in level set methods. The principal drawback is that the front location is represented only approximately. The thickness of the diffusive layer can be driven to zero to simulate the sharp interface, but this is costly from the numerical point of view. From the analytical point of view the study of the sharp interface limit requires an asymptotic analysis which can also be involved. It is actually an active field of research in the phase-field community; see, for instance, [4, 24] for the Allen–Cahn/Cahn–Hilliard system, [5] for structural optimization, and also [11, 14].

The first part of the present paper, from section 2 to the end of section 3, is dedicated to a thorough analysis of the smooth case. We show how the smooth perturbation of Ω_ϕ generated by a perturbation of ϕ can be described by the flow of a nonautonomous vector field V. In this way, we can relate the Gâteaux derivative of the objective functional with the shape derivative of the corresponding shape functional.

The second part of the paper, corresponding to section 4, deals with the analysis of the singular case, i.e., the case where $\nabla\phi$ may vanish at isolated points on the boundary $\partial\Omega_\phi$. In this case, topological changes such as splitting/merging or creation of an island/hole may occur. For the creation of a hole or an island, we provide an asymptotic expansion of the cost functional and establish a link with the notion of topological derivative. For splitting/merging, we study the two-dimensional case for volume and boundary integrals. We show that the cost functionals are not differentiable but are continuous with respect to the splitting/merging, and we provide an asymptotic expansion. The main ingredient for analyzing the case of splitting/merging is to use a parameterized Morse lemma, to transform ϕ into a quadratic function locally around a nondegenerate critical point.

2. Shape derivative. In shape optimization, one studies continuity and differentiability properties of *shape functionals* $\mathcal{J} : \Omega \mapsto \mathcal{J}(\Omega) \in \mathbb{R}$, where $\Omega \subset \mathbb{R}^d$. The concept of *shape derivative* [8, 29] is based on the *speed method* (also known as the *velocity method*), which is used for building a parameterized family of shapes Ω_t. When $\Omega = \Omega_\phi$ is the subzero level set of a smooth function ϕ, we can consider ϕ as the variable; i.e., we introduce the functional $J(\phi) := \mathcal{J}(\Omega_\phi)$. The objective of sections 2 and 3 is to determine the flow of the subzero level set Ω_ϕ, as expressed in the speed method, which corresponds to a small perturbation of ϕ. In this way, we can relate the Gâteaux derivative of J with respect to ϕ with the shape derivative of $\mathcal{J}(\Omega_\phi)$.

First we recall the notions of Eulerian semiderivative and shape derivative of a shape functional. Let $\mathscr{P}(\mathcal{D})$ be the set of subsets of $\mathcal{D} \subset \mathbb{R}^d$ compactly contained in $\mathcal{D}$, where $\mathcal{D} \subset \mathbb{R}^d$ is open and bounded. In this paper, we use the notation V for nonautonomous vector fields, i.e., vector fields which depend on t, and θ for autonomous vector fields. Define for $k \geq 0$ and $0 \leq \alpha \leq 1$

$$\mathcal{C}_c^{k,\alpha}(\mathcal{D}, \mathbb{R}^d) := \{\theta \in \mathcal{C}^{k,\alpha}(\mathcal{D}, \mathbb{R}^d) \mid \theta \text{ has compact support in } \mathcal{D}\}, \tag{2}$$

and define $\mathcal{C}_c^k(\mathcal{D}, \mathbb{R}^d)$ in a similar way. For $\tau > 0$, consider a vector field $V \in \mathcal{C}([0,\tau]; \mathcal{C}_c^{0,1}(\mathcal{D}, \mathbb{R}^d))$ and the associated flow $T_t^V : \mathcal{D} \to \mathbb{R}^d$, $t \in [0,\tau]$, defined for each $x_0 \in \mathcal{D}$ as $T_t^V(x_0) := x(t)$, where $x : [0,\tau] \to \mathbb{R}^d$ solves

$$\dot{x}(t) = V(x(t), t) \quad \text{for } t \in [0,\tau], \quad x(0) = x_0. \tag{3}$$

We will use the simpler notation $T_t = T_t^V$ when no confusion is possible. Since $V(\cdot, t) \in \mathcal{C}_c^{0,1}(\mathcal{D}, \mathbb{R}^d)$, we have by Nagumo's theorem [22] that for fixed $t \in [0,\tau]$ the flow T_t is a homeomorphism from $\mathcal{D}$ onto itself, and maps boundary onto boundary and interior onto interior. We also introduce the family of perturbed domains

$$\Omega_t := T_t^V(\Omega). \tag{4}$$

The following definitions can be found in [8].

Definition 2.1. *Let $\mathcal{J} : \mathscr{P}_0 \to \mathbb{R}$ be a shape function defined on some admissible set $\mathscr{P}_0 \subset \mathscr{P}(\mathcal{D})$:*

(i) *The Eulerian semiderivative of $\mathcal{J}$ at Ω in direction $V \in \mathcal{C}([0,\tau]; \mathcal{C}_c^{0,1}(\mathcal{D}, \mathbb{R}^d))$ is defined by, when the limit exists,*

$$d_E\mathcal{J}(\Omega)(V) := \lim_{t \searrow 0} \frac{\mathcal{J}(\Omega_t) - \mathcal{J}(\Omega)}{t}. \tag{5}$$

For $\theta \in \mathcal{C}_c^{0,1}(\mathcal{D}, \mathbb{R}^d)$ and $\Omega_t := T_t^\theta(\Omega)$, we define the Eulerian semiderivative $d_E\mathcal{J}(\Omega)(\theta)$ in the same way.

(ii) *$\mathcal{J}$ is shape differentiable at Ω if it has a Eulerian semiderivative at Ω for all $V \in \mathcal{C}([0,\tau]; \mathcal{C}_c^\infty(\mathcal{D}, \mathbb{R}^d))$ and the mapping*

$$d_E\mathcal{J}(\Omega) : \mathcal{C}([0,\tau]; \mathcal{C}_c^\infty(\mathcal{D}, \mathbb{R}^d)) \to \mathbb{R},\ V \mapsto d_E\mathcal{J}(\Omega)(V)$$

is linear and continuous. In this case, we define the shape derivative $d\mathcal{J}(\Omega)$ as $d\mathcal{J}(\Omega) := d_E\mathcal{J}(\Omega)$.

The following well-known result shows that the Eulerian semiderivative in direction V only depends on $V(\cdot, 0)$ if it is continuous in the appropriate topology. This result will be useful to prove Theorem 3, which states that the shape derivative of a shape function $\mathcal{J}(\Omega)$ coincides with its Gâteaux derivative with respect to a function ϕ when Ω is defined as the zero sublevel set of ϕ.

THEOREM 1. *Let $k \geq 0$. If for all $V \in \mathcal{C}([0,\tau];\mathcal{C}_c^k(\mathcal{D},\mathbb{R}^d))$, $d_E\mathcal{J}(\Omega)(V)$ exists and the map $V \mapsto d_E\mathcal{J}(\Omega)(V) : \mathcal{C}([0,\tau];\mathcal{C}_c^k(\mathcal{D},\mathbb{R}^d)) \to \mathbb{R}$ is continuous, then*

$$d_E\mathcal{J}(\Omega)(V(\cdot,0)) = d_E\mathcal{J}(\Omega)(V) \quad \text{for all } V \in \mathcal{C}([0,\tau];\mathcal{C}_c^k(\mathcal{D},\mathbb{R}^d)).$$

Proof. See [8, Theorem 3.1(ii), p. 474]. ∎

Next we recall the structure theorem of Zolésio, which states that the shape derivative only depends on the normal component of the trace of the perturbation field on $\partial\Omega$. This result will also be useful for the proof of Theorem 3.

THEOREM 2 (structure theorem). *Assume $\partial\Omega$ is compact and of class $\mathcal{C}^{k+1}$, $k \geq 0$. Assuming $\mathcal{J}$ is shape differentiable at Ω and the shape derivative $d\mathcal{J}(\Omega)$ is continuous for the $\mathcal{C}_c^k(\mathcal{D},\mathbb{R}^d)$-topology, then there exists a linear and continuous functional $g : \mathcal{C}^k(\partial\Omega) \to \mathbb{R}$ such that for all $\theta \in \mathcal{C}_c^k(\mathcal{D},\mathbb{R}^d)$,*

$$d\mathcal{J}(\Omega)(\theta) = g(\theta_{|\partial\Omega} \cdot n). \tag{6}$$

Proof. See [8, Corollary 1, pp. 480–481]. ∎

Notation. We use D for derivatives (or partial derivatives) with respect to the space variable x and D^2 for the second derivative with respect to x. When the function is scalar, we use ∇ instead of D for the first derivative with respect to x. The notation $(\cdot)^\mathsf{T}$ is used for the transpose of a matrix and $(\cdot)^{-\mathsf{T}}$ for the transpose of the inverse. We denote by $\mathbb{1} : \mathbb{R}^d \to \mathbb{R}^d, x \mapsto x$ the identity and by χ_A the indicator function of a set A. We denote by $x \mapsto \mathrm{ch}(x)$ the hyperbolic cosine function and by $x \mapsto \mathrm{sh}(x)$ the hyperbolic sine function. Throughout the paper we denote by c a generic positive constant which may vary from line to line.

3. Geometric flow corresponding to perturbations of the level set function.

Let $\Omega_\phi := \{x \in \mathcal{D} \mid \phi(x) < 0\}$, where $\phi \in \mathcal{C}^\infty(\mathbb{R}^d)$. In the rest of the paper, we will use the simpler notation $\Omega_\phi = \{\phi < 0\}$. In the paper, we assume that the boundary $\partial\Omega_\phi = \{\phi = 0\}$ does not intersect $\partial\mathcal{D}$. Given a shape functional $\mathcal{J}$, we may recast it as a functional of the level set function ϕ by introducing $J(\phi) := \mathcal{J}(\Omega_\phi)$. Typical functionals considered in this context are

$$J_1(\phi) = \int_{\Omega_\phi} F_1(x, u_\phi(x), \nabla u_\phi(x))\, dx \quad \text{and} \quad J_2(\phi) = \int_{\partial\Omega_\phi} F_2(x, u_\phi(x), \nabla u_\phi(x))\, ds_x,$$

where u_ϕ is a function which depends on ϕ through Ω_ϕ. Often, u_ϕ is the solution of a partial differential equation. In this paper, we treat the cases where F_1 and F_2 only depend on x and not on u_ϕ.

The advantage of recasting $\mathcal{J}$ as a function of ϕ is that we have access to the standard notions of derivatives in vector spaces. Let us assume for simplicity that $\phi \in H(\mathcal{D})$, where $H(\mathcal{D})$ is a vector space of functions on $\mathcal{D}$. For $h \in H(\mathcal{D})$, the *Gâteaux semiderivative* of J at ϕ in the direction h is defined as, if the limit exists,

$$d_G J(\phi)(h) := \lim_{t \searrow 0} \frac{J(\phi + th) - J(\phi)}{t}.$$

The functional J has a *Gâteaux derivative* if $h \mapsto d_G J(\phi)(h)$ is linear and continuous.

We may also define the *Fréchet derivative* $d_F J(\phi)(h)$ as

$$J(\phi + h) = J(\phi) + d_F J(\phi)(h) + o(\|h\|_{H(\mathcal{D})}).$$

In fact, all the usual notions of differentiation in vector spaces are available in this framework.

In this section, we study the case $|\nabla\phi| > 0$ on $\partial\Omega_\phi$. We show that the Gâteaux derivative of J corresponds to the shape derivative of $\mathcal{J}$ for certain vector fields θ depending on h. This is the main result of this section; see Theorem 3. For this, we first determine in Lemma 3.2 the geometric flow of the domain Ω_ϕ corresponding to perturbations $\phi + th$ of the level set function ϕ; i.e., we determine a transformation T which is the flow of a nonautonomous vector field V such that $\Omega_{\phi+th} = T(\Omega_\phi, t)$. When $|\nabla\phi|$ vanishes at an isolated point of $\partial\Omega_\phi$, a perturbation of ϕ may generate a topological change of Ω_ϕ, and the situation is more involved. In this case, the Gâteaux derivative of J does not always exist; see section 4. We start with a lemma which provides the auxiliary function $\bar\alpha$ used to define T in Lemma 3.2.

LEMMA 3.1. *Assume $\phi, h \in \mathcal{C}^\infty(\mathcal{D})$, $\partial\Omega_\phi \subset \mathcal{D}$, and $|\nabla\phi| > 0$ on $\partial\Omega_\phi$. Then there exist $\tau_0 > 0$ and a $\mathcal{C}^\infty$ function $\bar\alpha : \mathcal{D} \times (-\tau_0, \tau_0) \to \mathbb{R}$ satisfying the following:*
(i) *$\bar\alpha(x, 0) = 0$ for all $x \in \mathcal{D}$.*
(ii) *$\bar\alpha(\cdot, t) \in \mathcal{C}_c^\infty(\mathcal{D})$ for all $t \in (-\tau_0, \tau_0)$.*
(iii) *$(\phi + th)(x + \bar\alpha(x, t)\nabla\phi(x)) = 0$ for all $x \in \partial\Omega_\phi$ and $t \in (-\tau_0, \tau_0)$.*
(iv) *$\partial_t\bar\alpha(x, 0) = -h(x)|\nabla\phi(x)|^{-2}$ for all $x \in \partial\Omega_\phi$.*

Proof. Let $x_0 \in \partial\Omega_\phi$, and let $B(0, 1)$ be the unit ball of $\mathbb{R}^d$. Let $\xi = (\xi', \xi_d) \in B(0, 1)$, with $\xi' = (\xi_1, \dots, \xi_{d-1})$. Since $\partial\Omega_\phi$ is $\mathcal{C}^\infty$, there exist a neighborhood X_{x_0} of x_0 and a bijective map $\zeta \in \mathcal{C}^\infty(B(0, 1), X_{x_0})$, with $\zeta^{-1} \in \mathcal{C}^\infty(X_{x_0}, B(0, 1))$ and $\zeta(0) = x_0$, such that $\zeta(B(0, 1) \cap \{\xi_d = 0\}) = \partial\Omega_\phi \cap X_{x_0}$ and $\zeta(B(0, 1) \cap \{\xi_d < 0\}) = \operatorname{int}(\Omega_\phi) \cap X_{x_0}$. We apply the implicit function theorem with

$$\begin{aligned}\Phi : (B(0, 1) \cap \{\xi_d = 0\}) \times \mathbb{R} \times \mathbb{R} \to \mathbb{R},&\\ (\xi', t, \alpha) \mapsto (\phi + th)(\zeta(\xi', 0) + \alpha\nabla\phi(\zeta(\xi', 0))).&\end{aligned}$$

Note that Φ is $\mathcal{C}^\infty$, and we have $\Phi(0, 0, 0) = \phi(\zeta(0)) = \phi(x_0) = 0$ since $x_0 \in \partial\Omega_\phi$. We compute

$$\partial_\alpha\Phi(0, 0, 0) = \nabla\phi(x_0) \cdot \nabla\phi(x_0) = |\nabla\phi(x_0)|^2 > 0.$$

As a consequence, the implicit function theorem yields the existence of a neighborhood $\mathcal{V}_{x_0} \times (-\tau_{x_0}, \tau_{x_0})$, where $\mathcal{V}_{x_0}$ is a neighborhood of 0 in $\mathbb{R}^{d-1}$, and of a unique function $\alpha : \mathcal{V}_{x_0} \times (-\tau_{x_0}, \tau_{x_0}) \to \mathbb{R}$ of class $\mathcal{C}^\infty$ such that $\alpha(0, 0) = 0$ and

$$\Phi(\xi', t, \alpha(\xi', t)) = (\phi + th)(\zeta(\xi', 0) + \alpha(\xi', t)\nabla\phi(\zeta(\xi', 0))) = 0. \tag{7}$$

Taking $t = 0$ in (7), we get

$$\Phi(\xi', 0, \alpha(\xi', 0)) = \phi(\zeta(\xi', 0) + \alpha(\xi', 0)\nabla\phi(\zeta(\xi', 0))) = 0,$$

which implies that $\zeta(\xi', 0) + \alpha(\xi', 0)\nabla\phi(\zeta(\xi', 0)) \in \partial\Omega_\phi$. Since $\zeta(\xi', 0) \in \partial\Omega_\phi$, we obtain $|\nabla\phi(\zeta(\xi', 0))| \neq 0$. Reducing the neighborhood $\mathcal{V}_{x_0}$ if necessary, we then necessarily have $\alpha(\xi', 0) = 0$ for all ξ' in $\mathcal{V}_{x_0}$. Now, taking the derivative with respect to t of (7) at $t = 0$, and using $\alpha(\xi', 0) = 0$, we compute

$$h(\zeta(\xi', 0)) + \nabla\phi(\zeta(\xi', 0)) \cdot (\partial_t\alpha(\xi', 0)\nabla\phi(\zeta(\xi', 0))) = 0,$$

which yields

$$\partial_t\alpha(\xi', 0) = -h(\zeta(\xi', 0))|\nabla\phi(\zeta(\xi', 0))|^{-2} \quad \text{for all } \xi' \in \mathcal{V}_{x_0}. \tag{8}$$

Note that (8) is well-defined since $|\nabla\phi(\zeta(\xi',0))| \neq 0$. Introduce the notations

$$\widehat{\zeta}(x) := (\zeta_1(x), \dots, \zeta_{d-1}(x)), \qquad \widehat{\zeta}^{-1}(x) := (\zeta_1^{-1}(x), \dots, \zeta_{d-1}^{-1}(x)),$$

where ζ_j, ζ_j^{-1}, $j = 1, \dots, d$, are the components of ζ and ζ^{-1}, respectively, and the function

$$\widehat{\alpha} : \widehat{\zeta}(\mathcal{V}_{x_0}) \times (-\tau_{x_0}, \tau_{x_0}) \to \mathbb{R}, \qquad (x,t) \mapsto \alpha(\widehat{\zeta}^{-1}(x), t),$$

which is $\mathcal{C}^\infty$ by composition. Although α and ζ depend on x_0, we can show, using the uniqueness of α, that $\widehat{\alpha}$ is actually independent of x_0. Since $\partial\Omega_\phi$ is compact, using a partition of unity and the independence of $\widehat{\alpha}$ on x_0, we can define the function $\widehat{\alpha} : \partial\Omega_\phi \times (-\tau_0, \tau_0) \to \mathbb{R}$ for some $\tau_0 > 0$. Then for some $x \in \partial\Omega_\phi$ there exist x_0, ζ, α, and a neighborhood $X_{x_0} \ni x$ defined as above so that $\zeta^{-1}(x) = (\xi', 0)$ and $\widehat{\zeta}^{-1}(x) = \xi'$ for some $\xi' \in \mathbb{R}^{d-1}$. This yields, in view of (7),

$$\begin{aligned} &(\phi + th)(x + \widehat{\alpha}(x,t)\nabla\phi(x)) \\ &= (\phi + th)(\zeta(\xi',0) + \alpha(\xi',t)\nabla\phi(\zeta(\xi',0))) = 0 \quad \text{for } x \in \partial\Omega_\phi \text{ and } t \in (-\tau_0, \tau_0). \end{aligned} \tag{9}$$

Since $\partial\Omega_\phi$ is also $\mathcal{C}^\infty$ and $\partial\Omega_\phi \subset \mathcal{D}$, we can extend $\widehat{\alpha}$ to a $\mathcal{C}^\infty$ function $\bar{\alpha} : \mathcal{D} \times (-\tau_0, \tau_0) \to \mathbb{R}$ which satisfies $\bar{\alpha}(x, 0) = 0$ for all $x \in \mathcal{D}$ and $\bar{\alpha}(\cdot, t) \in \mathcal{C}_c^\infty(\mathcal{D})$ for all $t \in (-\tau_0, \tau_0)$, which proves items (i) and (ii). Item (iii) is due to (9). Item (iv) is a consequence of (8) and $x = \zeta(\xi', 0)$ for $x \in \partial\Omega_\phi$. ∎

LEMMA 3.2. *Assume $\phi, h \in \mathcal{C}^\infty(\mathcal{D})$, $\partial\Omega_\phi \subset \mathcal{D}$, and $|\nabla\phi| > 0$ on $\partial\Omega_\phi$. Then there exist $\tau_1 > 0$ and a transformation $T : \mathcal{D} \times (-\tau_1, \tau_1) \to \mathcal{D}$ such that the following hold:*
- (i) *$T \in \mathcal{C}^\infty(\mathcal{D} \times (-\tau_1, \tau_1), \mathcal{D})$.*
- (ii) *$T(x, 0) = x$ for $x \in \mathcal{D}$, and $T(x,t) = x$ for $(x,t) \in \partial\mathcal{D} \times (-\tau_1, \tau_1)$.*
- (iii) *$\partial_t T(x, 0) = -h(x)|\nabla\phi(x)|^{-2}\nabla\phi(x)$ for $x \in \partial\Omega_\phi$.*
- (iv) *$T(\cdot, t) : \mathcal{D} \to \mathcal{D}$ is bijective for all $t \in (-\tau_1, \tau_1)$.*
- (v) *$T(\Omega_\phi, t) = \Omega_{\phi+th}$ for all $t \in (-\tau_1, \tau_1)$.*
- (vi) *$T(\partial\Omega_\phi, t) = \partial\Omega_{\phi+th}$ for all $t \in (-\tau_1, \tau_1)$.*

Proof. We start with the proof of items (i), (ii), and (iii). Define the function

$$\begin{aligned} T : \mathcal{D} \times (-\tau_0, \tau_0) &\to \mathbb{R}^d, \\ (x,t) &\mapsto x + \bar{\alpha}(x,t)\nabla\phi(x), \end{aligned} \tag{10}$$

where $\bar{\alpha}$ and τ_0 are given by Lemma 3.1. In view of item (iii) of Lemma 3.1, we have

$$T(x,t) \in \partial\Omega_{\phi+th} \quad \text{for } x \in \partial\Omega_\phi. \tag{11}$$

The function T is $\mathcal{C}^\infty$ since $\bar{\alpha}$ and ϕ are $\mathcal{C}^\infty$. In view of items (i) and (ii) of Lemma 3.1, it satisfies $T(x,0) = x$ for $x \in \mathcal{D}$, and $T(x,t) = x$ for $(x,t) \in \partial\mathcal{D} \times (-\tau_0, \tau_0)$. Then, in view of item (iv) of Lemma 3.1, we have

$$\partial_t T(x,0) = \partial_t\bar{\alpha}(x,0)\nabla\phi(x) = -h(x)|\nabla\phi(x)|^{-2}\nabla\phi(x) \quad \text{for } x \in \partial\Omega_\phi. \tag{12}$$

This proves items (i), (ii), and (iii) for $\tau_1 \le \tau_0$.

Proof of item (iv). First we prove surjectivity. For $y \in \mathcal{D}$, define $g(x,t) := y - \bar{\alpha}(x,t)\nabla\phi(x)$. Using that $\bar{\alpha}(x,0) = 0$ for all $x \in \mathcal{D}$ we have

$$Dg(x,0) = -D[\bar{\alpha}(x,t)\nabla\phi(x)]_{|t=0} = -\nabla\phi(x) \otimes \nabla\bar{\alpha}(x,0) - \bar{\alpha}(x,0)D^2\phi(x) = 0.$$

This yields

$$
\begin{aligned}
&|g(x_1,t)-g(x_2,t)| = |Dg(x_2+\eta_x(x_1-x_2),t)(x_1-x_2)|\\
&= |Dg(x_2+\eta_x(x_1-x_2),0)(x_1-x_2) + tD\partial_t g(x_2+\eta_x(x_1-x_2),\eta_t t)(x_1-x_2)|\\
&= |tD\partial_t g(x_2+\eta_x(x_1-x_2),\eta_t t)(x_1-x_2)|,
\end{aligned}
$$

where $\eta_x \in (0,1)$ and $\eta_t \in (0,1)$. Thus we obtain, for $|t| \le \bar\tau_1 \le \tau_0$,

$$|g(x_1,t)-g(x_2,t)| \le |x_1-x_2|\cdot|t|\cdot\|D\partial_t(\bar\alpha\nabla\phi)\|_{L^\infty(\mathcal{D}\times(-\bar\tau_1,\bar\tau_1))}.$$

We can choose $\bar\tau_1 \le \tau_0$ sufficiently small to obtain $|t|\cdot\|D\partial_t(\bar\alpha\nabla\phi)\|_{L^\infty(\mathcal{D}\times(-\bar\tau_1,\bar\tau_1))} < 1$ for all $|t| \le \bar\tau_1$. Thus, for fixed t, g is a contraction on $\mathcal{D}$, which implies that there exists a fixed point $x \in \mathcal{D}$ such that $g(x,t) = x$, which yields $T(x,t) = x + \bar\alpha(x,t)\nabla\phi(x) = y$, so this shows that $T(\cdot,t) : \mathcal{D} \to \mathcal{D}$ is surjective.

Now we prove injectivity. Let x_1 and x_2 in $\mathcal{D}$ be such that

$$T(x_1,t) = x_1 + \bar\alpha(x_1,t)\nabla\phi(x_1) = x_2 + \bar\alpha(x_2,t)\nabla\phi(x_2) = T(x_2,t).$$

Similarly to the proof for surjectivity, this yields

$$
\begin{aligned}
|x_1-x_2| &= |\bar\alpha(x_1,t)\nabla\phi(x_1) - \bar\alpha(x_2,t)\nabla\phi(x_2)|\\
&\le |x_1-x_2|\cdot|t|\cdot\|D\partial_t(\bar\alpha\nabla\phi)\|_{L^\infty(\mathcal{D}\times(-\bar\tau_1,\bar\tau_1))} \le L|x_1-x_2|,
\end{aligned}
$$

where $L < 1$ for $\bar\tau_1$ small enough. Thus, we must have $x_1 = x_2$, which proves the injectivity, and so the bijectivity of $T(\cdot,t) : \mathcal{D} \to \mathcal{D}$ is proved for $\tau_1 \le \bar\tau_1$.

Proof of items (v) *and* (vi). Now we prove that $T(\Omega_\phi,t) = \Omega_{\phi+th}$. Define

$$S_\varepsilon := \{x \in \Omega_\phi \mid 0 < d(x,\partial\Omega_\phi) < \varepsilon\},$$

where $d(x,\partial\Omega_\phi)$ is the distance of x to the set $\partial\Omega_\phi$. Since Ω_ϕ is $\mathcal{C}^\infty$, and since $\phi(x) = 0$ and $|\nabla\phi(x)| \ne 0$ for $x \in \partial\Omega_\phi$, there exists $\varepsilon_0 > 0$ such that for $\varepsilon \le \varepsilon_0$, for each $x \in S_\varepsilon$, there exists a unique projection $x_0 \in \partial\Omega_\phi$ of x on $\partial\Omega_\phi$ and we have

$$x = x_0 - \frac{|x-x_0|}{|\nabla\phi(x_0)|}\nabla\phi(x_0). \tag{13}$$

Let us assume that $0 < \varepsilon \le \varepsilon_0$, and introduce the function

$$\mathcal{P} : \mathcal{D}\times(-\bar\tau_1,\bar\tau_1) \to \mathbb{R}, \qquad (x,t) \mapsto (\phi+th)(T(x,t)),$$

which is $\mathcal{C}^\infty$ by composition. Let $x \in S_\varepsilon$, which implies $\phi(x) < 0$, and let x_0 be its unique projection on $\partial\Omega_\phi$. We have $\mathcal{P}(x_0,t) = (\phi+th)(T(x_0,t)) = 0$, which follows immediately from (11). We proceed with the following Taylor expansions:

$$
\begin{aligned}
\mathcal{P}(x,t) &= \mathcal{P}(x_0,t) + (x-x_0)\cdot\nabla\mathcal{P}(x_0+\eta(x-x_0),t)\\
&= (x-x_0)\cdot\nabla\mathcal{P}(x_0,0) + (x-x_0)\cdot[\nabla\mathcal{P}(x_0+\eta(x-x_0),t) - \nabla\mathcal{P}(x_0,0)]\\
&= (x-x_0)\cdot\nabla\mathcal{P}(x_0,0)\,(1+L), \qquad (14)
\end{aligned}
$$

with $\eta \in (0,1)$ and

$$L := \frac{(x-x_0)\cdot[\nabla\mathcal{P}(x_0+\eta(x-x_0),t) - \nabla\mathcal{P}(x_0,0)]}{(x-x_0)\cdot\nabla\mathcal{P}(x_0,0)}.$$

We also observe that

$$\nabla \mathcal{P}(x_0, 0) = DT(x_0, 0)^{\mathsf{T}} \nabla \phi(T(x_0, 0))$$

and

$$DT(x_0, t) = \mathcal{I} + \nabla \phi(x_0) \otimes \nabla \bar{\alpha}(x_0, t) + \bar{\alpha}(x_0, t) D^2 \phi(x_0),$$

where $\mathcal{I}$ is the identity matrix. Since $\bar{\alpha}(x, 0) = 0$ for all $x \in \mathcal{D}$, we have $\nabla \bar{\alpha}(x_0, 0) = 0$, so we get $DT(x_0, 0) = \mathcal{I}$ and $\nabla \mathcal{P}(x_0, 0) = \nabla \phi(x_0)$. In view of (13), we have

$$(x - x_0) \cdot \nabla \phi(x_0) = -|x - x_0| \cdot |\nabla \phi(x_0)| < 0 \quad \text{for } x \in S_\varepsilon. \tag{15}$$

Now we define the constant

$$\eta_1 := \min \left(\frac{1}{2} \frac{\inf_{\bar{x} \in \partial \Omega_\phi} |\nabla \phi(\bar{x})|}{\sup_{\bar{x} \in \overline{\mathcal{D}}, \bar{t} \in (-\bar{\tau}_1, \bar{\tau}_1)} \|D^2 \mathcal{P}(\bar{x}, \bar{t})\|_2 + \sup_{\bar{x} \in \overline{\mathcal{D}}, \bar{t} \in (-\bar{\tau}_1, \bar{\tau}_1)} |\partial_t \nabla \mathcal{P}(\bar{x}, \bar{t})|}, \bar{\tau}_1 \right).$$

Note that the two suprema in the definition of η_1 are finite since $\mathcal{P}$ is $\mathcal{C}^\infty$ and $\overline{\mathcal{D}}$ is compact. Thus, $\eta_1 > 0$ since $\inf_{\bar{x} \in \partial \Omega_\phi} |\nabla \phi(\bar{x})| > 0$ due to the compactness of $\partial \Omega_\phi$. If we choose $|t| \le \eta_1$ and $\varepsilon \le \eta_1$, then we obtain, using (15), $\eta \in (0, 1)$, $|x - x_0| < \varepsilon \le \eta_1$, and the definitions of η_1 and L, the estimate

$$\begin{aligned} |L| &\le \frac{|x - x_0| \cdot |\nabla \mathcal{P}(x_0 + \eta(x - x_0), t) - \nabla \mathcal{P}(x_0, 0)|}{|x - x_0| \cdot |\nabla \phi(x_0)|} \\ &\le \frac{|\eta(x - x_0)| \sup_{\bar{x} \in \overline{\mathcal{D}}, \bar{t} \in (-\bar{\tau}_1, \bar{\tau}_1)} \|D^2 \mathcal{P}(\bar{x}, \bar{t})\|_2 + |t| \sup_{\bar{x} \in \overline{\mathcal{D}}, \bar{t} \in (-\bar{\tau}_1, \bar{\tau}_1)} |\partial_t \nabla \mathcal{P}(\bar{x}, \bar{t})|}{\inf_{\bar{x} \in \partial \Omega_\phi} |\nabla \phi(\bar{x})|} \\ &\le \frac{\eta_1}{2\eta_1} < 1. \end{aligned}$$

Thus we get, using (14), (15) and $\nabla \bar{\alpha}(x_0, 0) = 0$, and taking into account $|t| \le \eta_1$ and $\varepsilon \le \eta_1$, that for $x \in S_\varepsilon$,

$$\mathcal{P}(x, t) = (\phi + th)(T(x, t)) = (x - x_0) \cdot \nabla \phi(x_0)\,(1 + L) = -|x - x_0| \cdot |\nabla \phi(x_0)|(1 + L) < 0.$$

This implies that

$$T(x, t) \in \Omega_{\phi + th} \quad \text{for all } |t| \le \eta_1 \text{ and } x \in S_\varepsilon. \tag{16}$$

Now define $K_\varepsilon := \Omega_\phi \backslash S_\varepsilon$. Clearly, K_ε is compact. Let $x \in K_\varepsilon$; then we have $\phi(x) < 0$, and since $\mathcal{P}$ is $\mathcal{C}^\infty$, there exists $\eta_0(x) > 0$ such that $\mathcal{P}(x, t) = (\phi + th)(T(x, t)) < 0$ for $|t| \le \eta_0(x)$. Since K_ε is compact, we have $\eta_2 := \min_{x \in K_\varepsilon} \eta_0(x) > 0$. Thus, for $|t| \le \eta_2$ and $x \in K_\varepsilon$ we get $(\phi + th)(T(x, t)) < 0$. This implies that

$$T(x, t) \in \Omega_{\phi + th} \quad \text{for all } |t| \le \eta_2 \text{ and } x \in K_\varepsilon. \tag{17}$$

Combining (16) and (17), we obtain

$$T(\Omega_\phi, t) \subset \Omega_{\phi + th} \quad \text{for all } |t| \le \min(\eta_1, \eta_2). \tag{18}$$

Using a similar argument, we can show that there exists $\eta_3, \eta_4 > 0$ such that

$$T(\mathcal{D} \setminus \overline{\Omega_\phi}, t) \subset \mathcal{D} \setminus \overline{\Omega_{\phi + th}} \quad \text{for all } |t| \le \min(\eta_3, \eta_4). \tag{19}$$

Choosing $\tau_1 = \min(\eta_1, \eta_2, \eta_3, \eta_4) > 0$, and combining (18) and (19), we show that

$$T(\Omega_\phi, t) = \Omega_{\phi+th} \quad \text{for all } |t| < \tau_1 \tag{20}$$

and

$$T(\mathcal{D} \setminus \overline{\Omega_\phi}, t) = \mathcal{D} \setminus \overline{\Omega_{\phi+th}} \quad \text{for all } |t| < \tau_1. \tag{21}$$

Indeed, assume $y \in \Omega_{\phi+th}$. Since $T(\cdot, t)$ is bijective for $t < \bar{\tau}_1$, there exists $x \in \mathcal{D}$ such that $y = T(x,t)$, and x cannot be in $\mathcal{D} \setminus \overline{\Omega_\phi}$; otherwise, $y = T(x,t) \in \mathcal{D} \setminus \overline{\Omega_{\phi+th}}$ in view of (19), so $x \in \overline{\Omega_\phi}$. Now if $x \in \partial\Omega_\phi$, then we have proved in (11) that $y = T(x,t) \in \partial\Omega_{\phi+th}$, which is also impossible since $y \in \Omega_{\phi+th}$. Thus, $x \in \Omega_\phi$ and we get (20). Property (21) is obtained in a similar way. Since $T(\cdot,t)$ is a bijection for $t < \bar{\tau}_1$ and by using $\tau_1 \leq \bar{\tau}_1$, we also get

$$T(\partial\Omega_\phi, t) = \partial\Omega_{\phi+th} \quad \text{for all } |t| < \tau_1.$$

This proves item (vi) and concludes the proof. □

Let T be given by Lemma 3.2. We will sometimes use the notation T_t instead of $T(\cdot,t)$ for convenience. We denote by T_t^{-1} the inverse function of T_t for fixed t. Let us introduce the $\mathcal{C}^\infty$ vector field

$$\begin{aligned} V : \mathcal{D} \times (-\tau_1, \tau_1) &\to \mathbb{R}^d, \\ (x,t) &\mapsto \partial_t \bar{\alpha}(T_t^{-1}(x), t) \nabla\phi(T_t^{-1}(x)), \end{aligned} \tag{22}$$

where $\bar{\alpha}$ is given by Lemma 3.1. Observe that

$$V(x,0) = \partial_t \bar{\alpha}(T_0^{-1}(x), 0) \nabla\phi(T_0^{-1}(x)) = \partial_t \bar{\alpha}(x,0) \nabla\phi(x) \tag{23}$$

and, in view of item (iv) of Lemma 3.1,

$$V(x,0) = -h(x) |\nabla\phi(x)|^{-2} \nabla\phi(x) \quad \text{for } x \in \partial\Omega_\phi. \tag{24}$$

This leads to the main result of this section.

THEOREM 3. *Let $\phi \in \mathcal{C}^\infty(\mathcal{D})$, and let $|\nabla\phi| > 0$ on $\partial\Omega_\phi$. Let $h \in \mathcal{C}^\infty(\mathcal{D})$ and $\theta \in \mathcal{C}^\infty(\mathcal{D}, \mathbb{R}^d)$ be such that*

$$\theta = -h |\nabla\phi|^{-2} \nabla\phi \quad \text{on } \partial\Omega_\phi. \tag{25}$$

Let $\mathcal{J}$ be a shape functional, and assume that $\mathcal{J}$ is shape differentiable at Ω_ϕ and that the shape derivative $d\mathcal{J}(\Omega_\phi)$ is continuous for the $\mathcal{C}_c^k(\mathcal{D}, \mathbb{R}^d)$-topology for some $k \geq 0$. Then $J(\phi) := \mathcal{J}(\Omega_\phi)$ has a Gâteaux derivative at ϕ in direction h, which is equal to the shape derivative of $\mathcal{J}$ at Ω_ϕ in direction θ, i.e.,

$$d_G J(\phi)(h) = d\mathcal{J}(\Omega_\phi)(\theta). \tag{26}$$

Proof. Let $\bar{\alpha}$ be given by Lemma 3.1, let T be given by Lemma 3.2, and define V using (22). Note first that $V(\cdot, 0)$ and θ coincide on $\partial\Omega_\phi$ due to (24) but need not be equal outside of $\partial\Omega_\phi$. In view of (22), we have $V(T(x,t),t) = \partial_t \bar{\alpha}(x,t) \nabla\phi(x) = \partial_t T(x,t)$. Thus, the restriction of T to $\mathcal{D} \times [0, \tau_1)$, still denoted by T for convenience, is the solution of

$$\begin{aligned} \partial_t T(x,t) &= V(T(x,t),t) \quad \text{for } (x,t) \in \mathcal{D} \times [0, \tau_1), \\ T(x,0) &= x \quad \text{for } x \in \mathcal{D}. \end{aligned} \tag{27}$$

By hypothesis, the shape derivative of $\mathcal{J}$ at Ω_ϕ in direction V exists and is given by (see Definition 2.1(ii))

$$d\mathcal{J}(\Omega_\phi)(V) = \lim_{t\searrow 0} \frac{\mathcal{J}(T_t(\Omega_\phi)) - \mathcal{J}(\Omega_\phi)}{t}.$$

Using Theorem 1, we have $d\mathcal{J}(\Omega_\phi)(V(\cdot,0)) = d\mathcal{J}(\Omega_\phi)(V)$. In view of Theorem 2, (23), and the fact that $\bar{\alpha}(\cdot,t) \in \mathcal{C}_c^\infty(\mathcal{D})$ for all $t \in (-\tau_0, \tau_0)$, there exists a function g such that $d\mathcal{J}(\Omega_\phi)(V(\cdot,0)) = g(V(\cdot,0)_{|\partial\Omega_\phi} \cdot n)$, where n is the unit outward normal vector to Ω_ϕ. Now, since V satisfies (24) and θ satisfies (25), we obtain

$$d\mathcal{J}(\Omega_\phi)(V(\cdot,0)) = g(V(\cdot,0)_{|\partial\Omega_\phi} \cdot n) = g(\theta_{|\partial\Omega_\phi} \cdot n) = d\mathcal{J}(\Omega_\phi)(\theta).$$

This allows us to write

$$\begin{aligned} d_G J(\phi)(h) &= \lim_{t\searrow 0} \frac{J(\phi + th) - J(\phi)}{t} = \lim_{t\searrow 0} \frac{\mathcal{J}(T_t(\Omega_\phi)) - \mathcal{J}(\Omega_\phi)}{t} \\ &= d\mathcal{J}(\Omega_\phi)(V(\cdot,0)) = d\mathcal{J}(\Omega_\phi)(\theta). \end{aligned}$$

Thus, J has a Gâteaux semiderivative at ϕ in direction h. Since $\theta \mapsto d\mathcal{J}(\Omega_\phi)(\theta)$ is linear and continuous, and θ is linear and continuous with respect to h on $\partial\Omega_\phi$ in view of (25), we have that $h \mapsto d_G J(\phi)(h)$ is linear and continuous and J has a Gâteaux derivative at ϕ in direction h. ∎

Remark 1. Note that the vector field θ can be associated with a flow

$$\begin{aligned} \partial_t \widehat{T}(x,t) &= \theta(\widehat{T}(x)) \quad \text{for } (x,t) \in \mathcal{D} \times [0,\tau_1), \\ \widehat{T}(x,0) &= x \quad \text{for } x \in \mathcal{D}. \end{aligned}$$

The flow $\widehat{T}$ is in general different from T defined in (27), even though the shape derivatives $d\mathcal{J}(\Omega_\phi)(\theta)$ and $d\mathcal{J}(\Omega_\phi)(V(\cdot,0))$ are equal. Indeed, higher-order shape derivatives are in general different.

Remark 2. There are various ways to choose θ in Theorem 3. For instance,

$$\theta = -\frac{h\nabla\phi}{|\nabla\phi|^2 + \phi^2} \tag{28}$$

is an admissible choice, as it satisfies $\theta = -h|\nabla\phi|^{-2}\nabla\phi$ on $\partial\Omega_\phi$, and we also have $|\nabla\phi|^2 + \phi^2 > 0$ in $\mathcal{D}$ since $|\nabla\phi| > 0$ on $\{\phi = 0\}$.

Note that the relation (25) is directly related to the Hamilton–Jacobi equation in the level set method. Indeed, taking the scalar product of (25) with $\nabla\phi$ we obtain, rearranging the terms, $h + \theta \cdot \nabla\phi = 0$. In the traditional level set framework, ϕ is a function of time and space $\phi(x,t)$. To establish the correspondence with the Hamilton–Jacobi equation, the perturbation h of the level set function in our framework plays the role of the time derivative $\partial_t\phi$. Thus, we formally recover the Hamilton–Jacobi equation (see [25, 27]):

$$\partial_t\phi(x,t) + \theta(x) \cdot \nabla\phi(x,t) = 0 \quad \text{on } \partial\Omega_\phi. \tag{29}$$

Using that the outer normal vector to Ω_ϕ is given by $n = \nabla\phi|\nabla\phi|^{-1}$, one also recovers the level set equation in the usual way:

$$\partial_t\phi(x,t) + \theta(x) \cdot n(x)|\nabla\phi(x,t)| = 0 \quad \text{on } \partial\Omega_\phi. \tag{30}$$

This comparison shows more clearly the difference between the evolution approach and the approach where ϕ is perturbed. In the evolution approach, the vector field θ is given, for instance through the calculation of the shape derivative, and the corresponding perturbation of $\partial_t\phi$ of the level set function can be computed using (29) or (30), as is done, for instance, in [1, 12, 16, 18, 21]. In the converse approach, one first considers a perturbation h of the level set and deduces the corresponding boundary perturbation θ. So the two points of view are somehow the reverse of each other, as was observed in [26]. In fact, in the approach where ϕ is perturbed, the computation of θ is only an intermediary step, and eventually the Gâteaux derivative of J depends only on h.

Then one can use the particular structure of the shape derivative. On one hand, if Ω_ϕ has enough regularity, it is often possible to write the shape derivative in the form of a boundary expression

$$d\mathcal{J}(\Omega_\phi)(\theta) = \int_{\partial\Omega_\phi} \mathscr{G}_\phi\, \theta \cdot n, \tag{31}$$

where $\mathscr{G}_\phi : \partial\Omega_\phi \to \mathbb{R}$. On the other hand, a more general way to write the shape derivative is to use a domain expression of the type

$$d\mathcal{J}(\Omega_\phi)(\theta) = \int_{\Omega_\phi} \mathscr{S}_{1,\phi} : D\theta + \mathscr{S}_{0,\phi} \cdot \theta, \tag{32}$$

where $\mathscr{S}_{1,\phi}$ and $\mathscr{S}_{0,\phi}$ are appropriate tensors; see [10, 13, 18, 19] for details. In view of (26), and replacing θ satisfying (25) in (31), we obtain the explicit expression for the Gâteaux derivative

$$d_G J(\phi)(h) = -\int_{\partial\Omega_\phi} \mathscr{G}_\phi h |\nabla\phi|^{-2}\nabla\phi \cdot n = -\int_{\partial\Omega_\phi} \mathscr{G}_\phi h |\nabla\phi|^{-1}, \tag{33}$$

where we have used that $n = \nabla\phi|\nabla\phi|^{-1}$ on $\partial\Omega_\phi$. Expression (33) shows how the Gâteaux derivative $d_G J(\phi)(h)$ can be written explicitly as a function of h. If one uses expression (32) to compute $d_G J(\phi)(h)$, it seems that the Gâteaux derivative depends on the choice of θ. However, this is not the case since the shape derivative (32) satisfies Theorem 2; indeed, this implies that the shape derivative only depends on $\theta_{|\partial\phi} = -h|\nabla\phi|^{-2}\nabla\phi$ in view of (25).

For instance, one may choose θ as in (28), and using (32) we obtain another possible explicit expression for the Gâteaux derivative:

$$d_G J(\phi)(h) = -\int_{\Omega_\phi} \mathscr{S}_{1,\phi} : D\left(\frac{h\nabla\phi}{|\nabla\phi|^2 + \phi^2}\right) + \mathscr{S}_{0,\phi} \cdot \left(\frac{h\nabla\phi}{|\nabla\phi|^2 + \phi^2}\right). \tag{34}$$

Expressions (33) and (34) may be used to find a descent direction h for a minimization algorithm.

To close this section, we prove a variant of Lemma 3.2, which will be needed to treat the case where $\nabla\phi$ is allowed to vanish at an isolated point on the boundary $\partial\Omega_\phi$.

LEMMA 3.3. *Assume $\phi, h \in \mathcal{C}^\infty(\mathcal{D})$, $|\nabla\phi| > 0$ on $\partial\Omega_\phi \setminus \{p\}$ and $\nabla\phi(p) = 0$. Let $\mathcal{A} \subset \mathcal{D}$ be an open set containing p and such that $\partial\Omega_\phi \setminus \mathcal{A}$ is a smooth manifold with boundary. Then there exist $\tau_1 > 0$ and $T : \mathcal{D} \times (-\tau_1, \tau_1) \to \mathcal{D}$ such that the following hold:*

(i) $T \in \mathcal{C}^\infty(\mathcal{D} \times (-\tau_1, \tau_1), \mathcal{D})$.
(ii) $T(x, 0) = x$ *for* $x \in \mathcal{D}$, *and* $T(x, t) = x$ *for* $(x, t) \in \partial\mathcal{D} \times (-\tau_1, \tau_1)$.
(iii) $\partial_t T(x, 0) = -h(x)|\nabla\phi(x)|^{-2}\nabla\phi(x)$ *for* $x \in \partial\Omega_\phi \setminus \mathcal{A}$.
(iv) $T(\cdot, t) : \mathcal{D} \to \mathcal{D}$ *is bijective for all* $t \in (-\tau_1, \tau_1)$.
(v) $T(\Omega_\phi \setminus \mathcal{A}, t) = \Omega_{\phi+th} \setminus T(\mathcal{A}, t)$ *for all* $t \in (-\tau_1, \tau_1)$.
(vi) $T(\partial\Omega_\phi \setminus \mathcal{A}, t) = \partial\Omega_{\phi+th} \setminus T(\mathcal{A}, t)$ *for all* $t \in (-\tau_1, \tau_1)$.

Proof. The proof is an adaptation of the proofs of Lemmas 3.1 and 3.2. Since $\partial\Omega_\phi \setminus \mathcal{A}$ is compact, we obtain similarly to Lemma 3.1 a $\mathcal{C}^\infty$ function $\hat{\alpha} : (\partial\Omega_\phi \setminus \mathcal{A}) \times (-\tau_0, \tau_0) \to \mathbb{R}$ for some $\tau_0 > 0$, such that

$$(\phi + th)(x + \hat{\alpha}(x, t)\nabla\phi(x)) = 0 \quad \text{for } (x, t) \in (\partial\Omega_\phi \setminus \mathcal{A}) \times (-\tau_0, \tau_0). \tag{35}$$

Since $\partial\Omega_\phi \setminus \mathcal{A}$ is assumed to be a smooth manifold with boundary, we can extend $\hat{\alpha}$ to a $\mathcal{C}^\infty$ function $\bar{\alpha} : \mathcal{D} \times (-\tau_0, \tau_0) \to \mathbb{R}$ which satisfies $\bar{\alpha}(x, 0) = 0$ for all $x \in \mathcal{D}$ and $\bar{\alpha}(\cdot, t) \in \mathcal{C}_c^\infty(\mathcal{D})$ for all $t \in (-\tau_0, \tau_0)$. Then the function T can be defined as in (10). Note that, contrarily to Lemma 3.2, we now have $T(\Omega_\phi, t) \neq \Omega_{\phi+th}$ in general since we do not control the behavior of T inside the set $\mathcal{A}$.

Properties (i), (ii), (iii), and (iv) follow immediately or in the same way as in the proof of Lemma 3.2. Properties (v) and (vi) can be obtained by a small modification of the corresponding part of the proof of Lemma 3.2 that we describe here. Starting from a point $x \in \Omega_\phi \setminus \mathcal{A}$, we prove in the same way as for (18) that

$$T(\Omega_\phi \setminus \mathcal{A}, t) \subset \Omega_{\phi+th} \setminus T(\mathcal{A}, t) \quad \text{for all } |t| \leq \min(\eta_1, \eta_2). \tag{36}$$

Similarly to (19), we also get

$$T((\mathcal{D} \setminus \overline{\Omega_\phi}) \setminus \mathcal{A}, t) \subset (\mathcal{D} \setminus \overline{\Omega_{\phi+th}}) \setminus T(\mathcal{A}, t) \quad \text{for all } |t| \leq \min(\eta_3, \eta_4). \tag{37}$$

Defining $\tau_1 := \min(\eta_1, \eta_2, \eta_3, \eta_4) > 0$, we obtain from (36) and (37) that

$$T(\Omega_\phi \setminus \mathcal{A}, t) = \Omega_{\phi+th} \setminus T(\mathcal{A}, t) \quad \text{for all } |t| < \tau_1, \tag{38}$$

$$T((\mathcal{D} \setminus \overline{\Omega_\phi}) \setminus \mathcal{A}, t) = (\mathcal{D} \setminus \overline{\Omega_{\phi+th}}) \setminus T(\mathcal{A}, t) \quad \text{for all } |t| < \tau_1. \tag{39}$$

To prove (38), take, for instance, $y \in \Omega_{\phi+th} \setminus T(\mathcal{A}, t)$. Since $T(\cdot, t)$ is bijective, there exists $x \in \mathcal{D}$ such that $y = T(x, t)$. The point x cannot belong to $(\mathcal{D} \setminus \overline{\Omega_\phi}) \setminus \mathcal{A}$; otherwise, $y = T(x, t)$ would belong to $(\mathcal{D} \setminus \overline{\Omega_{\phi+th}}) \setminus T(\mathcal{A}, t)$ according to (37), which is impossible. We also cannot have $x \in \mathcal{A}$; otherwise, $y = T(x, t) \in T(\mathcal{A}, t)$. Also $x \in \partial\Omega_\phi \setminus \mathcal{A}$ is impossible; otherwise, $y = T(x, t) \in \partial\Omega_{\phi+th}$ in view of (35). This implies $x \in \Omega_\phi \setminus \mathcal{A}$, which proves (38). One can prove (39) in a similar way, and (v) and (vi) immediately follow. ∎

4. Analyzing topological changes of the level set. In Theorem 3, it is clear that the crucial assumption is $|\nabla\phi| > 0$ on $\partial\Omega_\phi$. In level set methods, the same condition is required, and often ϕ is initialized as a distance function, so we have $|\nabla\phi| = 1$ at $t = 0$ and ϕ is regularly reinitialized so that $|\nabla\phi|$ stays close to 1 in numerical methods. Note that for the analysis of section 3, the value of $|\nabla\phi|$ is irrelevant, as long as it remains positive, but for a numerical implementation of this approach, keeping $|\nabla\phi| \approx 1$ might be useful for stability.

As explained in the introduction, the Hamilton–Jacobi equation does not allow one to consider topological changes on a theoretical level. Still, topological changes are a natural feature of level set methods if one considers only ϕ as the variable instead of considering variations of the level set Ω_ϕ. Consider, for instance, the situation where the graph of ϕ presents two bumps facing downwards and $\phi > 0$. Then there exist critical times $t_1 > t_0 > 0$ such that $\Omega_{\phi-t}$ has two connected components for $t_1 > t > t_0$ and only one component for $t > t_1$; i.e., these two components merge at $t = t_1$. In this example, a very simple variation of ϕ leads to a topological change of Ω_ϕ, but it is unclear how this topological change could be modeled precisely using the Hamilton–Jacobi equation.

Since the topological changes seem to occur in a continuous manner for smooth perturbations of ϕ, we naturally expect $J(\phi)$ to be continuous with respect to the variation of ϕ. For the optimization procedure, we also need to determine whether $J(\phi)$ is differentiable with respect to ϕ when a topological change occurs, which is a more difficult question to handle. Indeed, several different types of topological changes may occur depending on the properties of ϕ and h. For instance, if $J(\phi)$ depends on the solution u_ϕ of a partial differential equation defined on Ω_ϕ, then the differentiability of $J(\phi)$ will depend on the differentiability of u_ϕ with respect to ϕ, and this requires a different asymptotic analysis for each type of partial differential equation.

In this section, we will see that, in two dimensions and for volume integrals, topological changes of the type "creation of a island" and "drilling of a hole" lead to differentiability of the functional, whereas topological changes of the type "splitting/merging" lead to nondifferentiability but are continuous. For boundary integrals, splitting or merging also lead to nondifferentiability. When the functional is not differentiable, we can still compute an asymptotic expansion with respect to t.

To study the differentiability of $J(\phi)$ in cases of topological changes, the main idea is to use a parameterized Morse lemma in the vicinity of the point where the topological change occurs; see [17]. Topological changes occur in the neighborhood of points p where $\phi(p) = 0$ and $\nabla\phi(p) = 0$, if ϕ is sufficiently smooth. Since $\nabla\phi(p) = 0$ for some point p of the boundary, this explains why we introduced Lemma 3.3. In a small neighborhood of p, if the Hessian of ϕ is not singular, the function ϕ can be approximated by a quadratic function $D^2\phi(p)x \cdot x$, and we can use this property to compute an asymptotic expansion of $J(\phi + th)$ with respect to t.

A *critical point* p satisfies $\nabla\phi(p) = 0$ and a *degenerate critical point* is a critical point such that $\det D^2\phi(p) = 0$. If $\det D^2\phi(p) \neq 0$, then the critical point is *nondegenerate*. When a critical point is nondegenerate, we can use Morse's lemma to find a local coordinate system such that ϕ can be written in a standard form. We recall here this classical result for the convenience of the reader; see, for instance, [20] for a proof.

THEOREM 4 (Morse lemma). *Let p be a nondegenerate critical point of $\phi \in \mathcal{C}^\infty(\mathbb{R}^d)$. Then there exist $0 \leq q \leq d$ and a diffeomorphism ψ in a neighborhood X of p such that*

$$\phi(\psi(x)) = -\sum_{i=1}^{q} x_i^2 + \sum_{i=q+1}^{d} x_i^2 + \phi(p). \tag{40}$$

The integer q in Theorem 4 is called the *index* of the nondegenerate critical point p, and the right-hand side of (40) is the *normal form* of ϕ locally around p. Depending on the value of q, the perturbation $\phi + th$, with $h(p) \neq 0$, may induce several types of topological changes. In the case $d = 2$, for t small enough, we separate three different cases. When $q = 0$, the topological change corresponds to the creation of a new small connected component, a so-called island. When $q = 1$, the topological change is a merging or a splitting of two components which are connected by a single point at $t = 0$. The nature of the topological change (merging or splitting) depends on the value of $h(p)$. When $q = 2$, the topological change corresponds to the creation of a "hole" in Ω_ϕ.

In this paper, we treat the case where p is a nondegenerate critical point. The case where p is degenerate could also be interesting, but is more difficult since $\det D^2\phi(x) = 0$ and ϕ cannot be represented as a quadratic function in a neighborhood of p. In this case, we would have more complicated topological changes of Ω_ϕ. However, it is not clear yet whether the case of a degenerate p would be useful for applications.

Since we are interested in the situation where the perturbed level set function $\phi + th$ depends on t, we now give a parameterized version of the Morse lemma which will be useful for our analysis. Without loss of generality, we assume in the rest of the paper that the critical point p coincides with the origin $0 \in \mathbb{R}^d$.

THEOREM 5 (Morse lemma with parameters). *Let $F : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$ be a smooth map in a neighborhood of $(0, 0)$, where we use coordinates x_i in $\mathbb{R}^d$ and t in $\mathbb{R}$, and $(0, 0)$ means $x_i = 0$ for $1 \le i \le d$ and $t = 0$. Assume that $\nabla F(0, 0) = 0$ and $D^2F(0, 0)$ is nonsingular. Then there exist a neighborhood $\widehat{X} = X \times (-\tau_2, \tau_2)$ of $(0, 0)$ in $\mathbb{R}^d \times \mathbb{R}$ and a map $\psi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^d$ with the following properties:*

(i) *We have that $\psi(0, 0) = 0$, $\psi_{|\widehat{X}}$ is smooth, and $\psi(\cdot, t)$ is a diffeomorphism of X onto $\psi(X, t)$ for each $t \in (-\tau_2, \tau_2)$. Denoting by $\psi^{-1}(\cdot, t)$ the inverse function of $\psi(\cdot, t)$ for fixed t, the function $(x, t) \mapsto \psi^{-1}(x, t)$ is smooth on $\bigcup_{t\in(-\tau_2,\tau_2)} \psi(X, t) \times \{t\}$.*

(ii) *We have the normal form*

$$F(\psi(x, t), t) = F(0, 0) - \sum_{i=1}^{q} x_i^2 + \sum_{i=q+1}^{d} x_i^2 + v(t), \tag{41}$$

where $0 \le q \le d$ and $v : (-\tau_2, \tau_2) \to \mathbb{R}$ is a smooth map satisfying $v(0) = 0$ and $v'(0) = \partial_t F(0, 0)$.

(iii) *We have*

$$|\det D\psi(0, t)| = \frac{2^{d/2}}{\sqrt{(-1)^q \det D^2F(\psi(0, t), t)}}. \tag{42}$$

Proof. The normal form (41) can be found, for instance, in [6, p. 97]. However, in [6], the regularity with respect to t of ψ and item (iii) are not discussed; therefore, we provide here the additional results. The proofs of (i) and (ii) that we present here follow the ideas from [6, p. 97] and [20, pp. 224–228].

Proofs of (i) *and* (ii). We prove (i) and (ii) for the case $d = 2$. For $d \ge 3$, the result can be proved by induction; see [6]. Define $\widehat{F}(x, t) := F(x, t) - F(0, t)$. We have $\widehat{F}(0, t) = 0$ for all t. Due to the assumptions on F, we have $\nabla\widehat{F}(0, 0) = 0$ and $D^2\widehat{F}(0, 0)$ is nonsingular. Applying the implicit function theorem, there exist $\eta_0 > 0$ and a smooth function $w : (-\eta_0, \eta_0) \to \mathbb{R}^2$ with $w(0) = 0$ such that $\nabla\widehat{F}(w(t), t) = 0$. Next, we introduce the function

$$\mathfrak{F}(x, t) := \widehat{F}(x + w(t), t) - \widehat{F}(w(t), t). \tag{43}$$

We compute $\mathfrak{F}(0, t) = 0$, which yields

$$\mathfrak{F}(x, t) = \int_0^1 \frac{d}{ds}\mathfrak{F}(sx, t)ds = x \cdot \int_0^1 \nabla\mathfrak{F}(sx, t)ds = x_1g_1(x, t) + x_2g_2(x, t),$$

where

$$g_i(x,t) := \int_0^1 \partial_{x_i}\mathfrak{F}(sx,t)ds \quad \text{for } i = 1,2.$$

Observe that the g_i's are smooth in x and t. We also have

$$g_i(0,t) := \int_0^1 \partial_{x_i}\mathfrak{F}(0,t)ds = \partial_{x_i}\widehat{F}(w(t),t) = 0 \quad \text{for } i = 1,2.$$

Using the same method, we obtain smooth functions $\mathfrak{g}_i : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ such that $g_i(x,t) = x \cdot \mathfrak{g}_i(x,t)$. Denoting $\mathfrak{g}_{i1}$ and $\mathfrak{g}_{i2}$ the components of $\mathfrak{g}_i$, we get $\mathfrak{F}(x,t) = \sum_{i,j=1}^2 x_i x_j \mathfrak{g}_{ij}(x,t)$. Defining $\mathfrak{G}_{ij} := \frac{1}{2}(\mathfrak{g}_{ij} + \mathfrak{g}_{ji})$, we obtain $\mathfrak{G}_{ij} = \mathfrak{G}_{ji}$ and

$$\mathfrak{F}(x,t) = \sum_{i,j=1}^{2} x_i x_j \mathfrak{G}_{ij}(x,t). \tag{44}$$

Differentiating (44) twice at $x = 0$, we get

$$\mathfrak{G}_{ij}(0,t) = \frac{1}{2}\partial^2_{x_i x_j}\mathfrak{F}(0,t), \qquad i,j = 1,2. \tag{45}$$

We compute $D^2\mathfrak{F}(0,t) = D^2\widehat{F}(w(t),t)$. Since $D^2\mathfrak{F}(0,0) = D^2\widehat{F}(0,0)$ is nonsingular and $\mathfrak{F}$ is smooth, we have that $D^2\mathfrak{F}(0,t)$ is invertible for all $t \in (-\eta_0,\eta_0)$, reducing η_0 if necessary. This shows that $\det \mathfrak{G}(0,t) \neq 0$ for all $t \in (-\eta_0,\eta_0)$, where the entries of $\mathfrak{G}$ are the $\mathfrak{G}_{ij}$, $i,j = 1,2$. By continuity, there also exists a neighborhood X_0 of 0 such that $\det \mathfrak{G}(x,t) \neq 0$ for $(x,t) \in X_0 \times (-\eta_0,\eta_0)$.

Assume now that $|\mathfrak{G}_{11}(0,0)| > |\mathfrak{G}_{22}(0,0)|$. If $|\mathfrak{G}_{22}(0,0)| > |\mathfrak{G}_{11}(0,0)|$, one can proceed first to the change of variables $y_1 = x_2$, $y_2 = x_1$. Then we have $\mathfrak{G}_{11}(0,0) \neq 0$. Reducing η_0 and X_0 if necessary, we also have that $\mathfrak{G}_{11}(x,t) \neq 0$ for $(x,t) \in X_0 \times (-\eta_0,\eta_0)$. In view of (44), we have the following identity:

$$\mathfrak{F}(x,t) = \frac{(x_1\mathfrak{G}_{11} + x_2\mathfrak{G}_{12})^2 + (\mathfrak{G}_{11}\mathfrak{G}_{22} - \mathfrak{G}_{12}^2)x_2^2}{\mathfrak{G}_{11}} \quad \text{for } (x,t) \in X_0 \times (-\eta_0,\eta_0). \tag{46}$$

Introduce the smooth function

$$\begin{aligned} u_0 &: \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2, \\ &(x,t) \mapsto (x_1\mathfrak{G}_{11}(x_1,x_2,t) + x_2\mathfrak{G}_{12}(x_1,x_2,t), x_2), \end{aligned} \tag{47}$$

which satisfies $u_0(0,t) = 0$. The Jacobian matrix of u_0 at $x = 0$ is

$$Du_0(0,t) = \begin{pmatrix} \mathfrak{G}_{11}(0,t) & \mathfrak{G}_{12}(0,t) \\ 0 & 1 \end{pmatrix}.$$

Since $\mathfrak{G}_{11}(0,t) \neq 0$ for all $t \in (-\eta_0,\eta_0)$, the matrix $Du_0(0,t)$ is invertible for $t \in (-\eta_0,\eta_0)$. Consider the function

$$\begin{aligned} \Phi &: \mathbb{R}^2 \times \mathbb{R}^2 \times (-\eta_0,\eta_0) \to \mathbb{R}^2, \\ &\qquad (x,y,t) \mapsto u_0(x,t) - y, \end{aligned}$$

which satisfies $\Phi(0,0,0) = 0$. Since $D\Phi(0,0,0) = Du_0(0,0)$ is invertible, applying the implicit function theorem we obtain a neighborhood $X_1 \times (-\eta_1,\eta_1)$ of $(0,0)$, with

$0 < \eta_1 \leq \eta_0$ and $X_1 \subset X_0$, and a smooth function $\hat{u}_0 : X_1 \times (-\eta_1, \eta_1) \to \mathbb{R}^2$, with $\hat{u}_0(0,0) = 0$, such that

$$\Phi(\hat{u}_0(y,t), y, t) = u_0(\hat{u}_0(y,t), t) - y = 0,$$

which yields $u_0(\hat{u}_0(y,t), t) = y$. Then we compute, using (46) and (47),

$$\mathfrak{F}(\hat{u}_0(y,t), t) = \frac{y_1^2}{\mathfrak{G}_{11} \circ \hat{u}_0} + y_2^2 \left[\frac{\mathfrak{G}_{11}\mathfrak{G}_{22} - \mathfrak{G}_{12}^2}{\mathfrak{G}_{11}} \right] \circ \hat{u}_0. \tag{48}$$

Now introduce the function

$$\begin{aligned} &u_1 : X_1 \times (-\eta_1, \eta_1) \to \mathbb{R}^2, \\ &\qquad (y,t) \mapsto \left(\frac{y_1}{|\mathfrak{G}_{11} \circ \hat{u}_0|^{1/2}}, y_2 \left| \frac{\mathfrak{G}_{11}\mathfrak{G}_{22} - \mathfrak{G}_{12}^2}{\mathfrak{G}_{11}} \right|^{1/2} \circ \hat{u}_0 \right). \end{aligned} \tag{49}$$

Reducing X_1 and η_1 if necessary, u_1 is smooth on its domain of definition due to $\mathfrak{G}_{11}(0,0) \neq 0$ and the smoothness of $\mathfrak{G}$ and $\hat{u}_0$. The Jacobian matrix (with respect to y) at $y = 0$ is

$$Du_1(0,t) = \begin{pmatrix} |\mathfrak{G}_{11} \circ \hat{u}_0|^{-1/2} & 0 \\ 0 & \left| \frac{\mathfrak{G}_{11}\mathfrak{G}_{22} - \mathfrak{G}_{12}^2}{\mathfrak{G}_{11}} \right|^{1/2} \circ \hat{u}_0 \end{pmatrix},$$

which is nonsingular. Proceeding similarly as in the case of u_0, we apply the implicit function theorem and we obtain a neighborhood $X_2 \times (-\eta_2, \eta_2)$, with $0 < \eta_2 \leq \eta_1$, and a smooth function $\hat{u}_1 : X_2 \times (-\eta_2, \eta_2) \to X_1$, with $\hat{u}_1(0,0) = 0$, such that $u_1(\hat{u}_1(z,t), t) = z$. Then we compute, using (48) and (49),

$$\mathfrak{F}(\hat{u}_0(\hat{u}_1(z,t), t), t) = \sigma_1 z_1^2 + \sigma_2 z_2^2,$$

where $\sigma_i = \pm 1$ for $i = 1, 2$.

Now consider the case $|\mathfrak{G}_{11}(0,0)| = |\mathfrak{G}_{22}(0,0)|$. On one hand, the subcase $|\mathfrak{G}_{11}(0,0)| > 0$ can be treated as above; on the other hand, the subcase $|\mathfrak{G}_{11}(0,0)| = 0$ can be reduced to the former case using a linear coordinate change; see [20, p. 227].

Using the definition (43), we get

$$\mathfrak{F}(\hat{u}_0(\hat{u}_1(z,t), t), t) = \widehat{F}(\hat{u}_0(\hat{u}_1(z,t), t) + w(t), t) - \widehat{F}(w(t), t) = \sigma_1 z_1^2 + \sigma_2 z_2^2. \tag{50}$$

Introducing the function

$$\begin{aligned} &\psi : X_2 \times (-\eta_2, \eta_2) \to \mathbb{R}^2, \\ &\qquad (z,t) \mapsto \hat{u}_0(\hat{u}_1(z,t), t) + w(t) \end{aligned}$$

and using $\widehat{F}(x,t) = F(x,t) - F(0,t)$, we get, in view of (50),

$$F(\psi(z,t), t) - F(w(t), t) = \sigma_1 z_1^2 + \sigma_2 z_2^2,$$

which yields (41) for $d = 2$, $\tau_2 = \eta_2$, and $v(t) := F(w(t), t) - F(0,0)$ and considering that the index q in (41) is the number of negative eigenvalues of $D^2F(0,0)$; see [20, p. 228].

We also compute

$$v'(0) := \partial_t F(w(0), 0) + \nabla F(w(0), 0) \cdot w'(0) = \partial_t F(0,0) + \nabla F(0,0) \cdot w'(0) = \partial_t F(0,0),$$

where we have used the fact that $\nabla F(0,0) = 0$.

For fixed $t \in (-\tau_2, \tau_2)$, we have that $\hat{u}_1(\cdot,t)$ is a diffeomorphism of X_2 onto $\hat{u}_1(X_2,t)$ with inverse $u_1(\cdot,t)$ since $u_1(\hat{u}_1(z,t),t) = z$. Also, $\hat{u}_0(\cdot,t)$ is a diffeomorphism of $\hat{u}_1(X_2,t)$ onto $\hat{u}_0(\hat{u}_1(X_2,t),t)$ with inverse $u_0(\cdot,t)$ since $u_0(\hat{u}_0(y,t),t) = y$. Thus, for fixed $t \in (-\tau_2,\tau_2)$, $\psi(\cdot,t)$ is a diffeomorphism of X_2 onto $\hat{u}_0(\hat{u}_1(X_2,t),t)+w(t)$ with inverse $\psi^{-1}(\cdot,t) : x \mapsto u_1(u_0(x-w(t),t),t)$. Choosing $X = X_2$, we have that $(x,t) \mapsto \psi^{-1}(x,t)$ is smooth on $\bigcup_{t\in(-\tau_2,\tau_2)} \psi(X,t) \times \{t\}$, and with $\psi(0,0) = \hat{u}_0(\hat{u}_1(0,0),0) + w(0) = 0$ we have proved (i).

Proof of (iii). Differentiating (41) with respect to x, we get

$$D\psi(x,t)^{\mathsf{T}} \nabla F(\psi(x,t),t) = (-x_1, -x_2, \ldots, -x_q, x_{q+1}, \ldots, x_d)^{\mathsf{T}}. \tag{51}$$

At $x = 0$ this yields $D\psi(0,t)^{\mathsf{T}} \nabla F(\psi(0,t),t) = 0$. According to (i), the Jacobian matrix $D\psi(0,t)$ is nonsingular on $(-\tau_2,\tau_2)$, which yields

$$\nabla F(\psi(0,t),t) = 0. \tag{52}$$

Now we differentiate two times (41) with respect to x and take $x = 0$, which yields

$$D^2\psi(0,t)\nabla F(\psi(0,t),t) + D\psi(0,t)^{\mathsf{T}} D^2F(\psi(0,t),t) D\psi(0,t) = 2\mathcal{M}, \tag{53}$$

where $\mathcal{M} \in \mathbb{R}^{d\times d}$ is a diagonal matrix with the first q entries equal to -1 and the other entries equal to 1. Using (52), we get

$$D\psi(0,t)^{\mathsf{T}} D^2F(\psi(0,t),t) D\psi(0,t) = 2\mathcal{M}. \tag{54}$$

Note that (54) does not allow us to determine $D\psi(0,t)$ in a unique way in general. This is due to the fact that there is not a unique ψ satisfying (41).

Denote by λ_i, $i = 1,\ldots,d$, the eigenvalues of $D^2F(0,0)$, ordered such that

$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_q < 0 < \lambda_{q+1} \le \cdots \le \lambda_d.$$

Note that $\lambda_i \neq 0$ for all $i = 1,\ldots,n$ since $D^2F(0,0)$ is nonsingular. Taking the determinant of (54) yields (42). Note that

$$\det D^2F(\psi(0,0),0) = \det D^2F(0,0) = \prod_{i=1}^d \lambda_i = (-1)^q \prod_{i=1}^d |\lambda_i|, \tag{55}$$

so that for t small enough, the square root in (42) is well-defined. □

At $t = 0$, (54) yields the following expression of $D^2F(0,0)$:

$$D^2F(0,0) = 2D\psi(0,0)^{-\mathsf{T}} \mathcal{M} D\psi(0,0)^{-1}. \tag{56}$$

This leads to the following lemma, which states that $D^2F(0,0)$ has the same eigenvalues as $H := 2D\psi(0,0)^{-1}D\psi(0,0)^{-\mathsf{T}}\mathcal{M}$. This result is useful in sections 4.3 and 4.5 (see also Lemma A.2) for calculating asymptotic expansions of cost functions defined as boundary integrals; indeed, the matrix H appears naturally in these calculations.

LEMMA 4.1. *Let F, ψ, and q be as in Theorem* 5. *Let $\mathcal{M} \in \mathbb{R}^{d\times d}$ be a diagonal matrix with the first q entries equal to* -1 *and the other entries equal to* 1, *and let $H := 2D\psi(0,0)^{-1}D\psi(0,0)^{-\mathsf{T}}\mathcal{M}$. Then H and $D^2F(0,0)$ have the same eigenvalues λ_i, $1 \le i \le d$, and the eigenvectors w_i of H associated with λ_i satisfy*

$$\langle w_i, \mathcal{M}w_j\rangle = 0 \quad \textit{for all } 1 \le i \neq j \le d. \tag{57}$$

Proof. For two nonsingular square matrices H_1 and H_2, it is known that H_1H_2 and H_2H_1 are similar and have the same eigenvalues. Choosing $H_1 := 2D\psi(0,0)^{-1}$ and $H_2 := D\psi(0,0)^{-\mathsf{T}}\mathcal{M}$, we obtain in view of (56) that $D^2F(0,0) = H_2H_1$ and $H = H_1H_2$ have the same eigenvalues.

Since $D^2F(0,0)$ is symmetric, there exists an orthonormal basis of eigenvectors u_i associated with λ_i. So we have

$$2D\psi(0,0)^{-\mathsf{T}}\mathcal{M}D\psi(0,0)^{-1}u_i = D^2F(0,0)u_i = \lambda_i u_i.$$

Multiplying by $D\psi(0,0)^{-1}$ on both sides, we get

$$HD\psi(0,0)^{-1}u_i = \lambda_i D\psi(0,0)^{-1}u_i,$$

which shows that $w_i := D\psi(0,0)^{-1}u_i \neq 0$ is an eigenvector of H associated with λ_i. The converse statement is proven in a similar way.

Finally, we compute for $i \neq j$,

$$\begin{aligned}\langle w_i, \mathcal{M}w_j\rangle &= \langle D\psi(0,0)^{-1}u_i, \mathcal{M}D\psi(0,0)^{-1}u_j\rangle = \langle D\psi(0,0)^{-\mathsf{T}}\mathcal{M}D\psi(0,0)^{-1}u_i, u_j\rangle \\ &= \frac{1}{2}\langle D^2F(0,0)u_i, u_j\rangle = \frac{\lambda_i}{2}\langle u_i, u_j\rangle = 0,\end{aligned}$$

which proves the claim. □

Since our objective is to compute integrals depending on $\Omega_{\phi+th} = \{\phi + th < 0\}$, formula (42) for the Jacobian determinant will be useful with $F(x,t) = \phi(x) + th(x)$. Thus, we rewrite Theorem 5 with $F(x,t) = \phi(x) + th(x)$ below for convenience. Since $D^2F(0,0) = D^2\phi(0)$, the eigenvalues of $D^2\phi(0)$ are denoted by λ_i.

COROLLARY 4.2. *Let* 0 *be a nondegenerate critical point of* $\phi : \mathbb{R}^d \to \mathbb{R}$. *Then there exist a neighborhood* $\widehat{X} = X \times (-\tau_2, \tau_2)$ *of* $(0,0)$ *in* $\mathbb{R}^d \times \mathbb{R}$ *and a map* $\psi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}^d$ *with the following properties:*

(i) *We have that* $\psi(0,0) = 0$, $\psi_{|\widehat{X}}$ *is smooth, and* $\psi(\cdot,t)$ *is a diffeomorphism of* X *onto* $\psi(X,t)$ *for each* $t \in (-\tau_2,\tau_2)$. *Denoting by* $\psi^{-1}(\cdot,t)$ *the inverse function of* $\psi(\cdot,t)$ *for fixed* t, *the function* $(x,t) \mapsto \psi^{-1}(x,t)$ *is smooth on* $\bigcup_{t\in(-\tau_2,\tau_2)} \psi(X,t) \times \{t\}$.

(ii) *We have the normal form*

$$\phi(\psi(x,t)) + th(\psi(x,t)) = \phi(0) - \sum_{i=1}^{q} x_i^2 + \sum_{i=q+1}^{d} x_i^2 + v(t), \tag{58}$$

where $0 \leq q \leq d$ *and* $v : (-\tau_2,\tau_2) \to \mathbb{R}$ *is a smooth map satisfying* $v(0) = 0$ *and* $v'(0) = h(0)$.

(iii) *We have*

$$|\det D\psi(0,t)| = \frac{2^{d/2}}{\sqrt{(-1)^q \det[D^2\phi(\psi(0,t)) + tD^2h(\psi(0,t))]}}. \tag{59}$$

4.1. Creation of an island: Case of volume integrals. In this section, we assume $q = 0$, and $p = 0$ is a nondegenerate critical point of ϕ. In order to obtain a topological change with a small perturbation of ϕ, we also assume that $\phi(0) = 0$. Let $f \in \mathcal{C}^\infty(\mathcal{D})$, and consider the volume functional

$$J_1(\phi) := \int_{\Omega_\phi} f(x)dx. \tag{60}$$

In view of Theorem 4, since $q = 0$, the point $p = 0$ is a strict local minimum of ϕ and $\det D^2\phi(0) > 0$. Let $\widehat{X} = X \times (-\tau_2, \tau_2)$ be the neighborhood given by Corollary 4.2. If necessary, $\widehat{X}$ can be reduced so that $\phi(x) > 0$ for all $x \in X \setminus \{0\}$. We choose the function h with a compact support in X.

If $h(0) > 0$, then we have for $t > 0$ small enough

$$\Omega_{\phi+th} = \{x \in \mathcal{D} \mid \phi(x) + th(x) < 0\} = \{x \in \mathcal{D} \mid \phi(x) < 0\} = \Omega_\phi \text{ a.e.}$$

Thus, in this case, the following Gâteaux semiderivative exists:

$$d_G J_1(\phi)(h) := \lim_{t \searrow 0} \frac{J_1(\phi + th) - J_1(\phi)}{t} = 0. \tag{61}$$

If $h(0) < 0$ and $t > 0$, then the set $\Omega_{\phi+th}$ is different from Ω_ϕ and we have, in fact, for t small enough, that $\Omega_{\phi+th} \setminus \Omega_\phi = \Omega_{\phi+th} \cap X$, and the Gâteaux semiderivative is not zero. Using Corollary 4.2, we get, using the change of variables $x \mapsto \psi(x,t)$,

$$J_1(\phi + th) - J_1(\phi) = \int_{\Omega_{\phi+th} \cap X} f(x)dx = \int_{\mathcal{B}_t} f(\psi(x,t))|\det D\psi(x,t)|dx,$$

where $\mathcal{B}_t := \psi_t^{-1}(\Omega_{\phi+th} \cap X)$. In view of (58), $\phi(0) = 0$, and $q = 0$, we observe that

$$\mathcal{B}_t = \left\{ \sum_{i=1}^d x_i^2 < -v(t) \right\}. \tag{62}$$

Note that for t small enough, $\mathcal{B}_t$ is not empty since $v(0) = 0$ and $v'(0) = h(0) < 0$. Using a Taylor expansion about $(0,0)$, we get

$$\int_{\mathcal{B}_t} f(\psi(x,t))|\det D\psi(x,t)|\,dx = \int_{\mathcal{B}_t} f(\psi(0,0))|\det D\psi(0,0)|dx + R(t), \tag{63}$$

where $R(t)$ is a small remainder. Using (59) at $t = 0$ and $\psi(0,0) = 0$, we get

$$\begin{aligned} J_1(\phi + th) - J_1(\phi) &= f(0)\frac{2^{d/2}}{\sqrt{(-1)^q \det D^2\phi(0)}}|\mathcal{B}_t| + R(t) \\ &= f(0)2^{d/2}\prod_{i=1}^d |\lambda_i|^{-1/2}|B(0, \sqrt{-v(t)})| + R(t), \end{aligned}$$

where $B(0, \sqrt{-v(t)})$ is the ball of radius $\sqrt{-v(t)}$ and center 0. We also observe that

$$\prod_{i=1}^d |\lambda_i|^{-1/2}|B(0, \sqrt{-v(t)})| = |v(t)|^{d/2}|\mathfrak{E}| = \prod_{i=1}^d |\lambda_i|^{-1/2}\frac{(\pi)^{d/2}}{\Gamma(\frac{d}{2}+1)}|v(t)|^{d/2},$$

where Γ is the Gamma function, $\mathfrak{E}$ denotes the d-dimensional ellipsoid with semi-axis $\lambda_1^{-1/2}, \dots, \lambda_d^{-1/2}$, and $|\mathfrak{E}|$ is the volume of $\mathfrak{E}$.

In view of Corollary 4.2(ii), we have $v(t) = th(0) + o(t)$. Writing the next term of the Taylor expansion in (63), one gets $R(t) = o(|B(0, \sqrt{-v(t)})|)$. Thus we obtain the following result.

THEOREM 6. *Let $f, h, \phi \in \mathcal{C}^\infty(\mathcal{D})$, and let J_1 be defined in (60). Let 0 be a nondegenerate critical point of ϕ with index $q = 0$, $\phi(0) = 0$, $t > 0$, and $h(0) < 0$. Let $\mathfrak{E}$ be the d-dimensional ellipsoid with semi-axis $\lambda_1^{-1/2}, \dots, \lambda_d^{-1/2}$, where λ_i, $i = 1, \dots, d$, are the eigenvalues of $D^2\phi(0)$. We have the expansion*

$$J_1(\phi + th) - J_1(\phi) = f(0)|2h(0)|^{d/2}|\mathfrak{E}|t^{d/2} + o(t^{d/2}). \tag{64}$$

We observe that in $d = 2$ dimensions, we obtain the Gâteaux semiderivative

$$d_G J_1(\phi)(h) = \lim_{t \searrow 0} \frac{J_1(\phi + th) - J_1(\phi)}{t} = 2f(0)|h(0)| \cdot |\mathfrak{E}|. \tag{65}$$

In view of (61), the semiderivative is not linear with respect to h; therefore, the Gâteaux derivative does not exist in two dimensions. However, in higher dimensions $d \geq 3$, we see from (64) that the main term is of order $t^{d/2}$; therefore, we get

$$d_G J_1(\phi)(h) = \lim_{t \searrow 0} \frac{J_1(\phi + th) - J_1(\phi)}{t} = 0.$$

Combining this result with (61), we see that in dimension $d \geq 3$, J_1 admits a Gâteaux derivative

$$d_G J_1(\phi)(h) = \lim_{t \to 0} \frac{J_1(\phi + th) - J_1(\phi)}{t} = 0$$

since the Gâteaux semiderivative is trivially linear and continuous with respect to h.

This result shows that in dimension $d \geq 3$, the topological perturbation corresponding to the creation of an island is "too weak" to appear in the derivative of J_1. One obtains a semiderivative $d_G J_1(\phi)(h)$ different from zero only in two dimensions. We can expect this property to be true also for certain shape functionals depending on the solution of a partial differential equation. Also, even if the Gâteaux derivative is zero, an asymptotic expansion such as (64) is useful from an optimization perspective, as it can be used to find a descent direction. Basically, we observe that the sign of $J_1(\phi + th) - J_1(\phi)$ in (64) depends only on the sign of $f(0)$, which is the expected result for functional (60). Expansion (64) also shows that when d is odd, the $\frac{d+1}{2}$th-semiderivative does not exist.

There is a natural connection between expansion (64) and the notion of *topological derivative* [28] that we discuss now. Fix $\omega \subset \mathbb{R}^2$, and set $\omega_\varepsilon := \{y \in \mathbb{R}^2 : \varepsilon^{-1}y \in \omega\}$. Assume that there exist $d_T\mathcal{J}(0) \in \mathbb{R}$ and $\rho(\varepsilon) > 0$ such that $\rho(\varepsilon) \to 0$ as $\varepsilon \to 0$, and the following expansion is valid:

$$\mathcal{J}(\Omega \cup \omega_\varepsilon) - \mathcal{J}(\Omega) = \rho(\varepsilon) d_T\mathcal{J}(0) + o(\rho(\varepsilon)). \tag{66}$$

Then $d_T\mathcal{J}(0)$ is called the topological derivative of $\mathcal{J}$ at 0. In the case of the functional

$$\mathcal{J}(\Omega) = \int_\Omega f(x)dx,$$

it is easy to see that we have, up to a scaling factor, $d_T\mathcal{J}(0) = f(0)$ and $\rho(\varepsilon) = |\omega_\varepsilon| = O(\varepsilon^d)$. Therefore, comparing $d_T\mathcal{J}(0)$ with (65), we see that in two dimensions $d_T\mathcal{J}(0)$ and $d_G J_1(\phi)(h)$ only differ by the multiplication with a positive constant. In fact, we expect this property to also be true when the functional $\mathcal{J}$ depends on the solution of a partial differential equation. From an optimization perspective, this means the two derivatives provide similar descent directions. However, in dimension

$d \geq 3$, $d_T\mathcal{J}(0)$ and $d_G J_1(\phi)(h)$ do not coincide since $d_G J_1(\phi)(h) = 0$. Still, $d_T\mathcal{J}(0)$ coincides (still up to the multiplication by a positive constant) with the first term of the expansion of (64). Note that the topological derivative is not a derivative in the usual sense; it is in fact the first term of an asymptotic expansion, as seen in (66), so it is more meaningful to compare $d_T\mathcal{J}(0)$ with the first term of the expansion of (64) rather than $d_G J_1(\phi)(h)$. The conclusion is that there is a large intersection between the concept of the Gâteaux derivative of $J_1(\phi)$ and the concept of the topological derivative for shape functionals.

4.2. Creation of a hole: Case of volume integrals. Here we assume $q = d$, so that $p = 0$ is a strict local maximum of ϕ and $\det(D^2\phi(0)) > 0$. The procedure to compute the Gâteaux derivative of J_1 is the same as in section 4.1. Thus we obtain the following result.

THEOREM 7. *Let $f, h, \phi \in \mathcal{C}^\infty(\mathcal{D})$, let J_1 be defined as in* (60), *and let $\mathfrak{E}$ be defined as in Theorem* 6. *Let* 0 *be a nondegenerate critical point of ϕ with index $q = d$, $\phi(0) = 0$, $t > 0$, and $h(0) > 0$. Then we have the expansion*

$$J_1(\phi + th) - J_1(\phi) = -f(0)|2h(0)|^{d/2}|\mathfrak{E}|t^{d/2} + o(t^{d/2}). \tag{67}$$

From Theorem 7, we can draw conclusions similar to those in section 4.1 about the existence of the Gâteaux derivative of J_1, depending on the dimension, and the similarity with the topological derivative. Note that in this case, the topological derivative $d_T\mathcal{J}(0)$ is defined as

$$\mathcal{J}(\Omega \setminus \omega_\varepsilon) - \mathcal{J}(\Omega) = \rho(\varepsilon) d_T\mathcal{J}(0) + o(\rho(\varepsilon)), \tag{68}$$

which yields for this functional $d_T\mathcal{J}(0) = -f(0)$.

4.3. Creation of an island: Case of boundary integrals. In this section, we make the same assumptions as in section 4.1 and consider the boundary integral

$$J_2(\phi) := \int_{\partial\Omega_\phi} f(x)\, ds_x. \tag{69}$$

If $h(0) > 0$ and $t > 0$, we have $d_G J_2(\phi)(h) = 0$, as in section 4.1. If $h(0) < 0$ and $t > 0$, then using Corollary 4.2 and the change of variables $x \mapsto \psi(x,t)$, we get

$$J_2(\phi + th) - J_2(\phi) = \int_{\partial\Omega_{\phi+th} \cap X} f(x)\, ds_x = \int_{\partial\mathcal{B}_t} f(\psi(x,t)) z(t)\, ds_x,$$

with $\mathcal{B}_t$ given by (62), and $z(t) := |M(x,t) n_{\mathcal{B}_t}|$, where $n_{\mathcal{B}_t}$ is the unit outward normal vector to $\mathcal{B}_t$ and $M(x,t) := \det D\psi(x,t) D\psi(x,t)^{-\mathsf{T}}$ is the cofactor matrix of $D\psi(x,t)$. Using a Taylor expansion about $(0,0)$, we get

$$\begin{aligned} &\int_{\partial\mathcal{B}_t} f(\psi(x,t)) |\det D\psi(x,t)| \cdot |D\psi(x,t)^{-\mathsf{T}} n_{\mathcal{B}_t}|\ ds_x \\ &= \int_{\partial\mathcal{B}_t} f(\psi(0,0)) |\det D\psi(0,0)| \cdot |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{B}_t}|\, ds_x + R(t), \end{aligned} \tag{70}$$

where $R(t)$ is a small remainder. Considering the next terms in the asymptotic expansion (70), we can show that $R(t) = o(t^{(d-1)/2})$. Using (59) at $t = 0$, $\psi(0,0) = 0$, and $q = 0$, we get

$$J_2(\phi + th) - J_2(\phi) = f(0) \frac{2^{d/2}}{\sqrt{\det D^2\phi(0)}} \int_{\partial\mathcal{B}_t} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{B}_t}|\, ds_x + R(t).$$

Let $\mathcal{M}$ and H be as in Lemma 4.1. We have here $\mathcal{M} = \mathcal{I}$ due to $q = 0$. Then, in view of Lemma 4.1, we have

$$|D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{B}_t}|^2 = \langle D\psi(0,0)^{-1} D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{B}_t}, n_{\mathcal{B}_t}\rangle = \frac{1}{2}\langle H n_{\mathcal{B}_t}, n_{\mathcal{B}_t}\rangle.$$

Due to $\mathcal{M} = \mathcal{I}$, the matrix H is symmetric, and there exists an orthogonal matrix Q such that $H = Q\mathfrak{D}Q^{\mathsf{T}}$, with $\mathfrak{D} := \operatorname{diag}(\lambda_1, \ldots, \lambda_d)$. Thus, we obtain

$$\int_{\partial\mathcal{B}_t} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{B}_t}|\, ds_x = \frac{1}{\sqrt{2}} \int_{\partial\mathcal{B}_t} \langle \mathfrak{D}Q^{\mathsf{T}} n_{\mathcal{B}_t}, Q^{\mathsf{T}} n_{\mathcal{B}_t}\rangle^{1/2}\, ds_x.$$

Define $\mathcal{G}(x) := Qx$. Since Q is an orthogonal matrix, we have $\mathcal{G}^{-1}(x) := Q^{-1}x = Q^{\mathsf{T}}x$, $\mathcal{G}^{-1}(\partial\mathcal{B}_t) = \partial\mathcal{B}_t$, $|\det D\mathcal{G}(x)| = 1$ on $\partial\mathcal{B}_t$, and $|D\mathcal{G}(x)^{-\mathsf{T}} n_{\mathcal{G}^{-1}(\partial\mathcal{B}_t)}(x)| = 1$ on $\partial\mathcal{B}_t$. Using the change of variables $x \mapsto \mathcal{G}(x)$ and the fact that $n_{\mathcal{B}_t}(x) = |v(t)|^{-1/2}x$, we obtain

$$\begin{aligned}
&\frac{1}{\sqrt{2}} \int_{\partial\mathcal{B}_t} \langle \mathfrak{D}Q^{\mathsf{T}} n_{\mathcal{B}_t}, Q^{\mathsf{T}} n_{\mathcal{B}_t}\rangle^{1/2}\, ds_x \\
&= \frac{1}{\sqrt{2}} \int_{\mathcal{G}^{-1}(\partial\mathcal{B}_t)} \langle \mathfrak{D}Q^{\mathsf{T}}Q n_{\mathcal{B}_t}, Q^{\mathsf{T}}Q n_{\mathcal{B}_t}\rangle^{1/2} |\det D\mathcal{G}(x)| \cdot |D\mathcal{G}(x)^{-\mathsf{T}} n_{\mathcal{G}^{-1}(\partial\mathcal{B}_t)}(x)|\, ds_x \\
&= \frac{1}{\sqrt{2}} \int_{\partial\mathcal{B}_t} \langle \mathfrak{D} n_{\mathcal{B}_t}, n_{\mathcal{B}_t}\rangle^{1/2}\, ds_x = \frac{(-v(t))^{(d-1)/2}}{\sqrt{2}} \int_{\partial\mathcal{B}_1} \langle \mathfrak{D} n_{\mathcal{B}_1}, n_{\mathcal{B}_1}\rangle^{1/2}\, ds_x,
\end{aligned}$$

with $\mathcal{B}_1 := \left\{ \sum_{i=1}^d x_i^2 < 1 \right\}$. This yields, using $v(t) = th(0) + o(t)$,

$$J_2(\phi + th) - J_2(\phi) = f(0) \frac{(-2th(0))^{(d-1)/2}}{\sqrt{\det D^2\phi(0)}} \int_{\partial\mathcal{B}_1} \langle \mathfrak{D} n_{\mathcal{B}_1}, n_{\mathcal{B}_1}\rangle^{1/2}\, ds_x + R(t). \tag{71}$$

Thus, the main term in the asymptotic expansion (71) is independent of ψ, as expected.

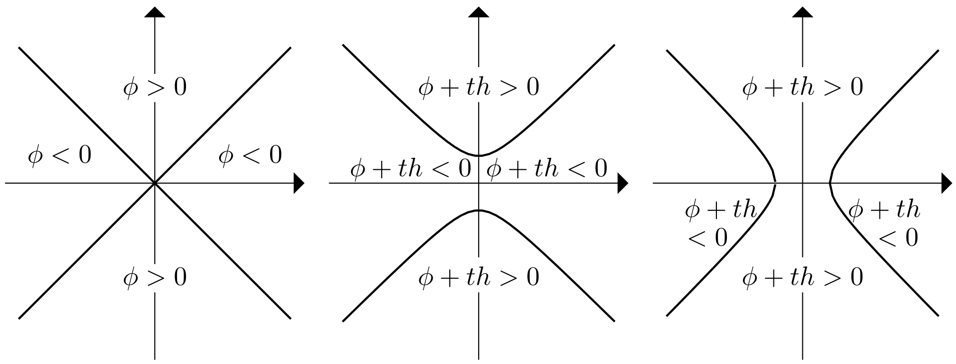
Further, define $\mathcal{F}(x) := \mathfrak{D}^{-1/2}x$. Note that $\mathfrak{D}^{-1/2}$ is well-defined since the eigenvalues are positive due to $q = 0$. We have $D\mathcal{F}(x) = \mathfrak{D}^{-1/2}$. Using the change of variables $x \mapsto \mathcal{F}(x)$, we obtain

$$\begin{aligned}
\mathcal{S}_{\mathfrak{E}} &:= \int_{\partial\mathfrak{E}} 1\, ds_x = \int_{\mathcal{F}^{-1}(\partial\mathfrak{E})} |\det D\mathcal{F}(x)| \cdot |D\mathcal{F}(x)^{-\mathsf{T}} n_{\mathcal{B}_1}(x)|\, ds_x \\
&= \prod_{i=1}^d |\lambda_i|^{-1/2} \int_{\partial\mathcal{B}_1} \langle \mathfrak{D} n_{\mathcal{B}_1}, n_{\mathcal{B}_1}\rangle^{1/2}\, ds_x \\
&= \frac{1}{\sqrt{\det D^2\phi(0)}} \int_{\partial\mathcal{B}_1} \langle \mathfrak{D} n_{\mathcal{B}_1}, n_{\mathcal{B}_1}\rangle^{1/2}\, ds_x,
\end{aligned} \tag{72}$$

where the ellipsoid $\mathfrak{E}$ is defined in Theorem 6. Finally, combining (72) and (71), we obtain the following result.

THEOREM 8. *Let $f, h, \phi \in \mathcal{C}^\infty(\mathcal{D})$, let J_2 be defined as in (69), and let $\mathcal{S}_{\mathfrak{E}}$ be defined as in (72). Let 0 be a nondegenerate critical point of ϕ with index $q = 0$, $\phi(0) = 0$, $t > 0$, and $h(0) < 0$. Then we have the expansion*

$$J_2(\phi + th) - J_2(\phi) = f(0)|2h(0)|^{(d-1)/2} \mathcal{S}_{\mathfrak{E}} t^{(d-1)/2} + o(t^{(d-1)/2}). \tag{73}$$



(a) Initial configuration when $t = 0$.
(b) Merging at $t > 0$ and $h(0) < 0$.
(c) Splitting at $t > 0$ and $h(0) > 0$.

FIG. 1. *Topological changes of the type splitting/merging (also known as Morse transitions) of the set* $\Omega_{\phi+th} = \{\phi + th < 0\}$ *occurring in the neighborhood of a point* p *with Morse index* $q = 1$ *in two dimensions.*

We observe that for $d = 2$, the Gâteaux semiderivative of $J_2(\phi+th)$ does not exist in general due to the term $t^{1/2}$ in (73), and for $d = 3$, we have Gâteaux semiderivatives but no Gâteaux derivative. For $d \geq 4$, the Gâteaux derivative exists and is equal to zero.

The case of a creation of a hole for boundary integrals, i.e., for $q = d$ and $h(0) > 0$, can be treated analogously. We obtain the same expansion as (73) but with a minus sign.

4.4. The splitting/merging case for domain integrals. In this section, we treat the case where the Morse index satisfies $0 < q < d$, which leads to a merging or splitting in the vicinity of the point where $\nabla\phi$ vanishes; see Figure 1. The results of [17, Theorem 2] show that for J_1 given by (60) and $f \equiv 1$, we have that $J_1(\phi+th) - J_1(\phi)$ is not differentiable with respect to t for $d = 2$ but is differentiable for $d \geq 3$. For arbitrary f, with $f(0) \neq 0$, we should obtain the same result. In any dimension, the variation of the cost functional far from the splitting/merging point yields a term of order t; indeed, this corresponds to the situation studied in Lemma 3.3. This term is similar to the usual shape derivative. On one hand, the expansion of the cost functional in a small neighborhood of the splitting/merging point yields a term of order $t|\ln t|$ in $d = 2$ dimensions; therefore, the variation of the cost functional far from this point is negligible and goes into the remainder. On the other hand, the variation of the cost functional far from the splitting/merging point in $d \geq 3$ dimensions is no longer negligible since $J_1(\phi + th)$ is differentiable. Therefore, the procedure for the asymptotic expansion for $d = 2$ is different from the case $d \geq 3$.

In this paper, we compute the asymptotic expansion for the case $d = 2$, which implies $q = 1$. This means that the nondegenerate critical point $p = 0$ is a saddle point of ϕ, and, in view of Theorem 4, ϕ is locally diffeomorphic to a function $\phi \circ \psi$ whose zero level set is the union of two cones connected at their vertex; see Figure 1. The main result of this section is the asymptotic expansion of a domain integral in the splitting/merging case.

THEOREM 9. *Let* $d = 2$*,* $q = 1$*, and* $f, h \in \mathcal{C}^\infty(\mathcal{D})$*. Let* $J_1(\phi)$ *be given by* (60)*, and let* $0 \in \partial\Omega_\phi$ *be a critical, nondegenerate point of* ϕ*. Assume that* $f(0) \neq 0$*,*

$h(0) \neq 0$, *and* $|\nabla\phi| > 0$ *on* $\partial\Omega_\phi \setminus \{0\}$. *Then* $\det D^2\phi(0) < 0$ *and we have*

$$J_1(\phi + th) - J_1(\phi) = -\frac{2h(0)f(0)}{|\det D^2\phi(0)|^{1/2}} t|\ln(t)| + \mathcal{O}(t). \tag{74}$$

Remark 3. In Theorem 9, the assumption $h(0) \neq 0$ is required so that merging or splitting occurs. The case $h(0) < 0$ corresponds to a merging locally around 0, and the case $h(0) > 0$ corresponds to a splitting of Ω_ϕ; see Figure 1.

Proof. Since $q = 1$, applying Corollary 4.2, there exists a set $\widehat{X} = X \times (-\tau_2, \tau_2)$ such that

$$\phi(\psi(x,t)) + th(\psi(x,t)) = \phi(0) - x_1^2 + x_2^2 + v(t) \quad \text{ for all } (x,t) \in \widehat{X}.$$

For convenience, we use the notation $\psi_t := \psi(\cdot, t)$ and the notation ψ_t^{-1} for the inverse function of ψ_t for fixed t. Let $\mathcal{X} \subset X$ be open and such that $0 \in \mathcal{X}$. Let τ_3 be such that $0 < \tau_3 < \min(\tau_1, \tau_2)$, where τ_1 is given by Lemma 3.3. Introduce, for $0 < t \leq \tau_3$,

$$\omega_0 := \psi_0^{-1}(\Omega_\phi) \cap \mathcal{X} = \{x \in \mathcal{X} \mid -x_1^2 + x_2^2 < 0\},$$
$$\omega_t := \psi_t^{-1}(\Omega_{\phi+th}) \cap \mathcal{X} = \{x \in \mathcal{X} \mid -x_1^2 + x_2^2 < -v(t)\}.$$

In the proof, we assume $h(0) < 0$; the case $h(0) > 0$ can be treated in a similar way. In view of Corollary 4.2(ii) and $t \geq 0$, we have $v(t) \leq 0$ for t sufficiently small. Therefore, $\omega_0 \subset \omega_t$. We shall continue with the decomposition

$$J_1(\phi + th) - J_1(\phi) = I_1 + I_2 + I_3,$$

where

$$I_1 := \int_{\Omega_{\phi+th} \setminus \psi_t(\mathcal{X})} f(x)dx - \int_{\Omega_\phi \setminus \psi_0(\mathcal{X})} f(x)dx, \qquad I_2 := g(0,t) \int_{\omega_t \setminus \overline{\omega_0}} 1dx,$$
$$I_3 := \int_{\omega_t \setminus \overline{\omega_0}} g(x,t) - g(0,t)dx,$$

where we have used the changes of variables $x \to \psi(x,t)$ and $x \to \psi(x,0)$ inside the integrals and we use the notation

$$g(x,t) := f(\psi(x,t))|\det D\psi(x,t)|.$$

Next we estimate the terms I_i, $i = 1, 2, 3$. We show that the term of order $t|\ln(t)|$ in (74) comes from I_2, while the other terms are of order t and enter the remainder. To compute I_2, we need the expansion of the volume $|\omega_t \setminus \overline{\omega_0}|$. It has been shown in [17] that in two dimensions, this expansion is of order $t\ln(t)$, and therefore $J(\phi + th)$ is not differentiable. Our goal here is to compute the precise value of the coefficient of the expansion of I_2.

Step 1: *Calculation of* I_2. In view of the simple geometry of ω_t, we can use explicit calculations to estimate I_2. We introduce the rotation $r(u) = x = (x_1, x_2)$, with $u = (u_1, u_2)$, $x_1 = (u_1 - u_2)/\sqrt{2}$, and $x_2 = (u_1 + u_2)/\sqrt{2}$, so that $2u_1u_2 = x_2^2 - x_1^2$. This yields

$$r^{-1}(\omega_t \setminus \overline{\omega_0}) = \{(u_1, u_2) \in r^{-1}(\mathcal{X}) \mid 0 < 2u_1u_2 < -v(t)\}.$$

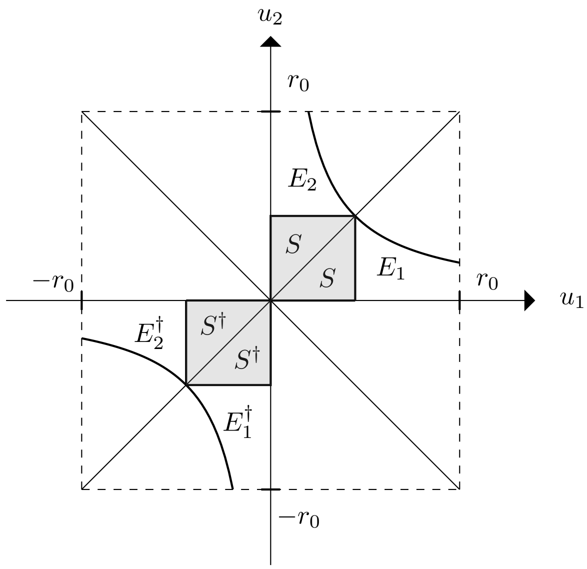


FIG. 2. *The sets* E_1, E_2, S, $E_1^\dagger$, $E_2^\dagger$, *and* $S^\dagger$.

We can now choose the neighborhood $\mathcal{X}$ such that $r^{-1}(\mathcal{X}) = (-r_0, r_0)^2$ for some $r_0 > 0$. Since r is a rotation, we take

$$\mathcal{X} := r((-r_0, r_0)^2) = \{x \in \mathbb{R}^2 \mid |x_1| + |x_2| < \sqrt{2}r_0\}. \tag{75}$$

Since the intersection of the line $u_2 = u_1$ and of the curve $u_2 = -v(t)/2u_1$ for $u_1 > 0$ is the point $(\sqrt{-v(t)/2}, \sqrt{-v(t)/2})$, we can partition $r^{-1}(\omega_t \setminus \overline{\omega_0})$ into six regions

$$r^{-1}(\omega_t \setminus \overline{\omega_0}) = E_1 \cup E_2 \cup S \cup E_1^\dagger \cup E_2^\dagger \cup S^\dagger, \tag{76}$$

where $S := \left[0, \sqrt{-v(t)/2}\right]^2$,

$$E_1 := \left\{ (u_1, u_2) \in \mathbb{R}^2 \;\middle|\; \sqrt{\frac{-v(t)}{2}} < u_1 < r_0 \text{ and } 0 < u_2 < \frac{-v(t)}{2u_1} \right\},$$

and E_2 is the image of E_1 for the reflection with respect to the line $u_2 = u_1$, while $E_1^\dagger$, $E_2^\dagger$, $S^\dagger$ are the images of E_1, E_2, S for the reflection with respect to the line $u_2 = -u_1$, respectively; see Figure 2. Using (76) and a change of variables inside the integral, it is easy to see that

$$\begin{aligned}\int_{\omega_t \setminus \overline{\omega_0}} 1 dx = \int_{r^{-1}(\omega_t \setminus \overline{\omega_0})} 1 du = 2|S| + 4|E_1| = -2\frac{v(t)}{2} + 4\int_{\sqrt{\frac{-v(t)}{2}}}^{r_0} \frac{-v(t)}{2u_1} du_1 \\ = -v(t) - 2v(t)(\ln(r_0) - \ln(\sqrt{-v(t)/2})) = -h(0)t|\ln(t)| + \mathcal{O}(t),\end{aligned}$$

where we have used that $v(t) = th(0) + \mathcal{O}(t^2)$. Using (59) at $t = 0$ and the smoothness of ψ with respect to t, obtained in Corollary 4.2, we get

$$\begin{aligned}g(0,t) = f(\psi(0,t))|\det D\psi(0,t)| = f(\psi(0,0))|\det D\psi(0,0)| + \mathcal{O}(t) \\ = \frac{2f(0)}{\sqrt{-\det(D^2\phi(0))}} + \mathcal{O}(t).\end{aligned} \tag{77}$$

Observe that $-\det(D^2\phi(0)) > 0$ since $q = 1$. Finally, we obtain

$$I_2 = -\frac{2h(0)f(0)}{\sqrt{-\det(D^2\phi(0))}} t|\ln(t)| + \mathcal{O}(t).$$

Note that the leading term of I_2 is independent of the choice of the parameter r_0; indeed, all the terms depending on r_0 are in the remainder $\mathcal{O}(t)$.

Step 2: *Estimate of* I_3. Introducing $g_r(u,t) := g(r(u),t)$, we have

$$\begin{aligned} I_3 &= \int_{\omega_t \setminus \overline{\omega_0}} g(x,t) - g(0,t)dx = \int_{r^{-1}(\omega_t \setminus \overline{\omega_0})} g_r(u,t) - g_r(0,t)du \\ &= \int_{r^{-1}(\omega_t \setminus \overline{\omega_0})} u \cdot \nabla g_r(\eta(u,t),t)du, \end{aligned}$$

where $\eta(u,t) \in r^{-1}(\omega_t \setminus \overline{\omega_0})$. A straightforward explicit calculation provides

$$|I_3| \le \sum_{i=1}^{2} \|\partial_{u_i} g_r\|_{L^\infty((-r_0,r_0)^2 \times [0,\tau_3])} \int_{r^{-1}(\omega_t \setminus \overline{\omega_0})} |u_i| du = \mathcal{O}(t).$$

Step 3: *Estimate of* I_1. We use the decomposition $I_1 = I_{11} + I_{12}$, with

$$\begin{aligned} I_{11} &:= \int_{\Omega_{\phi+th} \setminus T_t(\psi_0(\mathcal{X}))} f(x)dx - \int_{\Omega_\phi \setminus \psi_0(\mathcal{X})} f(x)dx, \\ I_{12} &:= \int_{\Omega_{\phi+th} \setminus \psi_t(\mathcal{X})} f(x)dx - \int_{\Omega_{\phi+th} \setminus T_t(\psi_0(\mathcal{X}))} f(x)dx, \end{aligned}$$

where T is the restriction to $\mathcal{D} \times [0,\tau_3]$ of T given by Lemma 3.3. We observe that the assumptions of Lemma 3.3 are satisfied, choosing $\mathcal{A} = \psi_0(\mathcal{X})$, since $|\nabla\phi| > 0$ on $\partial\Omega_\phi \setminus \psi_0(\mathcal{X})$. In view of item (v) of Lemma 3.3, we have

$$T(\Omega_\phi \setminus \psi_0(\mathcal{X}), t) = \Omega_{\phi+th} \setminus T(\psi_0(\mathcal{X}), t).$$

Using the change of variables $x \to T_t(x)$, we get

$$I_{11} = \int_{\Omega_\phi \setminus \psi_0(\mathcal{X})} f(T(x,t))|\det DT(x,t)| - f(x)dx. \tag{78}$$

In view of Lemma 3.3, we have $T \in \mathcal{C}^\infty(\mathcal{D} \times [0,\tau_3], \mathcal{D})$ and $T(\cdot,0) = \mathcal{I}$. Thus, reducing τ_3 if necessary, we have $|\det DT(x,t)| = \det DT(x,t) > 0$ for all $(x,t) \in \mathcal{D} \times [0,\tau_3]$, and using a Taylor expansion, we get

$$|I_{11}| \le t|\Omega_\phi \setminus \psi_0(\mathcal{X})| \cdot \|\partial_t (f \circ T \det DT)\|_{L^\infty(\mathcal{D} \times [0,\tau_3])}.$$

For I_{12}, we can write $|I_{12}| \le |I_{121}| + |I_{122}|$, where

$$\begin{aligned} I_{121} &:= \int_{\Omega_{\phi+th} \cap \psi_t(\mathcal{X})^c} f(x)dx - \int_{\Omega_{\phi+th} \cap \psi_0(\mathcal{X})^c} f(x)dx, \\ I_{122} &:= \int_{\Omega_{\phi+th} \cap \psi_0(\mathcal{X})^c} f(x)dx - \int_{\Omega_{\phi+th} \cap (T_t(\psi_0(\mathcal{X})))^c} f(x)dx. \end{aligned}$$

Then we also have

$$I_{121} = \int_{\Omega_{\phi+th}} f(x)(\chi_{\psi_t(\mathcal{X})^c} - \chi_{\psi_0(\mathcal{X})^c})dx = -\int_{\Omega_{\phi+th}} f(x)(\chi_{\psi_t(\mathcal{X})} - \chi_{\psi_0(\mathcal{X})})dx$$
$$= \int_{\Omega_{\phi+th}\cap(\psi_t(\mathcal{X})\triangle\psi_0(\mathcal{X}))} f(x)(\chi_{\psi_0(\mathcal{X})} - \chi_{\psi_t(\mathcal{X})})dx,$$

where $\triangle$ denotes the symmetric difference of two sets. To estimate $|I_{121}|$, we proceed with the change of variables $x \to \psi_0(x)$ inside the integral. Note that, if necessary, we can reduce the size of $\mathcal{X}$ and τ_3 to have $\psi_t(\mathcal{X})\triangle\psi_0(\mathcal{X}) \subset \psi_0(X)$ for $t \in [0, \tau_3]$ since $\mathcal{X} \subset X$. Thus, we have $\psi_0^{-1}(\Omega_{\phi+th} \cap (\psi_t(\mathcal{X})\triangle\psi_0(\mathcal{X}))) \subset X$, and we can proceed with the change of variables $x \to \psi_0(x)$ in I_{121}. This yields

$$|I_{121}| \le \left| \int_{\psi_0^{-1}(\Omega_{\phi+th}\cap(\psi_t(\mathcal{X})\triangle\psi_0(\mathcal{X})))} g(x,0)\left(\chi_{\mathcal{X}} - \chi_{\widehat{\mathcal{X}}_t}\right) dx \right|$$
$$\le \|g(\cdot,0)\|_{L^\infty(X)} \int_X \left|\chi_{\mathcal{X}} - \chi_{\widehat{\mathcal{X}}_t}\right| dx,$$

where $\widehat{\mathcal{X}}_t := \psi_0^{-1}(\psi_t(\mathcal{X}))$. Applying Lemma A.1, with $\mathcal{V} = \overline{\mathcal{X}}$ and $\mathcal{T}(\cdot,t) = \psi_0^{-1} \circ \psi_t$, we get

$$d_H(\overline{\mathcal{X}}, \overline{\widehat{\mathcal{X}}_t}) \le c_1 t, \tag{79}$$

where $c_1 := \|\partial_t(\psi_0^{-1} \circ \psi)\|_{L^\infty(\overline{\mathcal{X}}\times[0,\tau_3])}$. To continue the estimate of $|I_{121}|$, introduce

$$\mathfrak{X}_t := \{x \in \mathbb{R}^2 \mid \sqrt{2}(r_0 - c_1 t) \le |x_1| + |x_2| \le \sqrt{2}(r_0 + c_1 t)\}.$$

Estimate (79) implies $\overline{\mathcal{X}} \triangle \overline{\widehat{\mathcal{X}}_t} \subset \mathfrak{X}_t$ and $\left|\chi_{\mathcal{X}} - \chi_{\widehat{\mathcal{X}}_t}\right| \le \chi_{\mathfrak{X}_t}$. It follows that

$$|I_{121}| \le \|g(\cdot,0)\|_{L^\infty(X)} \int_X \chi_{\mathfrak{X}_t} dx = \mathcal{O}(t).$$

We proceed in a similar way to estimate I_{122}, which yields

$$|I_{122}| \le \|g(\cdot,0)\|_{L^\infty(X)} \int_X \left|\chi_{\mathcal{X}} - \chi_{\psi_0^{-1}(T_t(\psi_0(\mathcal{X})))}\right| dx = \mathcal{O}(t).$$

Thus, we obtain $|I_{12}| \le |I_{121}| + |I_{122}| = \mathcal{O}(t)$. Finally, gathering the previous results, we obtain (74). ∎

4.5. The splitting/merging case for boundary integrals. The proof of Theorem 9 cannot be straightforwardly extended to the case of boundary integrals. Some of the ideas of the proof of Theorem 9 can be used, but most of the time we are facing more complicated estimates. The first term of the expansion for boundary integrals is of order $t^{1/2}$, which is more singular than the term $t|\ln(t)|$ obtained for domain integrals. The main result is the following.

THEOREM 10. *Let $d = 2$, $q = 1$, $t \ge 0$, and $f, h \in \mathcal{C}^\infty(\mathcal{D})$. Let $J_2(\phi)$ be given by (69), and let $0 \in \partial\Omega_\phi$ be a critical, nondegenerate point of ϕ. Assume that $f(0) \neq 0$, $h(0) \neq 0$, and $|\nabla\phi| > 0$ on $\partial\Omega_\phi \setminus \{0\}$. Denote by $\lambda^+ > 0 > \lambda^-$ the eigenvalues of $D^2\phi(0)$. Then* $\det D^2\phi(0) < 0$ *and we have*

$$J_2(\phi + th) - J_2(\phi) = c_\phi^h f(0) \left| \frac{h(0)}{\det(D^2\phi(0))} \right|^{1/2} t^{1/2} + o(t^{1/2}), \tag{80}$$

where $c^h_\phi := c_\phi(\lambda^+, -\lambda^-)$ *if* $h(0) < 0$ *and* $c^h_\phi := c_\phi(-\lambda^-, \lambda^+)$ *if* $h(0) > 0$*, with*

$$c_\phi(a,b) := 2\sqrt{2}\left[-(a+b)^{1/2} + \int_0^{+\infty} 2(a\,\mathrm{ch}(u)^2 + b\,\mathrm{sh}(u)^2)^{1/2} - e^u(a+b)^{1/2}du\right].$$

Remark 4. Using $0 \le -\lambda^- \mathrm{sh}(u)^2 < -\lambda^- \mathrm{ch}(u)^2$, we get for $h(0) < 0$,

$$\begin{aligned} c^h_\phi &< 2\sqrt{2}\left[-(\lambda^+ - \lambda^-)^{1/2} + \int_0^{+\infty} 2(\lambda^+ \mathrm{ch}(u)^2 - \lambda^- \mathrm{ch}(u)^2)^{1/2} - e^u(\lambda^+ - \lambda^-)^{1/2}du\right] \\ &< -2\sqrt{2}(\lambda^+ - \lambda^-)^{1/2} + 2\sqrt{2}(\lambda^+ - \lambda^-)^{1/2} = 0. \end{aligned}$$

In a similar way, we also have $c^h_\phi < 0$ for $h(0) > 0$. Thus, we observe that independently of the sign of $h(0)$, the sign of $J_2(\phi + th) - J_2(\phi)$ is equal to the sign of $-f(0)$. Indeed, roughly speaking, Ω_ϕ is similar to two cones touching at their vertex locally around 0. After a merging or a splitting, the two cones are rounded at their vertex or are merging, so that the perimeter decreases locally around 0; therefore, the perimeter of $\partial\Omega_\phi$ should be larger than the perimeter of $\partial\Omega_{\phi+th}$; see Figure 1.

Proof. Step 1: *Geometry and notations.* In view of Corollary 4.2, we can choose τ_3 with $\min(\tau_1, \tau_2) > \tau_3 > 0$, where τ_1 is given by Lemma 3.3, and a neighborhood $\mathcal{S}$ of 0 such that for all $0 < t \le \tau_3$, $\psi_t^{-1}(\partial\Omega_{\phi+th}) \cap \mathcal{S}$ coincides exactly with the points satisfying $-x_1^2 + x_2^2 = -v(t)$ in $\mathcal{S}$. Throughout the proof, we assume $h(0) < 0$; the case $h(0) > 0$ will be discussed in the conclusion. Thus, we have $-v(t) \ge 0$ for t sufficiently small.

We choose

$$\mathcal{S} := [-s_1, s_1] \times [-s_2, s_2] \quad \text{and} \quad \varpi_t := \{x \in \mathcal{S} \mid -x_1^2 + x_2^2 = -v(t)\},$$

with $s_1 > 0$ sufficiently small and $s_2 := \sqrt{s_1^2 - v(\tau_3)} \ge s_1$ so that $\psi_t^{-1}(\partial\Omega_{\phi+th}) \cap \mathcal{S} = \varpi_t$. Let n_{ϖ_t} be a unit normal vector to ϖ_t, chosen such that $n_{\varpi_t}(x_1, x_2) \cdot (0,1) = \mathrm{sign}(x_2)$. Introduce

$$\begin{aligned} \varpi_t^{\mathrm{n}} &:= \{x \in \mathcal{S} \mid -x_1^2 + x_2^2 = -v(t) \text{ and } x_2 \ge 0\}, \\ \varpi_t^{\mathrm{s}} &:= \{x \in \mathcal{S} \mid -x_1^2 + x_2^2 = -v(t) \text{ and } x_2 \le 0\}. \end{aligned}$$

The exponents "n" and "s" stand for "north" and "south," respectively. Introduce, for $t > 0$, $\varpi_t^{\mathrm{ne}} := \{x \in \varpi_t^{\mathrm{n}} \mid x_1 \ge 0\}$ and $\varpi_t^{\mathrm{nw}} := \{x \in \varpi_t^{\mathrm{n}} \mid x_1 \le 0\}$, so that $\varpi_t^{\mathrm{n}} = \varpi_t^{\mathrm{ne}} \cup \varpi_t^{\mathrm{nw}}$, where the exponents "ne" and "nw" stand for "north-east" and "north-west," respectively. Let $0 < \delta < 1/2$, and introduce

$$\varpi_{t,\delta}^{\mathrm{ne}} := \{x \in \varpi_t^{\mathrm{ne}} \mid 0 \le x_1 \le \varepsilon^{1-\delta}\}.$$

The sets $\varpi_{t,\delta}^{\mathrm{nw}}$, ϖ_t^{se}, ϖ_t^{sw}, $\varpi_{t,\delta}^{\mathrm{se}}$, and $\varpi_{t,\delta}^{\mathrm{sw}}$ are defined in a similar way, with "se" and "sw" corresponding to "south-east" and "south-west," respectively. See Figure 3 for a description of the geometry.

We also define $\mathcal{C}_k := \{x_2 = (-1)^{k+1}x_1\} \cap \mathcal{S}$, $k = 1, 2$, $\mathcal{C}_1^{\mathrm{ne}} := \{x \in \mathcal{C}_1 \mid x_1 \ge 0\}$, $\mathcal{C}_1^{\mathrm{sw}} := \{x \in \mathcal{C}_1 \mid x_1 \le 0\}$, and $\mathcal{C}_{1,\delta}^{\mathrm{ne}} := \{x \in \mathcal{C}_1^{\mathrm{ne}} \mid \varepsilon^{1-\delta} \ge x_1 \ge 0\}$ and the normal vectors $n_{\mathcal{C}_k} = ((-1)^k, 1)/\sqrt{2}$.

Step 2: *Decomposition of* $J_2(\phi + th) - J_2(\phi)$. We write

$$J_2(\phi + th) - J_2(\phi) = I_1 + I_2 + I_3,$$

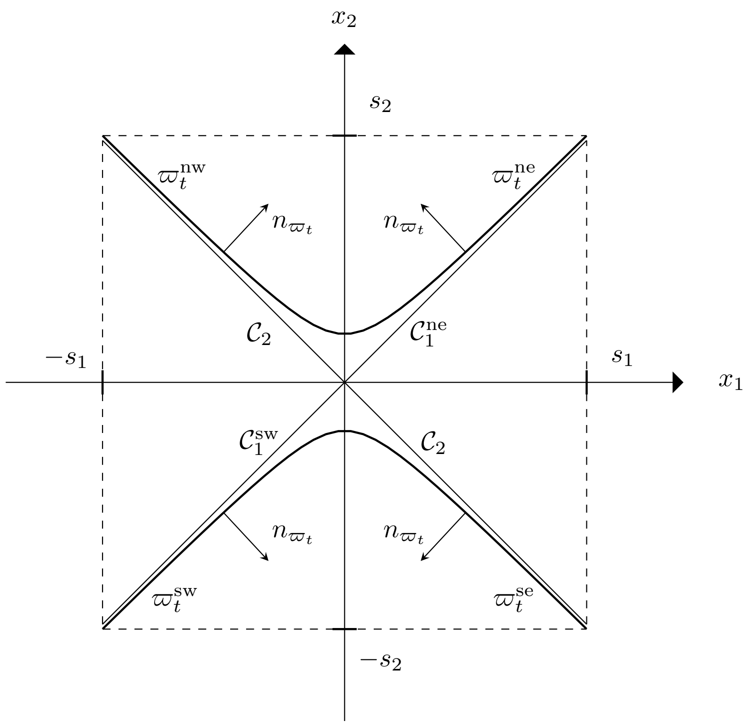


FIG. 3. *The sets* $\varpi_t = \varpi_t^{\mathrm{n}} \cup \varpi_t^{\mathrm{s}} = \varpi_t^{\mathrm{ne}} \cup \varpi_t^{\mathrm{nw}} \cup \varpi_t^{\mathrm{se}} \cup \varpi_t^{\mathrm{sw}}$ *and* $\mathcal{S} = [-s_1, s_1] \times [-s_2, s_2]$.

where

(81)
$$I_1 := \int_{\partial\Omega_{\phi+th}\setminus\psi_t(\mathcal{S})} f(x)\, ds_x - \int_{\partial\Omega_\phi\setminus\psi_0(\mathcal{S})} f(x)\, ds_x,$$
$$I_2 := \int_{\partial\Omega_{\phi+th}\cap\psi_t(\mathcal{S})} f(x)\, ds_x, \qquad I_3 := -\int_{\partial\Omega_\phi\cap\psi_0(\mathcal{S})} f(x)\, ds_x.$$

To compute I_3, we would like to use the change of variables $x \to \psi_0(x)$. However, the set $\partial\Omega_\phi \cap \psi_0(\mathcal{S})$ is not smooth since it has a pinch at the point 0; therefore, one needs to be careful with the change of variables. We also have $\nabla\phi(0) = 0$, so the normal vector $n_{\varpi_0}(0)$ is not well-defined. To define I_3 properly, consider the splitting

(82)
$$I_3 = -\int_{\partial\Omega_\phi\cap\psi_0(\mathcal{S})} f(x)\, ds_x = -\int_{\psi_0(\mathcal{C}_1)} f(x)\, ds_x - \int_{\psi_0(\mathcal{C}_2)} f(x)\, ds_x.$$

Then we can apply the change of variables $x \to \psi_0(x)$ in each integral; this gives

(83)
$$I_3 = -\int_{\mathcal{C}_1} g_{\mathcal{C}_1}(x)\, ds_x - \int_{\mathcal{C}_2} g_{\mathcal{C}_2}(x)\, ds_x,$$

where

(84)
$$g_{\mathcal{C}_k}(x) := f(\psi(x,0))|\det D\psi(x,0)| \cdot |D\psi(x,0)^{-\mathsf{T}} n_{\mathcal{C}_k}|, \qquad k = 1, 2.$$

Step 3: *Decomposition of* I_2. For $t > 0$, introduce the notation

(85)
$$g_\Gamma(x,t) := g_1(x,t)|g_2(x,t)g_3(x,t)|,$$

with $g_1(x,t) := f(\psi(x,t))|\det D\psi(x,t)|$, $g_2(x,t) := D\psi(x,t)^{-\mathsf{T}}$, $g_3(x,t) := n_{\varpi_t}(x)$. Using the change of variables $x \to \psi_t(x)$, we get

$$I_2 := \int_{\varpi_t} f(\psi(x,t))z(t)\, ds_x = \int_{\varpi_t} g_\Gamma(x,t)\, ds_x,$$

where $z(t) := |M(x,t)n_{\varpi_t}(x)|$ and $M(x,t) := \det(D\psi(x,t))D\psi(x,t)^{-\mathsf{T}}$ is the cofactor matrix of $D\psi(x,t)$.

A key feature of the proof is that the main term of the expansion of I_2 will cancel with I_3. We use the decomposition $I_2 = I_2^{\mathrm{n}} + I_2^{\mathrm{s}}$, where

$$I_2^{\mathrm{n}} := \int_{\varpi_t^{\mathrm{n}}} g_\Gamma(x,t)\, ds_x, \qquad I_2^{\mathrm{s}} := \int_{\varpi_t^{s}} g_\Gamma(x,t)\, ds_x.$$

Note that I_2^{s} can be computed similarly to I_2^{n} due to the symmetry, so we compute only I_2^{n} in what follows.

Now we use the decomposition $I_2^{\mathrm{n}} = I_{21}^{\mathrm{n}} + I_{22}^{\mathrm{n}} + I_{23}^{\mathrm{n}}$, where

$$\begin{aligned}
I_{21}^{\mathrm{n}} &:= \int_{\varpi_t^{\mathrm{n}}} (g_1(x,t) - g_1(x,0))|g_2(x,t)g_3(x,t)|\, ds_x,\\
I_{22}^{\mathrm{n}} &:= \int_{\varpi_t^{\mathrm{n}}} g_1(x,0)(|g_2(x,t)g_3(x,t)| - |g_2(x,0)g_3(x,t)|)\, ds_x,\\
I_{23}^{\mathrm{n}} &:= \int_{\varpi_t^{\mathrm{n}}} g_1(x,0)|g_2(x,0)g_3(x,t)|\, ds_x.
\end{aligned}$$

Step 4: *Estimates for I_{21}^{n} and I_{22}^{n}.* In view of Theorem 5(i), the functions ψ and $(x,t) \mapsto \psi^{-1}(x,t)$ are smooth in $\mathcal{S}\times[0,\tau_3]$ for τ_3 small enough. Hence, since $|n_{\varpi_t}(x)| = 1$, we have that $|g_2(x,t)g_3(x,t)| = |D\psi(x,t)^{-\mathsf{T}}n_{\varpi_t}(x)|$ is uniformly bounded on $\mathcal{S} \times [0,\tau_3]$. Also, g_1 is smooth for t sufficiently small, so we obtain

$$I_{21}^{\mathrm{n}} = \mathcal{O}(t). \tag{86}$$

For I_{22}^{n}, we compute

$$I_{22}^{\mathrm{n}} = \int_{\varpi_t^{\mathrm{n}}} g_1(x,0)\frac{\langle (g_2(x,t) - g_2(x,0))g_3(x,t), (g_2(x,t) + g_2(x,0))g_3(x,t)\rangle}{|g_2(x,t)g_3(x,t)| + |g_2(x,0)g_3(x,t)|}\, ds_x.$$

For s_1 and τ_3 sufficiently small, we have that $g_1(x,0)$, $g_3(x,t)$, and $g_2(x,t) + g_2(x,0)$ are uniformly bounded on $\mathcal{S} \times [0,\tau_3]$, and there exists a constant $c > 0$ such that

$$|g_2(x,t)g_3(x,t)| + |g_2(x,0)g_3(x,t)| \geq c \quad \text{ on } \mathcal{S} \times [0,\tau_3]$$

due to $D\psi(0,0)$ being nonsingular. Since g_2 is smooth in $\mathcal{S} \times [0,\tau_3]$, we obtain

$$I_{22}^{\mathrm{n}} = \mathcal{O}(t). \tag{87}$$

Step 5: *Estimate for I_{23}^{n}.* We proceed with the decomposition $I_{23}^{\mathrm{n}} = I_{23}^{\mathrm{ne}} + I_{23}^{\mathrm{nw}}$, where

$$I_{23}^{\mathrm{ne}} := \int_{\varpi_t^{\mathrm{ne}}} g_1(x,0)|g_2(x,0)g_3(x,t)|\, ds_x, \qquad I_{23}^{\mathrm{nw}} := \int_{\varpi_t^{\mathrm{nw}}} g_1(x,0)|g_2(x,0)g_3(x,t)|\, ds_x.$$

The integral I_{23}^{nw} can be estimated in the same way as I_{23}^{ne}, so we focus on I_{23}^{ne} in what follows.

Using the notation $\varepsilon := \sqrt{-v(t)}$, the curve ϖ_t^{ne} can be parameterized by

$$x(s,t) = \left(s, (s^2+\varepsilon^2)^{1/2}\right) \quad \text{for } 0 \le s \le s_1. \tag{88}$$

To simplify the notations, introduce $K := I_{23}^{\mathrm{ne}}$ and $G_i(s,t,t) := g_i(x(s,t),t)$ for $i = 1,2,3$. We have

$$\begin{aligned} I_{23}^{\mathrm{ne}} = K &= \int_0^{s_1} G_1(s,t,0)|G_2(s,t,0)G_3(s,t,t)| j_\varepsilon \, ds \\ &= K_1(0,t) + K_1(t,s_1) + K_2(0,t) + K_2(t,s_1) \\ &\quad + K_3(0,\varepsilon^{1-\delta}) + K_3(\varepsilon^{1-\delta}, s_1) + K_4, \end{aligned} \tag{89}$$

with

$$j_\varepsilon := \left(\frac{2s^2+\varepsilon^2}{s^2+\varepsilon^2}\right)^{1/2},$$

and

$$\begin{aligned} K_1(a_1,a_2) &:= \int_{a_1}^{a_2} (G_1(s,t,0) - G_1(s,0,0))|G_2(s,t,0)G_3(s,t,t)| j_\varepsilon \, ds, \\ K_2(a_1,a_2) &:= \int_{a_1}^{a_2} G_1(s,0,0) \left(|G_2(s,t,0)G_3(s,t,t)| - |G_2(s,0,0)G_3(s,t,t)|\right) j_\varepsilon \, ds, \\ K_3(a_1,a_2) &:= \int_{a_1}^{a_2} G_1(s,0,0) \left(|G_2(s,0,0)G_3(s,t,t)| - |G_2(s,0,0)n_{\mathcal{C}_1}|\right) j_\varepsilon \, ds, \\ K_4 &:= \int_0^{s_1} G_1(s,0,0)|G_2(s,0,0)n_{\mathcal{C}_1}| j_\varepsilon \, ds. \end{aligned}$$

Since the integrands in $K_1(0,t)$ and $K_2(0,t)$ are clearly uniformly bounded with respect to (s,t), we have

$$|K_1(0,t)| + |K_2(0,t)| = \mathcal{O}(t). \tag{90}$$

To estimate $K_1(t,s_1)$, we use $v'(0) = h(0)$ and we observe that there exists $\eta_t \in (0,t)$, with

$$\begin{aligned} G_1(s,t,0) - G_1(s,0,0) &= t\nabla g_1(x(s,\eta_t),0) \cdot \partial_t x(s,\eta_t) \\ &= t\partial_{x_2} g_1(x(s,\eta_t),0) \frac{-h(0)}{2(s^2-\eta_t h(0))^{1/2}}. \end{aligned}$$

Using the fact that $s^2 - \eta_t h(0) \ge s^2$, due to $h(0) < 0$, and the smoothness of g_1, we get the estimate, for some constant $c > 0$,

$$|K_1(t,s_1)| \le ct \int_t^{s_1} s^{-1} \, ds = ct(\ln(s_1) - \ln(t)) = \mathcal{O}(t|\ln(t)|). \tag{91}$$

To estimate $K_2(t,s_1)$, we write

$$K_2(t,s_1) = \int_t^{s_1} G_1(s,0,0) \frac{\langle \zeta_1^+, \zeta_1^- \rangle}{|G_2(s,t,0)G_3(s,t,t)| + |G_2(s,0,0)G_3(s,t,t)|} j_\varepsilon \, ds,$$

with $\zeta_1^{\pm} := (G_2(s,t,0) \pm G_2(s,0,0))G_3(s,t,t)$. Then we proceed as in the estimate for $K_1(t,s_1)$. We also need the fact that the denominator in $K_2(t,s_1)$ is bounded uniformly from below, which is done in a similar way as for the estimate of I_{22}^{n}; see (87). Thus, we obtain

$$|K_2(t,s_1)| = \mathcal{O}(t|\ln(t)|). \tag{92}$$

Step 6: *Estimate for* $K_3(\varepsilon^{1-\delta}, s_1)$. We have

$$K_3(\varepsilon^{1-\delta}, s_1) = \int_{\varepsilon^{1-\delta}}^{s_1} G_1(s,0,0) \frac{\langle \zeta_2^+, \zeta_2^- \rangle}{|G_2(s,0,0)G_3(s,t,t)| + |G_2(s,0,0)n_{\mathcal{C}_1}|} j_\varepsilon \, ds,$$

with $\zeta_2^{\pm} := G_2(s,0,0)(G_3(s,t,t) \pm n_{\mathcal{C}_1})$. For reasons similar to those in the estimate of $K_2(t,s_1)$, the denominator in $K_3(\varepsilon^{1-\delta}, s_1)$ is uniformly bounded from below. Then $G_1(s,0,0)$, $G_2(s,0,0)$, and $G_3(s,t,t) + n_{\mathcal{C}_1}$ are also uniformly bounded, so we get for some constant $c > 0$,

$$|K_3(\varepsilon^{1-\delta}, s_1)| \le c \int_{\varepsilon^{1-\delta}}^{s_1} |G_3(s,t,t) - n_{\mathcal{C}_1}| \, ds = c \int_{\varepsilon^{1-\delta}}^{s_1} |n_{\varpi_t}(x(s,t)) - n_{\mathcal{C}_1}| \, ds.$$

In view of the parameterization (88), a quick calculation yields

$$n_{\varpi_t}(x(s,t)) = \frac{(-s, (s^2+\varepsilon^2)^{1/2})}{2s^2+\varepsilon^2} \quad \text{for } x(s,t) \in \varpi_t^{\mathrm{ne}}, \tag{93}$$

and then

$$|K_3(\varepsilon^{1-\delta}, s_1)| \le c \int_{\varepsilon^{1-\delta}}^{s_1} \frac{\left[(\sqrt{2s^2+\varepsilon^2} - \sqrt{2s^2})^2 + (\sqrt{2s^2+2\varepsilon^2} - \sqrt{2s^2+\varepsilon^2})^2 \right]^{1/2}}{\sqrt{2s^2+\varepsilon^2}} \, ds.$$

Proceeding with the change of variables $s = \varepsilon u$, a straightforward calculation yields

$$K_3(\varepsilon^{1-\delta}, s_1) = \mathcal{O}(\varepsilon^{1+\delta}). \tag{94}$$

Step 7: *Estimate for* $K_3(0, \varepsilon^{1-\delta})$. We use the decomposition $K_3(0,\varepsilon^{1-\delta}) = K_{31} + K_{32} + K_{33} + K_{34}$, with

$$K_{31} := \int_0^{\varepsilon^{1-\delta}} (G_1(s,0,0) - g_1(0,0)) \left(|G_2(s,0,0)G_3(s,t,t)| - |G_2(s,0,0)n_{\mathcal{C}_1}| \right) j_\varepsilon \, ds,$$

$$K_{32} := \int_0^{\varepsilon^{1-\delta}} g_1(0,0) \left(|G_2(s,0,0)G_3(s,t,t)| - |g_2(0,0)G_3(s,t,t)| \right) j_\varepsilon \, ds,$$

$$K_{33} := \int_0^{\varepsilon^{1-\delta}} g_1(0,0) \left(|g_2(0,0)n_{\mathcal{C}_1}| - |G_2(s,0,0)n_{\mathcal{C}_1}| \right) j_\varepsilon \, ds,$$

$$K_{34} := \int_0^{\varepsilon^{1-\delta}} g_1(0,0) \left(|g_2(0,0)G_3(s,t,t)| - |g_2(0,0)n_{\mathcal{C}_1}| \right) j_\varepsilon \, ds.$$

To estimate K_{31}, we use

$$G_1(s,0,0) - g_1(0,0) = s\nabla g_1(x(\eta_s,0),0) \cdot \partial_s x(\eta_s,0) = s\nabla g_1(x(\eta_s,0),0) \cdot (1,1)$$

for some $\eta_s \in (0, \varepsilon^{1-\delta})$. Since $\nabla g_1(x(\eta_s, 0), 0)$ is uniformly bounded on $(0, \varepsilon^{1-\delta})$, we get

$$|K_{31}| \leq c \int_0^{\varepsilon^{1-\delta}} s\, ds = \mathcal{O}(\varepsilon^{2-2\delta}). \tag{95}$$

In a similar way, we get

$$|K_{32}| + |K_{33}| = \mathcal{O}(\varepsilon^{2-2\delta}). \tag{96}$$

Step 8: *Estimate for* K_{34}. Since $g_2(0,0) = D\psi(0,0)^{-\mathsf{T}}$, we have

$$K_{34} = g_1(0,0) \int_{\varpi_{t,\delta}^{\mathrm{ne}}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}| - g_1(0,0) \int_{\varpi_{t,\delta}^{\mathrm{ne}}} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_1}| = K_{341} + K_{342},$$

with

$$K_{341} := g_1(0,0) \int_{\varpi_{t,\delta}^{\mathrm{ne}}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}| - g_1(0,0) \int_{\mathcal{C}_{1,\delta}^{\mathrm{ne}}} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_1}|, \tag{97}$$

$$K_{342} := g_1(0,0) \int_{\mathcal{C}_{1,\delta}^{\mathrm{ne}}} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_1}| - g_1(0,0) \int_{\varpi_{t,\delta}^{\mathrm{ne}}} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_1}|. \tag{98}$$

Further, K_{341} contributes to the main term of the asymptotic expansion (80) , whereas K_{342} cancels with a part of K_4 from (89).

Step 9: *Estimate for* K_4 *and* I_3. We decompose (82) in the following way:

$$I_3 = -\int_{\psi_0(\mathcal{C}_1)} f(x)\, ds_x - \int_{\psi_0(\mathcal{C}_2)} f(x)\, ds_x = I_3^{\mathrm{ne}} + I_3^{\mathrm{sw}} + I_3^{\mathcal{C}_2}, \tag{99}$$

with

$$I_3^{\mathrm{ne}} := -\int_{\psi_0(\mathcal{C}_1^{\mathrm{ne}})} f(x)\, ds_x, \quad I_3^{\mathrm{sw}} := -\int_{\psi_0(\mathcal{C}_1^{\mathrm{sw}})} f(x)\, ds_x, \quad I_3^{\mathcal{C}_2} := -\int_{\psi_0(\mathcal{C}_2)} f(x)\, ds_x.$$

Now denote $L := K_4 + I_3^{\mathrm{ne}}$, where K_4 is defined in (89). Using a change of variables $x \to \psi_0(x)$ in I_3^{ne}, we can define $L = L_1 + L_2 + L_3 + L_4$, with

$$\begin{aligned}
L_1 &:= \int_{\varepsilon^{1-\delta}}^{s_1} G_1(s,0,0)|G_2(s,0,0)n_{\mathcal{C}_1}|(j_\varepsilon - \sqrt{2})\, ds,\\
L_2 &:= \int_0^{\varepsilon^{1-\delta}} (G_1(s,0,0) - g_1(0,0))|G_2(s,0,0)n_{\mathcal{C}_1}|(j_\varepsilon - \sqrt{2})\, ds,\\
L_3 &:= \int_0^{\varepsilon^{1-\delta}} g_1(0,0)\,(|G_2(s,0,0)n_{\mathcal{C}_1}| - |g_2(0,0)n_{\mathcal{C}_1}|)\,(j_\varepsilon - \sqrt{2})\, ds,\\
L_4 &:= \int_0^{\varepsilon^{1-\delta}} g_1(0,0)|g_2(0,0)n_{\mathcal{C}_1}|(j_\varepsilon - \sqrt{2})\, ds.
\end{aligned}$$

In the same way as we treated K_{31}, K_{32}, and K_{33} in step 7, we get

$$|L_2| + |L_3| = \mathcal{O}(\varepsilon^{2-2\delta}). \tag{100}$$

Now we have

$$L_1 = \int_{\varepsilon^{1-\delta}}^{s_1} G_1(s,0,0)|G_2(s,0,0)n_{\mathcal{C}_1}| \frac{(2s^2+\varepsilon^2)^{1/2} - (2s^2+2\varepsilon^2)^{1/2}}{(s^2+\varepsilon^2)^{1/2}}\, ds.$$

Using the fact that $G_1(s,0,0)$ and $G_2(s,0,0)$ are uniformly bounded on $[\varepsilon^{1-\delta}, s_1]$, and the change of variables $s = \varepsilon u$, we get

$$\begin{aligned}|L_1| &\le c\varepsilon \int_{\varepsilon^{-\delta}}^{s_1\varepsilon^{-1}} \frac{(2u^2+2)^{1/2} - (2u^2+1)^{1/2}}{(u^2+1)^{1/2}}\, du \\ &= c\varepsilon \int_{\varepsilon^{-\delta}}^{s_1\varepsilon^{-1}} \frac{1}{(u^2+1)^{1/2}((2u^2+2)^{1/2} + (2u^2+1)^{1/2})}\, du = \mathcal{O}(\varepsilon^{1+\delta}).\end{aligned} \tag{101}$$

Finally, in view of (98), it is easy to verify that

$$L_4 + K_{342} = 0. \tag{102}$$

Step 10: *Estimate of* I_2. Gathering the decompositions obtained in the previous steps, we have

$$\begin{aligned} I_2 + I_3 &= I_{21}^{\mathrm{n}} + I_{22}^{\mathrm{n}} + I_{23}^{\mathrm{ne}} + I_{23}^{\mathrm{nw}} + I_2^{\mathrm{s}} + I_3 \\ &= K_1(0,t) + K_1(t,s_1) + K_2(0,t) + K_2(t,s_1) + K_3(0,\varepsilon^{1-\delta}) + K_3(\varepsilon^{1-\delta}, s_1) + K_4 \\ &\quad + I_{21}^{\mathrm{n}} + I_{22}^{\mathrm{n}} + I_{23}^{\mathrm{nw}} + I_2^{\mathrm{s}} + I_3^{\mathrm{ne}} + I_3^{\mathrm{sw}} + I_3^{\mathcal{C}_2}, \end{aligned}$$

where we have used (89) and (99). Then using $K_4 + I_3^{\mathrm{ne}} = L = L_1 + L_2 + L_3 + L_4$, $K_3(0,\varepsilon^{1-\delta}) = K_{31} + K_{32} + K_{33} + K_{34}$, and $K_{34} = K_{341} + K_{342}$ we get

$$\begin{aligned} I_2 + I_3 = I_{21}^{\mathrm{n}} + I_{22}^{\mathrm{n}} &+ K_1(0,t) + K_1(t,s_1) + K_2(0,t) + K_2(t,s_1) + K_{31} + K_{32} + K_{33} \\ &+ K_{341} + K_{342} + K_3(\varepsilon^{1-\delta}, s_1) + I_{23}^{\mathrm{nw}} + I_2^{\mathrm{s}} + I_3^{\mathrm{sw}} + I_3^{\mathcal{C}_2} + L_1 + L_2 + L_3 + L_4. \end{aligned}$$

Gathering the estimates (86), (87), (90), (91), (92), (94), (95), (96), (100), (101), we obtain

$$\begin{aligned} |I_{21}^{\mathrm{n}}| + |I_{22}^{\mathrm{n}}| &= \mathcal{O}(t), \\ |K_1(0,t) + K_1(t,s_1) + K_2(0,t) + K_2(t,s_1) + K_3(\varepsilon^{1-\delta}, s_1)| &= \mathcal{O}(t|\ln(t)| + \varepsilon^{1+\delta}), \\ |K_{31} + K_{32} + K_{33}| + |L_2| + |L_3| &= \mathcal{O}(\varepsilon^{2-2\delta}), \\ |L_1| &= \mathcal{O}(\varepsilon^{1+\delta}). \end{aligned}$$

Using these estimates and (102), we get

$$I_2 + I_3 = K_{341} + I_{23}^{\mathrm{nw}} + I_2^{\mathrm{s}} + I_3^{\mathrm{sw}} + I_3^{\mathcal{C}_2} + \mathcal{R}_1, \quad \mathcal{R}_1 = \mathcal{O}(t + t|\ln(t)| + \varepsilon^{1+\delta} + \varepsilon^{2-2\delta}).$$

Regarding the sum $I_{23}^{\mathrm{nw}} + I_2^{\mathrm{s}} + I_3^{\mathrm{sw}} + I_3^{\mathcal{C}_2}$, observe that I_{23}^{nw} is similar to I_{23}^{ne}, except that the integral is on the north-west branch ϖ_t^{nw}. Also, I_2^{s} is similar to I_2^{n}, except that the integral is on the southern part of ϖ_t. Using the symmetries of ϖ_t, the estimates obtained in the previous steps can be straightforwardly adapted. This yields three other terms similar to K_{341} but with the integrals on the other branches "nw," "sw," and "se." Thus, we get, in view of (97),

$$I_2 + I_3 = \mathcal{K} + \mathcal{R}_2, \quad \text{with} \quad \mathcal{R}_2 = \mathcal{O}(t + t|\ln(t)| + \varepsilon^{1+\delta} + \varepsilon^{2-2\delta}),$$

where

$$\mathcal{K} := g_1(0,0) \int_{\varpi_{t,\delta}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}| - g_1(0,0) \int_{\mathcal{C}_\delta} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}}|, \tag{103}$$

with $\mathcal{C}_\delta := \{x \in \mathcal{C} \mid |x_1| \le \varepsilon^{1-\delta}\}$, $\varpi_{t,\delta} := \{x \in \varpi_t \mid |x_1| \le \varepsilon^{1-\delta}\}$, and $n_{\mathcal{C}}$ being either $n_{\mathcal{C}_1}$ or $n_{\mathcal{C}_2}$. In view of Lemma A.2 and $h(0) < 0$, we have

$$I_2 + I_3 = \mathcal{K} + \mathcal{R}_2 = c_\phi^h g_1(0,0)\sqrt{-v(t)}/2 + \mathcal{R}_3, \tag{104}$$

with $g_1(0,0) = f(0)|\det D\psi(0,0)|$ and $\mathcal{R}_3 = \mathcal{O}(t|\ln(t)| + t^{(1+\delta)/2} + t^{1-\delta}) = o(t^{1/2})$.

Step 11: *Estimate of* I_1. In view of (81), we use the splitting $I_1 = I_{11} + I_{12}$, with

$$\begin{aligned} I_{11} &:= \int_{\partial\Omega_{\phi+th}\setminus T_t(\psi_0(\mathcal{S}))} f(x)\, ds_x - \int_{\partial\Omega_\phi\setminus\psi_0(\mathcal{S})} f(x)\, ds_x, \\ I_{12} &:= \int_{\partial\Omega_{\phi+th}\setminus\psi_t(\mathcal{S})} f(x)\, ds_x - \int_{\partial\Omega_{\phi+th}\setminus T_t(\psi_0(\mathcal{S}))} f(x)\, ds_x, \end{aligned}$$

where T is the restriction to $\mathcal{D}\times[0,\tau_3]$ of the function T given by Lemma 3.3 (using that $\tau_3 < \min(\tau_2,\tau_1)$), and we choose $\mathcal{A} = \psi_0(\mathcal{S})$ in Lemma 3.3. To compute I_{11}, we use the change of variables $x \to T_t(x)$ in the first integral; this yields

$$I_{11} = \int_{\partial\Omega_\phi\setminus\psi_0(\mathcal{S})} f(T(x,t))|\det DT(x,t)|\cdot|DT(x,t)^{-\mathsf{T}} n_1(x)| - f(x)\, ds_x,$$

where n_1 is the unit outward normal vector to $\Omega_\phi\setminus\psi_0(\mathcal{S})$. In view of Lemma 3.3, we have $T \in \mathcal{C}^\infty(\mathcal{D}\times[0,\tau_3],\mathcal{D})$ and $T(\cdot,0) = \mathbb{1}$. Thus, using a Taylor expansion we get

$$|I_{11}| \le t|\partial\Omega_\phi\setminus\psi_0(\mathcal{S})|\cdot\|\partial_t(f\circ T|\det DT|\cdot|DT^{-\mathsf{T}}n_1|)\|_{L^\infty(\mathcal{D}\times[0,\tau_3])} = \mathcal{O}(t). \tag{105}$$

Note that $|\det DT|$ and $|DT^{-\mathsf{T}}n_1|$ are smooth with respect to t if τ_3 is small enough since $T(\cdot,0) = \mathbb{1}$ and $|n_1| = 1$.

We also have

$$\begin{aligned} I_{12} &= \int_{\partial\Omega_{\phi+th}} f(x)(\chi_{\psi_t(\mathcal{S})^c} - \chi_{T_t(\psi_0(\mathcal{S}))^c})\, ds_x \\ &= -\int_{\partial\Omega_{\phi+th}} f(x)(\chi_{\psi_t(\mathcal{S})} - \chi_{T_t(\psi_0(\mathcal{S}))})\, ds_x \\ &= \int_{\partial\Omega_{\phi+th}\cap\mathcal{E}_t} f(x)(\chi_{T_t(\psi_0(\mathcal{S}))} - \chi_{\psi_t(\mathcal{S})})\, ds_x, \end{aligned}$$

where $\mathcal{E}_t := \psi_t(\mathcal{S})\triangle T_t(\psi_0(\mathcal{S}))$ and $\triangle$ denotes the symmetric difference of two sets. To estimate I_{12}, we proceed to the change of variables $x \to \psi_t(x)$ in the integral. This gives

$$I_{12} = \int_{\psi_t^{-1}(\partial\Omega_{\phi+th}\cap\mathcal{E}_t)} \widehat{g}_\Gamma(x,t)(\chi_{\widehat{\mathcal{S}}_t} - \chi_{\mathcal{S}})\, ds_x, \tag{106}$$

where $\widehat{g}_\Gamma(x,t) := f(\psi(x,t))|\det D\psi(x,t)|\cdot|D\psi(x,t)^{-\mathsf{T}}n_2(x)|$, with n_2 a unit outward normal vector to $\psi_t^{-1}(\Omega_{\phi+th})$, and $\widehat{\mathcal{S}}_t := \psi_t^{-1}(T_t(\psi_0(\mathcal{S})))$.

Applying Lemma A.1 with $\mathcal{V} = \mathcal{S}$ and $\mathcal{T}(\cdot,t) = \psi_t^{-1}\circ T_t\circ\psi_0$, we get

$$d_H(\mathcal{S},\widehat{\mathcal{S}}_t) \le c_3 t, \tag{107}$$

where $c_3 := \|\partial_t(\psi^{-1}\circ T\circ\psi_0)\|_{L^\infty(\mathcal{S}\times[0,\tau_3])}$. Thus, we have $\mathcal{S}\triangle\widehat{\mathcal{S}}_t \subset \mathfrak{S}_t$, where $\mathfrak{S}_t := \mathcal{S}_t^+\setminus\mathcal{S}_t^-$, with

$$\begin{aligned} \mathcal{S}_t^+ &:= [-s_1 - c_3 t, s_1 + c_3 t]\times[-s_2 - c_3 t, s_2 + c_3 t], \\ \mathcal{S}_t^- &:= [-s_1 + c_3 t, s_1 - c_3 t]\times[-s_2 + c_3 t, s_2 - c_3 t], \end{aligned}$$

and $|\chi_{\mathcal{S}} - \chi_{\widehat{\mathcal{S}}_t}| \leq \chi_{\mathfrak{S}_t}$. The set $\mathfrak{S}_t$ can be seen as a "thickened" boundary of $\mathcal{S}$. Using (106) and $\psi_t^{-1}(\partial\Omega_{\phi+th} \cap \mathcal{E}_t) \subset \mathcal{S} \triangle \widehat{\mathcal{S}}_t \subset \mathfrak{S}_t$, we get

$$
\begin{aligned}
|I_{12}| &\leq \|\widehat{g}_\Gamma\|_{L^\infty(\mathfrak{S}_{\tau_3}\times[0,\tau_3])} \int_{\psi_t^{-1}(\partial\Omega_{\phi+th}\cap\mathcal{E}_t)} \chi_{\mathfrak{S}_t}\, ds_x \\
&\leq \|\widehat{g}_\Gamma\|_{L^\infty(\mathfrak{S}_{\tau_3}\times[0,\tau_3])} \int_{\psi_t^{-1}(\partial\Omega_{\phi+th})\cap\mathfrak{S}_t} 1\, ds_x. \qquad (108)
\end{aligned}
$$

Reducing $\mathcal{S}$ and τ_3 if necessary, we have $\mathfrak{S}_t \subset X$ for $t \leq \tau_3$, where X is the neighborhood of 0 given by Corollary 4.2. Thus, in view of Corollary 4.2, we have the normal form (58) in $\mathfrak{S}_t$, so the set $\psi_t^{-1}(\partial\Omega_{\phi+th}) \cap \mathfrak{S}_t$ is the union of four arcs which can be parameterized using (58). For instance, the north-eastern arc can be parameterized by

$$\left(s, (s^2+\varepsilon^2)^{1/2}\right) \qquad \text{for } s \in [s_1 - c_3 t, s_1 + c_3 t].$$

Thus, we obtain

$$\int_{\psi_t^{-1}(\partial\Omega_{\phi+th})\cap\mathfrak{S}_t} 1\ ds_x \leq 4\int_{s_1-c_3t}^{s_1+c_3t} \left(\frac{2s^2+\varepsilon^2}{s^2+\varepsilon^2}\right)^{1/2} ds = \mathcal{O}(t).$$

Finally, in view of (108), we obtain

$$I_{12} = \mathcal{O}(t). \qquad (109)$$

Step 11: *Conclusion.* We gather (104), (105), (109) and use $v(t) = th(0) + o(t)$ to obtain

$$
\begin{aligned}
J_2(\phi+th) - J_2(\phi) &= I_1 + I_2 + I_3 = I_{11} + I_{12} + I_2 + I_3 \\
&= \frac{c_\phi^h f(0)|\det D\psi(0,0)| t^{1/2}\sqrt{-h(0)}}{2} + \mathcal{R}_4, \qquad (110)
\end{aligned}
$$

with $\mathcal{R}_4 = \mathcal{O}(t|\ln(t)| + t^{(1+\delta)/2} + t^{1-\delta}) = o(t^{1/2})$. We also have, in view of (59),

$$|\det D\psi(0,0)| = \frac{2^{d/2}}{\sqrt{(-1)^q \det D^2\phi(0)}} = \frac{2}{\sqrt{-\det D^2\phi(0)}}.$$

Observe that $h(0)$ and $\det D^2\phi(0)$ are both negative, so the square roots are well-defined, and we have proved (80) in the case $h(0) < 0$.

The case $h(0) > 0$ can be deduced from the case $h(0) < 0$ by observing that

$$\partial\Omega_{\phi+th} = \{\phi + th = 0\} = \{-\phi - th = 0\}.$$

Thus, replacing ϕ by $-\phi$, we can apply the previous results. We obtain the same asymptotic expansion as (110), except that c_ϕ^h is defined using the eigenvalues $\widehat{\lambda}^+ > 0 > \widehat{\lambda}^-$ of $-D^2\phi(0)$ instead of (λ^+, λ^-). Since $\widehat{\lambda}^+ = -\lambda^-$ and $\widehat{\lambda}^- = -\lambda^+$, we obtain (80). ∎

5. Conclusion. In this paper, we have shown how perturbing ϕ rather than Ω_ϕ in the level set method allows us to model and analyze both smooth and singular perturbations of the level set Ω_ϕ. For smooth perturbations, we have obtained results in any dimension and shown that the Gâteaux derivative with respect to ϕ coincides with the shape derivative.

For topological changes corresponding to the creation of an island or a hole, we have shown a correspondence with the notion of topological derivative in any dimension. For topological changes by merging and splitting, we have studied boundary and volume integrals in two dimensions. It is known that topological perturbations of the domain lead to smoother perturbations of the functionals when the dimension increases, so we also expect these functionals to be differentiable in three or higher dimensions. This expectation is reinforced by the results of [17], where it is shown that the volume functional is differentiable for $d \geq 3$.

For applications in shape optimization, one needs to perform the analysis of topological changes by splitting/merging when the objective functional depends on the solution to some partial differential equation. This would be useful, for instance, to analyze level set methods used in structural mechanics. These problems are beyond the scope of this paper but could be the topic of further research. The additional difficulty is that the asymptotic analysis of the solution of the partial differential equation around the splitting/merging point is required; see, for instance, [23] for a related problem. The boundary and volume integrals studied in the present paper, although not involving partial differential equations, are useful for applications since they often appear in applications, for instance to penalize the volume or perimeter.

Appendix A.

LEMMA A.1. *Let $\tilde{\tau} > 0$, and let $\mathcal{T} : \mathbb{R}^2 \times [0, \tilde{\tau}] \to \mathbb{R}^2$ be a smooth function satisfying $\mathcal{T}(\cdot, 0) = \mathbb{1}$. Let $\mathcal{V} \subset \mathbb{R}^2$ be compact, and denote $\widehat{\mathcal{V}}_t := \mathcal{T}(\mathcal{V}, t)$. Let d_H denote the Hausdorff distance for compact sets. Then*

$$d_H(\mathcal{V}, \widehat{\mathcal{V}}_t) \leq t \|\partial_t \mathcal{T}\|_{L^\infty(\mathcal{V}\times[0,\tilde{\tau}])}.$$

Proof. Let $y \in \widehat{\mathcal{V}}_t$; then there exists $x \in \mathcal{V}$ such that $y = \mathcal{T}(x, t)$, and thus

$$d(y, \mathcal{V}) \leq d(y, x) = |\mathcal{T}(x, t) - \mathcal{T}(x, 0)| \leq t \|\partial_t \mathcal{T}\|_{L^\infty(\mathcal{V}\times[0,\tilde{\tau}])}.$$

In a similar way, let $x \in \mathcal{V}$, and denote $y = \mathcal{T}(x, t)$. Then

$$d(x, \widehat{\mathcal{V}}_t) \leq d(x, y) = |\mathcal{T}(x, t) - \mathcal{T}(x, 0)| \leq t \|\partial_t \mathcal{T}\|_{L^\infty(\mathcal{V}\times[0,\tilde{\tau}])}.$$

Using the estimates above we get

$$d_H(\mathcal{V}, \widehat{\mathcal{V}}_t) = \max\left(\sup_{y\in\widehat{\mathcal{V}}_t} d(y, \mathcal{V}), \sup_{x\in\mathcal{V}} d(x, \widehat{\mathcal{V}}_t) \right) \leq t \|\partial_t \mathcal{T}\|_{L^\infty(\mathcal{V}\times[0,\tilde{\tau}])}. \qquad \square$$

LEMMA A.2. *Assuming $h(0) < 0$, and with $\mathcal{K}$ defined in (103), we have*

$$\mathcal{K} = c_\phi^h g_1(0, 0)\sqrt{-v(t)}/2 + \mathfrak{R},$$

with $\mathfrak{R} = \mathcal{O}(\varepsilon^{1+\delta})$ and

$$\begin{aligned} c_\phi^h :=& -2\sqrt{2}(\lambda^+ - \lambda^-)^{1/2} \\ &+ 2\sqrt{2}\int_0^{+\infty} 2(\lambda^+ \operatorname{ch}(u)^2 - \lambda^- \operatorname{sh}(u)^2)^{1/2} - e^u(\lambda^+ - \lambda^-)^{1/2} du. \end{aligned} \tag{111}$$

Proof. Let H be defined as in Lemma 4.1, and recall that $\mathcal{M} = \mathrm{diag}(-1,1)$. In view of Lemma 4.1, H is diagonalizable and has the same eigenvalues as $D^2\phi(0)$. Denote these eigenvalues by λ^-, λ^+, with $\lambda^- < 0 < \lambda^+$. Since H is diagonalizable, there exist matrices Q and $\mathfrak{D} := \mathrm{diag}(\lambda^+, \lambda^-)$, such that $H = Q\mathfrak{D}Q^{-1}$, where the first and second columns of Q are $D\psi(0,0)^{-1}u^+$ and $D\psi(0,0)^{-1}u^-$, respectively, where u^+, u^- are the eigenvectors of $D^2\phi(0)$ associated with λ^+, λ^-. We compute

$$
\begin{aligned}
|D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}| &= \langle D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}, D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}\rangle^{1/2} = \left\langle \frac{1}{2} H\mathcal{M} n_{\varpi_t}, n_{\varpi_t} \right\rangle^{1/2} \\
&= \frac{1}{\sqrt{2}} \langle \mathfrak{D} Q^{-1}\mathcal{M} n_{\varpi_t}, Q^{\mathsf{T}} n_{\varpi_t}\rangle^{1/2}.
\end{aligned}
$$

Let us denote β_{ij}, $1 \le i,j \le 2$, the coefficients of Q. Recall that $\varepsilon = \sqrt{-v(t)}$. We use the parameterization $x(s) = (\varepsilon\,\mathrm{sh}(s), \varepsilon\,\mathrm{ch}(s))$ of $\varpi^{\mathrm{ne}}_{t,\delta}$ for $t > 0$ and $s \in [0, \mathrm{argsh}\,\varepsilon^{-\delta}]$. This yields

$$
n_{\varpi_t^{\mathrm{ne}}} = \frac{(-\mathrm{sh}(s), \mathrm{ch}(s))}{(\mathrm{sh}(s)^2 + \mathrm{ch}(s)^2)^{1/2}},
$$

where $n_{\varpi_t^{\mathrm{ne}}}$ is the restriction of n_{ϖ_t} to ϖ_t^{ne}. A straightforward calculation gives

$$
|D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t^{\mathrm{ne}}}|^2 = \frac{1}{2} \frac{\lambda^+ P(\mathrm{sh}(s), \mathrm{ch}(s)) - \lambda^- P(\mathrm{ch}(s), \mathrm{sh}(s))}{\det Q(\mathrm{sh}(s)^2 + \mathrm{ch}(s)^2)},
$$

where $P(u,v) := -\beta_{11}\beta_{22}u^2 - \beta_{12}\beta_{21}v^2 + (\beta_{11}\beta_{12} + \beta_{21}\beta_{22})uv$. In view of Lemma 4.1, we have

$$
\langle D\psi(0,0)^{-1}u^+, \mathcal{M} D\psi(0,0)^{-1}u^-\rangle = 0.
$$

Since $D\psi(0,0)^{-1}u^+$ and $D\psi(0,0)^{-1}u^-$ are the two columns of Q, this yields $\beta_{11}\beta_{12} = \beta_{21}\beta_{22}$. Thus, we get

$$
(\beta_{11}\beta_{22})(\beta_{12}\beta_{21}) = (\beta_{11}\beta_{12})(\beta_{21}\beta_{22}) = (\beta_{11}\beta_{12})^2 \ge 0;
$$

consequently, $\beta_{11}\beta_{22}$ and $\beta_{12}\beta_{21}$ have the same sign. Further,

$$
\beta_{11}\beta_{12} + \beta_{21}\beta_{22} = 2\beta_{11}\beta_{12} = 2\sigma_1\sqrt{(\beta_{11}\beta_{12})(\beta_{21}\beta_{22})},
$$

where σ_1 is the sign of $\beta_{11}\beta_{12}$. This yields

$$
\begin{aligned}
P(u,v) &= -\beta_{11}\beta_{22}u^2 - \beta_{12}\beta_{21}v^2 + 2\sigma_1\sqrt{(\beta_{11}\beta_{12})(\beta_{21}\beta_{22})}uv. \\
&= \sigma_2(|\beta_{11}\beta_{22}|u^2 + |\beta_{12}\beta_{21}|v^2 + 2\sigma_1\sigma_2\sqrt{(\beta_{11}\beta_{12})(\beta_{21}\beta_{22})}uv) \\
&= \sigma_2(\sqrt{|\beta_{11}\beta_{22}|}u + \sigma\sqrt{|\beta_{12}\beta_{21}|}v)^2,
\end{aligned}
$$

with $\sigma_2 = \mathrm{sign}(-\beta_{11}\beta_{22})$ and $\sigma := \sigma_1\sigma_2$. Using this result, and denoting σ_Q the sign of $\det Q$, we get

$$
|D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t^{\mathrm{ne}}}|^2 = \frac{\sigma_2\sigma_Q\left[\lambda^+(\mu_1\,\mathrm{sh}(s) + \sigma\mu_2\,\mathrm{ch}(s))^2 - \lambda^-(\mu_1\,\mathrm{ch}(s) + \sigma\mu_2\,\mathrm{sh}(s))^2\right]}{2(\mathrm{sh}(s)^2 + \mathrm{ch}(s)^2)},
$$

with

$$
\mu_1 := \sqrt{\frac{|\beta_{11}\beta_{22}|}{|\det Q|}} \quad \text{and} \quad \mu_2 := \sqrt{\frac{|\beta_{12}\beta_{21}|}{|\det Q|}}.
$$

Since $\lambda^- < 0 < \lambda^+$ and $|D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t^{\rm ne}}|^2 > 0$, we must have $\sigma_2\sigma_Q = 1$ in view of the above expression. We also have

$$\mu_2^2 - \mu_1^2 = \frac{|\beta_{12}\beta_{21}| - |\beta_{11}\beta_{22}|}{|\det Q|}.$$

Since $\det Q = \beta_{11}\beta_{22} - \beta_{12}\beta_{21}$ and $\beta_{11}\beta_{22}$ has the same sign as $\beta_{12}\beta_{21}$, we get

$$\mu_2^2 - \mu_1^2 = \sigma_2\sigma_Q = 1.$$

Thus, there exists $\xi \in \mathbb{R}$ such that $\mu_1 = \mathrm{sh}(\xi)$ and $\mu_2 = \mathrm{ch}(\xi)$, and we have

$$\begin{aligned} &|D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t^{\rm ne}}|^2 \\ &= \frac{1}{2}\frac{\lambda^+(\mathrm{sh}(\xi)\,\mathrm{sh}(s) + \sigma\,\mathrm{ch}(\xi)\,\mathrm{ch}(s))^2 - \lambda^-(\mathrm{sh}(\xi)\,\mathrm{ch}(s) + \sigma\,\mathrm{ch}(\xi)\,\mathrm{sh}(s))^2}{\mathrm{sh}(s)^2 + \mathrm{ch}(s)^2}, \\ &= \frac{1}{2}\frac{\lambda^+\,\mathrm{ch}(s+\sigma\xi)^2 - \lambda^-\,\mathrm{sh}(s+\sigma\xi)^2}{\mathrm{sh}(s)^2 + \mathrm{ch}(s)^2}. \end{aligned}$$

Considering that the parameterization for $\varpi_{t,\delta}^{\rm ne}$ is $x(s) = (\varepsilon\,\mathrm{sh}(s), \varepsilon\,\mathrm{ch}(s))$ and using the result above yields

$$\begin{aligned} &\int_{\varpi_{t,\delta}^{\rm ne}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t^{\rm ne}}| \\ &= \frac{1}{\sqrt{2}}\int_0^{\mathrm{argsh}\,\varepsilon^{-\delta}} \left[\frac{\lambda^+\,\mathrm{ch}(s+\sigma\xi)^2 - \lambda^-\,\mathrm{sh}(s+\sigma\xi)^2}{\mathrm{sh}(s)^2 + \mathrm{ch}(s)^2}\right]^{1/2} \varepsilon(\mathrm{sh}(s)^2 + \mathrm{ch}(s)^2)^{1/2} ds \\ &= \frac{\varepsilon}{\sqrt{2}}\int_0^{\mathrm{argsh}\,\varepsilon^{-\delta}} \left[\lambda^+\,\mathrm{ch}(s+\sigma\xi)^2 - \lambda^-\,\mathrm{sh}(s+\sigma\xi)^2\right]^{1/2} ds. \end{aligned}$$

Now, using the change of variables $u = s + \sigma\xi$, we get

$$\int_{\varpi_{t,\delta}^{\rm ne}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t^{\rm ne}}| = \frac{\varepsilon}{\sqrt{2}}\int_{\sigma\xi}^{\mathrm{argsh}\,\varepsilon^{-\delta}+\sigma\xi} \left[\lambda^+\,\mathrm{ch}(u)^2 - \lambda^-\,\mathrm{sh}(u)^2\right]^{1/2} du.$$

For $\varpi_{t,\delta}^{\rm se}$, we use the parameterization $x(s) = (\varepsilon\,\mathrm{sh}(s), -\varepsilon\,\mathrm{ch}(s))$ for $s \in [0, \mathrm{argsh}\,\varepsilon^{-\delta}]$, which yields the normal vector

$$n_{\varpi_t^{\rm se}} = \frac{(-\mathrm{sh}(s), -\mathrm{ch}(s))}{((\mathrm{sh}(s)^2 + \mathrm{ch}(s)^2))^{1/2}}.$$

Thus, the calculation of the integral on the branch $\varpi_{t,\delta}^{\rm se}$ is the same as the calculation on $\varpi_{t,\delta}^{\rm ne}$, but with σ replaced by $-\sigma$, so we obtain

$$\int_{\varpi_{t,\delta}^{\rm se}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t^{\rm se}}| = \frac{\varepsilon}{\sqrt{2}}\int_{-\sigma\xi}^{\mathrm{argsh}\,\varepsilon^{-\delta}-\sigma\xi} \left[\lambda^+\,\mathrm{ch}(u)^2 - \lambda^-\,\mathrm{sh}(u)^2\right]^{1/2} du.$$

For the two other branches "nw" and "sw," we have, due to symmetries,

$$\begin{aligned} \int_{\varpi_{t,\delta}^{\rm nw}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}| &= \int_{\varpi_{t,\delta}^{\rm se}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}|, \\ \int_{\varpi_{t,\delta}^{\rm sw}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}| &= \int_{\varpi_{t,\delta}^{\rm ne}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}|. \end{aligned}$$

Now we compute the second integral appearing in $\mathcal{K}$; see (103). Recalling the definition $\mathcal{C}_{1,\delta}^{\rm ne} = \{x \in \mathcal{C}_1 \mid \varepsilon^{1-\delta} \geq x_1 \geq 0\}$, we have

$$\begin{aligned}
\int_{\mathcal{C}_{1,\delta}^{\rm ne}} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_1}| &= \sqrt{2}\varepsilon^{1-\delta}|D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_1}| = \varepsilon^{1-\delta}\langle \mathfrak{D}Q^{-1}\mathcal{M}n_{\mathcal{C}_1}, Q^{\mathsf{T}} n_{\mathcal{C}_1}\rangle^{1/2}\\
&= \varepsilon^{1-\delta}\left[\frac{\lambda^+ P(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}}) - \lambda^- P(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}})}{\det Q}\right]^{1/2}\\
&= \frac{1}{\sqrt{2}}\varepsilon^{1-\delta}\left[\lambda^+(\mu_1+\sigma\mu_2)^2 - \lambda^-(\mu_1+\sigma\mu_2)^2\right]^{1/2}\\
&= \frac{1}{\sqrt{2}}\varepsilon^{1-\delta}\left[\lambda^+ - \lambda^-\right]^{1/2}|\operatorname{sh}(\xi) + \sigma\operatorname{ch}(\xi)| = \frac{1}{\sqrt{2}}\varepsilon^{1-\delta}\left[\lambda^+ - \lambda^-\right]^{1/2} e^{\sigma\xi}.
\end{aligned}$$

On $\mathcal{C}_{2,\delta}^{\rm se} := \{x \in \mathcal{C}_2 \mid \varepsilon^{1-\delta} \geq x_1 \geq 0\}$ we compute

$$\begin{aligned}
\int_{\mathcal{C}_{2,\delta}^{\rm se}} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_2}| &= \varepsilon^{1-\delta}\left[\frac{\lambda^+ P(-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}}) - \lambda^- P(\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}})}{\det Q}\right]^{1/2}\\
&= \frac{1}{\sqrt{2}}\varepsilon^{1-\delta}\left[\lambda^+(\mu_1-\sigma\mu_2)^2 - \lambda^-(\mu_1-\sigma\mu_2)^2\right]^{1/2}\\
&= \frac{1}{\sqrt{2}}\varepsilon^{1-\delta}\left[\lambda^+ - \lambda^-\right]^{1/2} e^{-\sigma\xi}.
\end{aligned}$$

Next we have

$$\begin{aligned}
\int_{\sigma\xi}^{\operatorname{argsh}\varepsilon^{-\delta}+\sigma\xi} e^u du &= e^{\operatorname{argsh}\varepsilon^{-\delta}+\sigma\xi} - e^{\sigma\xi} = e^{\sigma\xi}(\varepsilon^{-\delta} + \sqrt{1+\varepsilon^{-2\delta}} - 1)\\
&= \varepsilon^{-\delta}e^{\sigma\xi}(1+\sqrt{1+\varepsilon^{2\delta}}) - e^{\sigma\xi} = 2e^{\sigma\xi}\varepsilon^{-\delta} + \mathfrak{R}_1 - e^{\sigma\xi},
\end{aligned}$$

with $\mathfrak{R}_1 = \mathcal{O}(\varepsilon^\delta)$. Thus, we get

$$\begin{aligned}
\int_{\mathcal{C}_{1,\delta}^{\rm ne}} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_1}| &= \frac{1}{\sqrt{2}}\varepsilon^{1-\delta}\left[\lambda^+ - \lambda^-\right]^{1/2} e^{\sigma\xi}\\
&= \frac{\varepsilon}{2\sqrt{2}}\left[\lambda^+ - \lambda^-\right]^{1/2}\left(\int_{\sigma\xi}^{\operatorname{argsh}\varepsilon^{-\delta}+\sigma\xi} e^u du - \mathfrak{R}_1 + e^{\sigma\xi}\right).
\end{aligned}$$

Now we introduce the decomposition $\mathcal{K} = \mathcal{K}^{\rm sw} + \mathcal{K}^{\rm ne} + \mathcal{K}^{\rm se} + \mathcal{K}^{\rm nw}$, with

$$\begin{aligned}
\mathcal{K}^{\rm ne} &:= g_1(0,0)\int_{\varpi_{t,\delta}^{\rm ne}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}| - g_1(0,0)\int_{\mathcal{C}_{1,\delta}^{\rm ne}} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_1}|\\
&= g_1(0,0)\frac{\varepsilon}{\sqrt{2}}\left(\int_{\sigma\xi}^{\operatorname{argsh}\varepsilon^{-\delta}+\sigma\xi}\left[\lambda^+\operatorname{ch}(u)^2 - \lambda^-\operatorname{sh}(u)^2\right]^{1/2} - \left[\lambda^+ - \lambda^-\right]^{1/2}\frac{e^u}{2}du\right)\\
&\quad - g_1(0,0)\frac{\varepsilon}{2\sqrt{2}}\left[\lambda^+ - \lambda^-\right]^{1/2} e^{\sigma\xi} + \mathfrak{R}_2,
\end{aligned}$$

and $\mathfrak{R}_2 = \mathcal{O}(\varepsilon^{1+\delta})$, and a similar definition for the other terms. Then

$$\begin{aligned}&\int_{\sigma\xi}^{\operatorname{argsh}\varepsilon^{-\delta}+\sigma\xi} \left[\lambda^+ \operatorname{ch}(u)^2 - \lambda^- \operatorname{sh}(u)^2\right]^{1/2} - \left[\lambda^+ - \lambda^-\right]^{1/2} \frac{e^u}{2} du \\ &= \int_{\sigma\xi}^{\operatorname{argsh}\varepsilon^{-\delta}+\sigma\xi} \frac{(\lambda^+ - \lambda^-)e^{-2u} + 2(\lambda^+ + \lambda^-)}{4\left[\lambda^+ \operatorname{ch}(u)^2 - \lambda^- \operatorname{sh}(u)^2\right]^{1/2} + 2\left[\lambda^+ - \lambda^-\right]^{1/2} e^u} du \\ &= \Phi(\sigma\xi) + \mathfrak{R}_3,\end{aligned}$$

with

$$\Phi(\sigma\xi) := \int_{\sigma\xi}^{\infty} \frac{(\lambda^+ - \lambda^-)e^{-2u} + 2(\lambda^+ + \lambda^-)}{4\left[\lambda^+ \operatorname{ch}(u)^2 - \lambda^- \operatorname{sh}(u)^2\right]^{1/2} + 2\left[\lambda^+ - \lambda^-\right]^{1/2} e^u} du$$

and

$$\begin{aligned}|\mathfrak{R}_3| &= \left| \int_{\operatorname{argsh}\varepsilon^{-\delta}+\sigma\xi}^{\infty} \frac{(\lambda^+ - \lambda^-)e^{-2u} + 2(\lambda^+ + \lambda^-)}{4\left[\lambda^+ \operatorname{ch}(u)^2 - \lambda^- \operatorname{sh}(u)^2\right]^{1/2} + 2\left[\lambda^+ - \lambda^-\right]^{1/2} e^u} du \right| \\ &\leq c \int_{\operatorname{argsh}\varepsilon^{-\delta}+\sigma\xi}^{\infty} e^{-u} du = c e^{-\operatorname{argsh}\varepsilon^{-\delta} - \sigma\xi} = \frac{e^{-\sigma\xi}}{\varepsilon^{-\delta} + \sqrt{1+\varepsilon^{-2\delta}}} = \mathcal{O}(\varepsilon^{\delta}).\end{aligned}$$

Thus, we obtain

$$\mathcal{K}^{\mathrm{ne}} = g_1(0,0)\frac{\varepsilon}{\sqrt{2}}\Phi(\sigma\xi) - g_1(0,0)\frac{\varepsilon}{2\sqrt{2}}\left[\lambda^+ - \lambda^-\right]^{1/2} e^{\sigma\xi} + \mathfrak{R}_4,$$

with $\mathfrak{R}_4 = \mathcal{O}(\varepsilon^{1+\delta})$. We also have $\mathcal{K}^{\mathrm{sw}} = \mathcal{K}^{\mathrm{ne}}$ due to symmetries.

A similar calculation yields

$$\begin{aligned}\mathcal{K}^{\mathrm{se}} &:= g_1(0,0) \int_{\varpi_{t,\delta}^{\mathrm{se}}} |D\psi(0,0)^{-\mathsf{T}} n_{\varpi_t}| - g_1(0,0) \int_{\mathcal{C}_{2,\delta}^{\mathrm{se}}} |D\psi(0,0)^{-\mathsf{T}} n_{\mathcal{C}_2}| \\ &= g_1(0,0)\frac{\varepsilon}{\sqrt{2}}\Phi(-\sigma\xi) - g_1(0,0)\frac{\varepsilon}{2\sqrt{2}}\left[\lambda^+ - \lambda^-\right]^{1/2} e^{-\sigma\xi} + \mathfrak{R}_5,\end{aligned}$$

with $\mathfrak{R}_5 = \mathcal{O}(\varepsilon^{1+\delta})$ and $\mathcal{K}^{\mathrm{nw}} = \mathcal{K}^{\mathrm{se}}$. Finally, we obtain

$$\begin{aligned}\mathcal{K} &= \mathcal{K}^{\mathrm{sw}} + \mathcal{K}^{\mathrm{ne}} + \mathcal{K}^{\mathrm{se}} + \mathcal{K}^{\mathrm{nw}} \\ &= 2g_1(0,0)\frac{\varepsilon}{\sqrt{2}}(\Phi(-\sigma\xi) + \Phi(\sigma\xi)) - g_1(0,0)\frac{\varepsilon}{\sqrt{2}}\left[\lambda^+ - \lambda^-\right]^{1/2}(e^{\sigma\xi} + e^{-\sigma\xi}) + \mathfrak{R} \\ &= \mathcal{K}_0(\xi) + \mathfrak{R},\end{aligned}$$

with $\mathfrak{R} = \mathcal{O}(\varepsilon^{1+\delta})$ and

$$\mathcal{K}_0(\xi) := \sqrt{2}g_1(0,0)\varepsilon(\Phi(-\xi) + \Phi(\xi)) - \sqrt{2}g_1(0,0)\varepsilon\left[\lambda^+ - \lambda^-\right]^{1/2} \operatorname{ch}(\xi).$$

We compute

$$\begin{aligned}\frac{d\mathcal{K}_0(\xi)}{d\xi} &= \sqrt{2}g_1(0,0)\varepsilon(-\Phi'(-\xi) + \Phi'(\xi)) - \sqrt{2}g_1(0,0)\varepsilon\left[\lambda^+ - \lambda^-\right]^{1/2} \operatorname{sh}(\xi) \\ &= \sqrt{2}g_1(0,0)\varepsilon\left[-(\lambda^+ \operatorname{ch}(\xi)^2 - \lambda^- \operatorname{sh}(\xi)^2)^{1/2} + (\lambda^+ - \lambda^-)^{1/2}\frac{e^{\xi}}{2}\right] \\ &\quad + \sqrt{2}g_1(0,0)\varepsilon\left[(\lambda^+ \operatorname{ch}(\xi)^2 - \lambda^- \operatorname{sh}(\xi)^2)^{1/2} - (\lambda^+ - \lambda^-)^{1/2}\frac{e^{-\xi}}{2}\right] \\ &\quad - \sqrt{2}g_1(0,0)\varepsilon\left[\lambda^+ - \lambda^-\right]^{1/2} \operatorname{sh}(\xi) = 0.\end{aligned}$$

Thus, $\mathcal{K}_0(\xi)$ is constant and we have

$$\mathcal{K}_0(\xi) = \mathcal{K}_0(0) = 2\sqrt{2}g_1(0,0)\varepsilon\Phi(0) - \sqrt{2}g_1(0,0)\varepsilon\left[\lambda^+ - \lambda^-\right]^{1/2}.$$

Defining c_ϕ^h as in (111), we get $\mathcal{K}_0(0) = c_\phi^h g_1(0,0)\sqrt{-v(t)}/2$, proving the lemma. ∎

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