The Calculus of Boundary Variations and the Dielectric Boundary Force in the Poisson–Boltzmann Theory for Molecular Solvation

Bo Li * Zhengfang Zhang † Shenggao Zhou ‡ October 9, 2020

Abstract

In a continuum model of the solvation of charged molecules in an aqueous solvent, the classical Poisson-Boltzmann (PB) theory is generalized to include the solute point charges and the dielectric boundary that separates the high-dielectric solvent from the low-dielectric solutes. With such a setting, we construct an effective electrostatic freeenergy functional of ionic concentrations, where the solute point charges are regularized by a reaction field. We prove that such a functional admits a unique minimizer in a class of admissible ionic concentrations and that the corresponding electrostatic potential is the unique solution to the boundary-value problem of the dielectric-boundary PB equation. The negative first variation of this minimum free energy with respect to variations of the dielectric boundary defines the normal component of the dielectric boundary force. Together with the solute-solvent interfacial tension and van der Waals interaction forces, such boundary force drives an underlying charged molecular system to a stable equilibrium, as described by a variational implicit-solvent model. We develop an L^2 -theory for the continuity and differentiability of solutions to elliptic interface problems with respect to boundary variations, and derive an explicit formula of the dielectric boundary force. With a continuum description, our result of the dielectric boundary force confirms a molecular-level prediction that the electrostatic force points from the high-dielectric and polarizable aqueous solvent to the charged molecules. Our method of analysis is general as it does not rely on any variational principles.

Keywords: Molecular solvation, Poisson–Boltzmann equation, electrostatic free energy, point charges, dielectric boundary force, the calculus of boundary variations.

^{*}Department of Mathematics, University of California, San Diego, 9500 Gilman Drive, MC 0112, La Jolla, CA 92093-0112, USA. Email: bli@math.ucsd.edu

 $^{^\}dagger \text{College}$ of Science, Hangzhou Dianzi University, Hangzhou, Zhejiang 310018, China. Email: zhengfangzhang@hdu.edu.cn

[‡]Department of Mathematics and Mathematical Center for Interdiscipline Research, Soochow University, 1 Shizi Street, Suzhou 215006, Jiangsu, China. Email: sgzhou@suda.edu.cn

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1 Introduction

The classic Poisson–Boltzmann (PB) theory provides a continuum description of electrostatic interactions in an ionic solution through the PB equation [2, 6, 17, 23, 27]

$$\nabla \cdot \varepsilon \nabla \psi - B'(\psi) = -\rho \quad \text{in } \Omega_0, \tag{1.1}$$

where $\Omega_0 \subseteq \mathbb{R}^3$ is the region of the ionic solution, ε is the dielectric coefficient, $\rho: \Omega_0 \to \mathbb{R}$ represents the density of fixed charges, and $\psi: \Omega_0 \to \mathbb{R}$ is the electrostatic potential. In (1.1), the function $B: \mathbb{R} \to \mathbb{R}$ is defined by

$$B(s) = \beta^{-1} \sum_{j=1}^{M} c_j^{\infty} \left(e^{-\beta q_j s} - 1 \right) \qquad \forall s \in \mathbb{R}, \tag{1.2}$$

where $\beta = (k_B T)^{-1}$ with k_B the Boltzmann constant and T the temperature, M is the total number of ionic species, c_j^{∞} is the bulk ionic concentration of the jth ionic species, and $q_j = z_j e$ is the charge of an ion of the jth species with z_j the valence of such an ion and e the elementary charge. The PB equation (1.1) is a combination of Poisson's equation

$$\nabla \cdot \varepsilon \nabla \psi = -\left(\rho + \sum_{j=1}^{M} q_j c_j\right) \quad \text{in } \Omega_0,$$

where $c_j: \Omega_0 \to [0, \infty)$ is the ionic concentration of the jth ionic species, and the Boltzmann distributions for the equilibrium ionic concentrations

$$c_j(x) = c_j^{\infty} e^{-\beta q_j \psi(x)}, \qquad x \in \Omega_0, \ j = 1, \dots, M.$$

In modeling charged molecules (such as proteins) in an aqueous solvent (i.e., water or salted water) within an implicit-solvent (i.e., continuum-solvent) framework, the PB theory is generalized to include the point charges of the charged molecules and a dielectric boundary that separates the high-dielectric solvent region from the low-dielectric solute region [7, 14, 16, 34, 45, 48. To be more specific, let us assume that the entire solvation system occupies a region $\Omega \subset \mathbb{R}^3$. It is the union of three disjoint parts: the region of solutes (i.e., charged molecules) Ω_{-} ; the region of aqueous solvent Ω_{+} ; and the solute-solvent interface or dielectric boundary Γ , which is a closed surface with possibly multiple components, that separates Ω_{-} and Ω_+ ; cf. Figure 1. We denote by n the unit normal to the boundary Γ pointing from $\Omega_$ to Ω_+ and also the exterior unit normal to $\partial\Omega$, the boundary of Ω . The solute region $\Omega_$ contains all the solute atoms that are located at x_1, \ldots, x_N and that carry partial charges Q_1, \ldots, Q_N , respectively, where $N \geq 1$ is a given integer. The solvent region Ω_+ is the region of ionic solution, similar to Ω_0 in (1.1). As before, we assume that there are M species of ions in the solvent region Ω_+ with the valence z_j , charge $q_j = z_j e$, bulk concentration c_i^{∞} , and the local concentration $c_i:\Omega_+\to[0,\infty)$ for the j ionic species $(j=1,\ldots,M)$. The dielectric coefficients in the solute region Ω_{-} and solvent region Ω_{+} are denoted by ε_{-} and ε_+ , respectively. Typically, $\varepsilon_-=1$ and $\varepsilon_+=76\sim80$ in the unit of vacuum permittivity. Note that the density of fixed charges is now given by $\rho = \sum_{i=1}^{N} Q_i \delta_{x_i}$, where δ_{x_i} is the Dirac delta function at x_i .

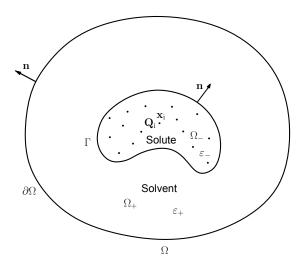


Figure 1: A schematic description of a solvation system with an implicit solvent.

We introduce the dielectric-boundary, electrostatic free-energy functional of the ionic con-

centrations $c = (c_1, \ldots, c_M)$ in the solvent region Ω_+ [7, 24, 34, 44]

$$F_{\Gamma}[c] = \frac{1}{2} \sum_{i=1}^{N} Q_{i}(\psi - \hat{\phi}_{C})(x_{i}) + \frac{1}{2} \int_{\Omega_{+}} \left(\sum_{j=1}^{M} q_{j} c_{j} \right) \psi \, dx$$
$$+ \beta^{-1} \sum_{j=1}^{M} \int_{\Omega_{+}} \left\{ c_{j} \left[\log(\Lambda^{3} c_{j}) - 1 \right] + c_{j}^{\infty} \right\} dx - \sum_{j=1}^{M} \int_{\Omega_{+}} \mu_{j} c_{j} \, dx, \tag{1.3}$$

where Λ is the thermal de Broglie wavelength, μ_j is the chemical potential for ions of the jth species, and $c_j^{\infty} = \Lambda^{-3}e^{\beta\mu_j}$ (j = 1, ..., M). In (1.3), $\psi : \Omega \to \mathbb{R}$ is the electrostatic potential. It is the unique weak solution to the boundary-value problem of Poisson's equation

$$\begin{cases}
\nabla \cdot \varepsilon_{\Gamma} \nabla \psi = -\left(\sum_{i=1}^{N} Q_{i} \delta_{x_{i}} + \chi_{+} \sum_{j=1}^{M} q_{j} c_{j}\right) & \text{in } \Omega, \\
\psi = \phi_{\infty} & \text{on } \partial \Omega,
\end{cases}$$
(1.4)

where the dielectric coefficient $\varepsilon_{\Gamma}:\Omega\to\mathbb{R}$ is defined by

$$\varepsilon_{\Gamma}(x) = \begin{cases} \varepsilon_{-} & \text{if } x \in \Omega_{-}, \\ \varepsilon_{+} & \text{if } x \in \Omega_{+}, \end{cases}$$
 (1.5)

 $\chi_+ = \chi_{\Omega_+}$ is the characteristic function of Ω_+ , and ϕ_{∞} is a given function on the boundary $\partial\Omega$. The function $\hat{\phi}_{\rm C}$ in (1.3) is the Coulomb potential arising from the point charges Q_i at x_i $(i=1,\ldots,N)$ in the medium with the dielectric coefficient ε_- , serving as a reference field. It is given by

$$\hat{\phi}_{\mathcal{C}}(x) = \sum_{i=1}^{N} \frac{Q_i}{4\pi\varepsilon_-|x-x_i|} \qquad \forall x \in \mathbb{R}^3 \setminus \{x_1, \dots, x_N\}.$$
 (1.6)

We prove that the functional $F_{\Gamma}[c]$ has a unique minimizer $c_{\Gamma} = (c_{\Gamma,1}, \ldots, c_{\Gamma,M})$ in a class of admissible concentrations, and derive the equilibrium conditions $\delta_{c_j} F_{\Gamma}[c_{\Gamma}] = 0$ $(j = 1, \ldots, M)$, which lead to the (modified) Botlzmann distributions

$$c_{\Gamma,j} = c_j^{\infty} e^{-\beta q_j(\psi_{\Gamma} - \phi_{\Gamma,\infty}/2)}$$
 in $\Omega_+, j = 1, \dots, M$,

where ψ_{Γ} is the corresponding electrostatic potential and $\phi_{\Gamma,\infty}:\Omega\to\mathbb{R}$ is the unique weak solution to the boundary-value problem

$$\begin{cases} \nabla \cdot \varepsilon_{\Gamma} \nabla \phi_{\Gamma,\infty} = 0 & \text{in } \Omega, \\ \phi_{\Gamma,\infty} = \phi_{\infty} & \text{on } \partial \Omega. \end{cases}$$
 (1.7)

We also prove that ψ_{Γ} is the unique solution to the boundary-value problem of the dielectric-boundary PB equation

$$\begin{cases}
\nabla \cdot \varepsilon_{\Gamma} \nabla \psi - \chi_{+} B' \left(\psi - \frac{\phi_{\Gamma, \infty}}{2} \right) = -\sum_{i=1}^{N} Q_{i} \delta_{x_{i}} & \text{in } \Omega, \\
\psi = \phi_{\infty} & \text{on } \partial \Omega,
\end{cases}$$
(1.8)

where B is given in (1.2); cf. Theorem 2.1 and Theorem 2.2. With the Boltzmann distributions, the minimum free energy min $F_{\Gamma}[\cdot] = F_{\Gamma}[c_{\Gamma}]$ can be expressed via the electrostatic potential ψ_{Γ} . We shall denote this minimum free energy by $E[\Gamma]$, as ultimately it depends on the dielectric boundary Γ .

We define the (normal component of the) dielectric boundary force to be $-\delta_{\Gamma}E[\Gamma]$, the negative first variation of the functional $E[\Gamma]$ with respect to the variation of the boundary Γ . The boundary variation is defined via a smooth vector field. Specifically, let $V: \mathbb{R}^3 \to \mathbb{R}^3$ be a smooth map vanishing outside a small neighborhood of the dielectric boundary Γ . Let x = x(t, X) be the solution map of the dynamical system defined by [3, 18, 30, 46]

$$\frac{dx(t,X)}{dt} = V(x(t,X)) \quad \forall t \in \mathbb{R} \quad \text{and} \quad x(0,X) = X \quad \forall X \in \mathbb{R}^3.$$

Such solution maps define a family of transformations $T_t : \mathbb{R}^3 \to \mathbb{R}^3$ $(t \in \mathbb{R})$ by $T_t(X) = x(t, X)$ for any $X \in \mathbb{R}^3$. The variational derivative (i.e., the shape derivative) of the functional $E[\Gamma]$ in the direction of $V : \mathbb{R}^3 \to \mathbb{R}^3$ is defined to be

$$\delta_{\Gamma,V} E[\Gamma] = \frac{d}{dt} E[\Gamma_t(V)] \bigg|_{t=0},$$

if it exists, where $\Gamma_t(V) = \{x(t,X) : X \in \Gamma\}$ and $E[\Gamma_t(V)]$ is defined similarly using $\Gamma_t(V)$ instead of Γ .

We prove that $\delta_{\Gamma,V}E[\Gamma]$ exists, and is an integral over Γ of the product of $V \cdot n$ and some function that is independent of V, where n is the unit normal along Γ , pointing from Ω_{-} to Ω_{+} . This function on Γ is identified as the variational derivative of $E[\Gamma]$ and is denoted by $\delta_{\Gamma}E[\Gamma]$. We obtain an explicit formula for $\delta_{\Gamma}E[\Gamma]$. If the boundary value $\phi_{\infty}=0$ on Γ , then

$$\delta_{\Gamma} E[\Gamma] = -\frac{1}{2} \left(\frac{1}{\varepsilon_{+}} - \frac{1}{\varepsilon_{-}} \right) \left| \varepsilon_{\Gamma} \partial_{n} \psi_{\Gamma} \right|^{2} + \frac{1}{2} (\varepsilon_{+} - \varepsilon_{-}) \left| \nabla_{\Gamma} \psi_{\Gamma} \right|^{2} + B(\psi_{\Gamma}), \tag{1.9}$$

where ψ_{Γ} is the unique solution to (1.8), $\varepsilon_{\Gamma}\partial_n\psi_{\Gamma}$ is the common value from both sides of Γ , and $\nabla_{\Gamma} = (I - n \otimes n)\nabla$ (with I the 3×3 identity matrix) is the tangential derivative along Γ . Additional terms arise from a general, inhomogeneous boundary value ϕ_{∞} ; cf. Theorem 3.2.

To describe the electrostatic free energy with point charges and to prove the main theorem, Theorem 3.2, we introduce various auxiliary functions that are weak solutions to the boundary-value problems of the operator $-\Delta$ or $-\nabla \cdot \varepsilon_{\Gamma} \nabla$, with or without the point charges $\sum_{i=1}^{N} Q_i \delta_{x_i}$ and with homogeneous or inhomogeneous Dirichlet boundary conditions. We also prove several lemmas, Lemmas 4.1–4.5, on the calculus of boundary variations. Lemma 4.1 is of its own interest. It states that if the vector field V satisfies $V \cdot n = 0$ on the boundary Γ , where n is the unit normal along Γ , then for $|t| \ll 1$ the set $\Gamma_t = \Gamma_t(V)$ is within an $O(t^2)$ -neighborhood of the boundary Γ . Lemmas 4.2–4.5 are on the continuity and differentiability of those functions with respect to boundary variations. Lemma 4.3 states that the " Γ -derivative" of the function $\phi_{\Gamma,\infty}$ which is defined in (1.7) is the unique weak solution

 $\zeta_{\Gamma,V} \in H_0^1(\Omega)$ to the elliptic interface problem $-\nabla \cdot \varepsilon_{\Gamma} \nabla \zeta_{\Gamma,V} = f$ in Ω , where f involves $\phi_{\Gamma,V}$ and V. Moreover,

$$\frac{\phi_{\Gamma_t(V),\infty} \circ T_t - \phi_{\Gamma,\infty}}{t} \to \zeta_{\Gamma,V} \quad \text{in } H^1(\Omega) \quad \text{as } t \to 0.$$

Lemma 4.4 and Lemma 4.5 generalize the result to other Γ -dependent functions, including the electrostatic potential ψ_{Γ} that is the unique soltuion to the boundary-value problem of the dielectric-boundary PB equation (1.8).

We now make several remarks on our results. In our model, we use an inhomogeneous Dirichlet boundary condition for the electrostatic potential (cf. (1.4) and (1.8)) that is common in modeling and analysis [7, 34, 53]. The nonzero Dirichlet boundary value leads to an extra term $\phi_{\Gamma,\infty}/2$ in the Boltzmann distribution and hence in the PB equation (1.8). If there are surface charges on the boundary $\partial\Omega$, then one can also use the Neumann boundary condition for the electrostatic potential on $\partial\Omega$. In that case, the electrostatic energy should include a boundary integral term involving the surface charge density; cf. [36, 41].

If we use the homogeneous Dirichlet boundary condition $\phi_{\infty} = 0$ for the electrostatic potential, then the dielectric boundary force points from the high dielectric solvent region Ω_{+} to the low dielectric solute region Ω_{-} ; cf. (1.9). Such prediction of a macroscopic property is consistent with a microscopic picture of molecular forces that charged solute molecules polarize the surrounding aqueous solvent, which is otherwise electrically neutral, generating an additional electric filed that attracts the solvent to the solutes [13]. In the limiting case where the region Ω_+ is conducting, i.e., the dielectric coefficient in Ω_+ is infinity, then it is expected that no bounded region Ω_{-} will minimize the sum of the electrostatic energy and the surface energy [42]. If a small, high-dielectric solvent region is surrounded by the low-dielectric solute molecules (such as a few water molecules buried in a protein), then the competition between the solute-solvent interfacial tension force and the dielectric boundary force results an equilibrium solute-solvent interface which is however unstable with long-wave perturbations, as shown in the stability analysis in [8]; cf. also [38]. Such analysis explains partially why water molecules in proteins are metastable [51,52]. It remains open to confirm if the dielectric boundary force still points from the high-dielectric solvent region to the low-dielectric solute region for a general inhomogeneous Dirichlet boundary value ϕ_{∞} .

In [4,5,50], the authors use the Maxwell stress tensor to define and derive the dielectric boundary force given an electrostatic potential that is determined by the dielectric-boundary PB equation. The existence of such a stress tensor in the presence of dielectric boundary is implicitly assumed. The shape derivative approach seems first introduced in [35] to define and derive the dielectric boundary force. However, approximations of point charges by smooth functions are made there, and the derivation of the boundary force utilizes heavily on the underlying variational principle that the electrostatic potential extremizes the dielectric-boundary PB free-energy functional. This approach is applied to the electrostatic force acting on membranes [43]. Here, we use the direct calculations to derive the boundary force, which is a more general approach.

Our study of the dielectric boundary force is closely related to the development of a variational implicit-solvent model (VISM) for biomolecules [19,20] (cf. also [9–11,49,53,54]).

Central in the VISM is an effective free-energy functional of all possible dielectric boundaries that consists mainly of the surface energy of solute molecules, solute-solvent van der Waals interaction energy, and continuum electrostatic free energy. Minimization of the free-energy functional with respect to the dielectric boundary yields optimal solute-solvent interfaces, as well as the solvation free energy. Numerical implementation of such minimization requires a formula of the first variation of the VISM function, particularly, the dielectric boundary force. In [37], the authors use the matched asymptotic analysis to derive the sharp-interface limit of a phase-field VISM [47]. In [15], the authors prove the convergence of the free energy and force in the phase-field VISM to their sharp-interface counterparts. In particular, they prove the general result that the variation of the van der Waals-Cahn-Hilliard functional converges to the mean curvature which is the variation of surface area. The recent work [26] is a detailed analysis of the electrostatics in molecular solvation through different scaling regimes arising from the large-number limit of solute particles.

The rest of the paper is organized as follows: In Section 2, we first state our assumptions and introduce some auxiliary functions. We then prove the existence, uniqueness, and bounds for the solution to the boundary-value problem of the dielectric-boundary PB equation. We finally study the electrostatic free-energy functionals of ionic concentrations and electrostatic potentials, respectively, with a given set of point charges and a dielectric boundary. In Section 3, we reformulate the minimum electrostatic free energy, define the dielectric boundary force, and present the main formula for such force. In Section 4, we prove several lemmas on the calculus of boundary variations. These lemmas are needed for the proof of the main theorem on the dielectric boundary force. Finally, in Section 5, we prove the main theorem (Theorem 3.2) of the dielectric boundary force.

2 The Poisson–Boltzmann Equation and Free-Energy Functional

2.1 Assumptions and Auxiliary Functions

Unless otherwise stated, we assume the following throughout the rest of the paper:

A1. The set $\Omega \subset \mathbb{R}^3$ is non-empty, bounded, open, and connected. The sets $\Omega_- \subset \mathbb{R}^3$ and $\Omega_+ \subset \mathbb{R}^3$ are non-empty, bounded, and open, and satisfy that $\overline{\Omega_-} \subset \Omega$ and $\Omega_+ = \Omega \setminus \overline{\Omega_-}$. The interface $\Gamma = \partial \Omega_- = \overline{\Omega_-} \cap \overline{\Omega_+}$ and the boundary $\partial \Omega$ are of the class C^3 and C^2 , respectively. The unit normal vector at the boundary Γ exterior to Ω_- and that at $\partial \Omega$ exterior to Ω are both denoted by n. The N points x_1, \ldots, x_N for some integer $N \geq 1$ belong to Ω_- ; cf. Figure 1. Moreover, there exists a constant $s_0 > 0$ such that

$$\operatorname{dist}\left(\Gamma,\partial\Omega\right) \ge s_0;\tag{2.1}$$

A2. All the integer $M \geq 2$, and real numbers $\beta > 0$, $\Lambda > 0$, $Q_i \in \mathbb{R}$ $(1 \leq i \leq N)$, $q_j \neq 0$ and $\mu_j \in \mathbb{R}$ $(1 \leq j \leq M)$, and $\varepsilon_- > 0$ and $\varepsilon_+ > 0$ are given. Moreover, $\varepsilon_- \neq \varepsilon_+$. The parameter c_j^{∞} is defined by $c_j^{\infty} = \Lambda^{-3}e^{\beta\mu_j}$ (j = 1, ..., M). The parameters q_j and c_j^{∞}

 $(1 \le j \le M)$ satisfy the condition of charge neutrality

$$\sum_{j=1}^{M} q_j c_j^{\infty} = 0; (2.2)$$

A3. The function $B: \mathbb{R} \to \mathbb{R}$ is defined in (1.2). The function $\varepsilon_{\Gamma} \in L^{\infty}(\Omega)$ is defined in (1.5). The boundary data ϕ_{∞} is the trace of a given function, also denoted by ϕ_{∞} , in $C^2(\overline{\Omega})$. (We use the standard notation for Sobolev spaces and other function spaces; cf. [1,22,25].)

Note that the function B defined in (1.2) satisfies that $B \in C^{\infty}(\mathbb{R})$. Since

$$B'(s) = -\sum_{j=1}^{M} q_j c_j^{\infty} e^{-\beta q_j s} \quad \text{and} \quad B''(s) = \sum_{j=1}^{M} \beta q_j^2 c_j^{\infty} e^{-\beta q_j s} > 0, \quad \forall s \in \mathbb{R},$$

the function B is strictly convex, and the charge neutrality (2.2) implies that B'(0) = 0. Hence, s = 0 is the unique minimum point for B with B(s) > B(0) = 0 for all $s \neq 0$. By the fact that $M \geq 2$ and the charge neutrality (2.2), there exist some $q_j > 0$ and some $q_k < 0$. Hence, $B(\pm \infty) = \infty$. Similar arguments show that $B'(\infty) = \infty$ and $B'(-\infty) = -\infty$.

We now introduce several auxiliary functions to treat the point-charge singularities, the dielectric discontinuity Γ , and the inhomogeneous boundary data ϕ_{∞} on $\partial\Omega$. We first recall that the Coulomb field $\hat{\phi}_{\rm C}$ is defined in (1.6). Let $\hat{\phi} \in \hat{\phi}_{\rm C} + H^1(\Omega)$ be defined by

$$\int_{\Omega} \varepsilon_{-} \nabla \hat{\phi} \cdot \nabla \eta \, dx = \sum_{i=1}^{N} Q_{i} \eta(x_{i}) \qquad \forall \eta \in C_{c}^{1}(\Omega), \tag{2.3}$$

where $C_{\rm c}^1(\Omega)$ denotes the class of $C^1(\Omega)$ -functions that are compactly supported in Ω . Clearly, we can modify the value of $\hat{\phi}$ on a set of zero Lebesgue measure, if necessary, so that $\hat{\phi}$ is a C^{∞} -function in $\Omega \setminus \{x_1, \ldots, x_N\}$. Moreover, $\Delta \hat{\phi} = 0$ in $\Omega \setminus \{x_1, \ldots, x_N\}$ and $\Delta(\hat{\phi} - \hat{\phi}_{\rm C}) = 0$ in Ω . There are infinitely many such functions. We will only use three of them. One of them is the Coulomb field $\hat{\phi} = \hat{\phi}_{\rm C}$. The other two are $\hat{\phi} = \hat{\phi}_{\rm 0}$ and $\hat{\phi} = \hat{\phi}_{\infty}$. They are uniquely determined by the boundary conditions

$$\hat{\phi}_0 = 0 \quad \text{on } \partial\Omega \quad \text{and} \quad \hat{\phi}_{\infty} = \phi_{\infty} \quad \text{on } \partial\Omega,$$
 (2.4)

respectively. Since $\partial\Omega$ is C^2 and $\phi_{\infty} \in C^2(\overline{\Omega})$, we have $\hat{\phi} - \hat{\phi}_{\mathrm{C}} \in H^2(\Omega)$; cf. Chapter 8 in [25]. Therefore, all these three functions belong to $\hat{\phi}_{\mathrm{C}} + H^2(\Omega) \cap C^{\infty}(\Omega) \subset W^{1,1}(\Omega)$.

We remark that $\eta \in C^1_c(\Omega)$ in (2.3) can be replaced by $\eta \in H^1_0(\Omega)$ with $\eta|_{\Omega_-} \in C^1(\Omega_-)$. To see this, we first note that (2.3) holds true if $\hat{\phi}$ is replaced by $\hat{\phi}_C$ (cf. (1.6)). Thus,

$$\int_{\Omega} \varepsilon_{-} \nabla (\hat{\phi} - \hat{\phi}_{C}) \cdot \nabla \eta \, dx = 0 \qquad \forall \eta \in H_{0}^{1}(\Omega),$$

as $\hat{\phi} - \hat{\phi}_{\mathcal{C}} \in H^1(\Omega)$ and $C^1_{\mathcal{C}}(\Omega)$ is dense in $H^1(\Omega)$. If $\eta \in H^1_0(\Omega)$ also satisfies $\eta|_{\Omega_-} \in C^1(\Omega_-)$, then $\nabla \hat{\phi}_{\mathcal{C}} \cdot \nabla \eta$, hence $\nabla \hat{\phi} \cdot \nabla \eta$, is integrable in Ω . Moreover,

$$\int_{\Omega} \varepsilon_{-} \nabla \hat{\phi} \cdot \nabla \eta \, dx = \int_{\Omega} \varepsilon_{-} \nabla \hat{\phi}_{C} \cdot \nabla \eta \, dx = \sum_{i=1}^{N} Q_{i} \eta(x_{i}),$$

where the second equality follows from straight forward calculations using the definition of $\hat{\phi}_{\rm C}$ (cf. (1.6)).

We recall that the function $\phi_{\Gamma,\infty} \in H^1(\Omega)$ is the unique weak solution to the boundary-value problem (1.7), defined by $\phi_{\Gamma,\infty} = \phi_{\infty}$ on $\partial\Omega$ and

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla \phi_{\Gamma,\infty} \cdot \nabla \eta \, dx = 0 \qquad \forall \eta \in H_0^1(\Omega). \tag{2.5}$$

By the regularity theory, we have, after modifying possibly the value of $\phi_{\Gamma,\infty}$ on a set of zero Lebesgue measure, that

$$\phi_{\Gamma,\infty} \in C(\overline{\Omega}) \cap W^{1,\infty}(\Omega) \quad \text{and} \quad \phi_{\Gamma,\infty}|_{\Omega_s} \in C^{\infty}(\Omega_s) \cap H^2(\Omega_s) \quad \text{for } s = -, +.$$
 (2.6)

Moreover, there exists a constant $C = C(\Omega, \varepsilon_+, \varepsilon_-, \phi_\infty) > 0$, independent of Γ , such that

$$\|\phi_{\Gamma,\infty}\|_{W^{1,\infty}(\Omega)} \le C. \tag{2.7}$$

See [25] (Theorem 8.16) and [39] (Theorem 1.1 and the beginning part of proof of Theorem 1.1) (also [12]) for the global $C(\overline{\Omega})$ and $W^{1,\infty}$ regularities, and the $W^{1,\infty}(\Omega)$ estimate, and [32] (Section 16 of Chapter 3) and [28,29] for the piecewise H^2 -regularity. By (2.5), we have

$$\Delta \phi_{\Gamma,\infty} = 0 \quad \text{in } \Omega_- \cup \Omega_+. \tag{2.8}$$

This implies the piecewise C^{∞} -regularity in (2.6). Moreover, since $\phi_{\Gamma,\infty} \in H_0^1(\Omega)$, routine calculations by (2.5) and the Divergence Theorem imply that [34]

$$\llbracket \phi_{\Gamma,\infty} \rrbracket_{\Gamma} = 0$$
 and $\llbracket \varepsilon_{\Gamma} \partial_n \phi_{\Gamma,\infty} \rrbracket_{\Gamma} = 0.$ (2.9)

Throughout, for any function u on Ω that has trace on Γ , we denote

$$u^{+} = u|_{\Omega_{+}}, \qquad u^{-} = u|_{\Omega_{-}}, \qquad \text{and} \qquad [\![u]\!]_{\Gamma} = u^{+} - u^{-} \qquad \text{on } \Gamma.$$
 (2.10)

Let $\hat{\phi}_{\Gamma,\infty} \in \hat{\phi}_{\mathcal{C}} + H^1(\Omega)$ be the unique function such that $\hat{\phi}_{\Gamma,\infty} = \phi_{\infty}$ on $\partial\Omega$ and

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \eta \, dx = \sum_{i=1}^{N} Q_{i} \eta(x_{i}) \qquad \forall \eta \in C_{c}^{1}(\Omega);$$
(2.11)

cf. [21,40]. If $\hat{\phi} = \hat{\phi}_C$, or $\hat{\phi}_0$, or $\hat{\phi}_\infty$, then (2.11) is equivalent to

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla (\hat{\phi}_{\Gamma,\infty} - \hat{\phi}) \cdot \nabla \eta \, dx = -(\varepsilon_{+} - \varepsilon_{-}) \int_{\Omega_{+}} \nabla \hat{\phi} \cdot \nabla \eta \, dx$$

$$= (\varepsilon_{+} - \varepsilon_{-}) \int_{\Gamma} \partial_{n} \hat{\phi} \, \eta \, dS \qquad \forall \eta \in H_{0}^{1}(\Omega), \tag{2.12}$$

where the unit normal n at Γ points from Ω_{-} to Ω_{+} . If $\eta \in H_0^1(\Omega)$ satisfies $\eta|_{\Omega_{-}} \in C^1(\Omega_{-})$, then it follows from (2.12) that

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \eta \, dx = \int_{\Omega} \varepsilon_{\Gamma} \nabla \hat{\phi} \cdot \nabla \eta \, dx - (\varepsilon_{+} - \varepsilon_{-}) \int_{\Omega_{+}} \nabla \hat{\phi} \cdot \nabla \eta \, dx
= \int_{\Omega} \varepsilon_{-} \nabla \hat{\phi} \cdot \nabla \eta \, dx
= \sum_{i=1}^{N} Q_{i} \eta(x_{i}).$$

Therefore, we can replace $\eta \in C^1_c(\Omega)$ in (2.11) by $\eta \in H^1_0(\Omega)$ that satisfies $\eta|_{\Omega_-} \in C^1(\Omega_-)$.

By (2.11) and (2.12), we have, after possibly modifying the value of $\hat{\phi}_{\Gamma,\infty}$ on a set of zero Lebesgue measure, that

$$\Delta(\hat{\phi}_{\Gamma,\infty} - \hat{\phi}) = 0 \quad \text{in } \Omega_{-} \quad \text{and} \quad \Delta\hat{\phi}_{\Gamma,\infty} = 0 \quad \text{in } (\Omega_{-} \setminus \{x_1, \dots, x_N\}) \cup \Omega_{+}, \tag{2.13}$$

$$[\![\hat{\phi}_{\Gamma,\infty}]\!]_{\Gamma} = 0 \quad \text{and} \quad [\![\varepsilon_{\Gamma}\partial_n\hat{\phi}_{\Gamma,\infty}]\!]_{\Gamma} = 0 \quad \text{on } \Gamma.$$
 (2.14)

Moreover, it follows from the elliptic regularity theory [12, 21, 25, 28, 29, 32, 39, 40] that

$$\hat{\phi}_{\Gamma,\infty} - \hat{\phi} \in C(\overline{\Omega}) \cap W^{1,\infty}(\Omega), \quad (\hat{\phi}_{\Gamma,\infty} - \hat{\phi})^- \in C^{\infty}(\Omega_-) \cap H^2(\Omega_-), \quad \hat{\phi}_{\Gamma,\infty}^+ \in C^{\infty}(\Omega_+) \cap H^2(\Omega_+). \tag{2.15}$$

Further, then there exists a constant C > 0 that may depend on Ω , x_i and Q_i $(1 \le i \le N)$, $\varepsilon_+, \varepsilon_-, \phi_\infty$, and $\hat{\phi}$, but does not depend on Γ , such that

$$\|\hat{\phi}_{\Gamma,\infty} - \hat{\phi}\|_{W^{1,\infty}(\Omega)} \le C. \tag{2.16}$$

These results (2.15) and (2.16) follow from the same arguments used above (cf. the description below (2.7)) applied to (2.11) with $\eta \in C_c^1(\Omega)$ so chosen that the support of η is in a neighborhood of Γ that excluding the signilarities x_i (i = 1, ..., N).

For any $g \in H^{-1}(\Omega)$, let $L_{\Gamma}g \in H_0^1(\Omega)$ be the unique weak solution (defined using test functions in $H_0^1(\Omega)$) to the boundary-value problem

$$\nabla \cdot \varepsilon_{\Gamma} \nabla L_{\Gamma} g = -g \quad \text{in } \Omega \quad \text{and} \quad L_{\Gamma} g = 0 \quad \text{on } \partial \Omega.$$
 (2.17)

This defines a linear, continuous, and self-adjoint operator $L_{\Gamma}: H^{-1}(\Omega) \to H_0^1(\Omega)$. The map

$$g \mapsto \|g\|_{L_{\Gamma}} := \sqrt{\langle g, L_{\Gamma}g \rangle_{H^{-1}(\Omega), H_0^1(\Omega)}} = \left[\int_{\Omega} \varepsilon_{\Gamma} |\nabla(L_{\Gamma}g)|^2 dx \right]^{1/2} \tag{2.18}$$

defines a norm on $H^{-1}(\Omega)$ which is equivalent to the $H^{-1}(\Omega)$ -norm. If $g \in L^1(\Omega)$, then we define $g \in L^1(\Omega) \cap H^{-1}(\Omega)$ if

$$\sup \left\{ \int_{\Omega} gu \, dx : u \in H_0^1(\Omega) \cap L^{\infty}(\Omega) \text{ and } ||u||_{H^1(\Omega)} = 1 \right\} < \infty.$$
 (2.19)

In this case, the action of g on $H_0^1(\Omega)$ is defined first for any $u \in H_0^1(\Omega) \cap L^{\infty}(\Omega)$ by the integral of gu over Ω and then extended for any $u \in H_0^1(\Omega)$ by (2.19) and the fact that $H_0^1(\Omega) \cap L^{\infty}(\Omega)$ is dense in $H_0^1(\Omega)$.

2.2 The Poisson–Boltzmann Equation

We now study the well-posedness of the boundary-value problem of the Poisson–Boltzmann (PB) equation (1.8) with a dielectric boundary and point charges.

Definition 2.1. A function $\psi \in \hat{\phi}_C + H^1(\Omega)$ is a weak solution to the boundary-value problem of the dielectric-boundary PB equation (1.8), if $\psi = \phi_{\infty}$ on $\partial\Omega$, $\chi_+B'(\psi - \phi_{\Gamma,\infty}/2) \in L^1(\Omega) \cap H^{-1}(\Omega)$, and

$$\int_{\Omega} \left[\varepsilon_{\Gamma} \nabla \psi \cdot \nabla \eta + \chi_{+} B' \left(\psi - \frac{\phi_{\Gamma, \infty}}{2} \right) \eta \right] dx = \sum_{i=1}^{N} Q_{i} \eta(x_{i}) \qquad \forall \eta \in C_{c}^{1}(\Omega).$$
 (2.20)

Note that we can replace $\eta \in C^1_{\rm c}(\Omega)$ in (2.20) by $\eta \in H^1_0(\Omega)$ that satisfies $\eta^- \in C^1(\Omega_-)$; cf. the remark below (2.12). The theorem below provides the existence and uniqueness of the solution to the boundary-value problem of the dielectric-boundary PB equation, and an equivalent formulation of such a boundary-value problem. These results are essentially proved in [35]. Here we sketch the proof and add some points that are not included in the previous proof due to some minor differences between the current and previous statements. Note that $\hat{\phi}_{\rm C} + H^1(\Omega) = \hat{\phi}_{\Gamma,\infty} + H^1(\Omega)$. So, we can replace $\hat{\phi}_{\rm C}$ by $\hat{\phi}_{\Gamma,\infty}$ in the above definition. Note also that there is a variational principle for the PB equation; cf. Theorem 3.1.

Theorem 2.1. (1) There exists a unique weak solution $\psi_{\Gamma} \in \hat{\phi}_{\Gamma,\infty} + H_0^1(\Omega)$ of the boundary-value problem of the dielectric-boundary PB equation (1.8). Moreover, after a possible modification of ψ_{Γ} on a set of zero Lebesgue measure, $\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty} \in C(\overline{\Omega}) \cap W^{1,\infty}(\Omega)$, $(\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})^- \in C^{\infty}(\Omega_-) \cap H^2(\Omega_-)$, and $\psi_{\Gamma}^+ \in C^{\infty}(\Omega_+) \cap H^2(\Omega_+)$. Further, there exists a constant C > 0 that may depend on Ω , x_i and Q_i $(1 \le i \le N)$, ε_+ , ε_- , ϕ_∞ , and B, but does not depend on Γ , such that

$$\|\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}\|_{W^{1,\infty}(\Omega)} \le C. \tag{2.21}$$

(2) A function $\psi \in \hat{\phi}_{\Gamma,\infty} + H^1(\Omega)$ with $\chi_+ B'(\psi - \phi_{\Gamma,\infty}/2) \in L^1(\Omega) \cap H^{-1}(\Omega)$ is the weak solution to the boundary-value problem of the dielectric-boundary PB equation (1.8) if and only if it is the unique solution to the following elliptic interface problem:

$$\begin{cases} \Delta(\psi - \hat{\phi}_{\Gamma,\infty}) = 0 & \text{in } \Omega_{-}, \\ \varepsilon_{+} \Delta \psi - B' \left(\psi - \frac{\phi_{\Gamma,\infty}}{2} \right) = 0 & \text{in } \Omega_{+}, \\ \llbracket \psi \rrbracket_{\Gamma} = 0 & \text{and} & \llbracket \varepsilon_{\Gamma} \partial_{n} \psi \rrbracket_{\Gamma} = 0 & \text{on } \Gamma, \\ \psi = \psi_{\infty} & \text{on } \partial \Omega. \end{cases}$$

$$(2.22)$$

Proof. (1) With $u = \psi - \hat{\phi}_{\Gamma,\infty}$ and by (2.11) and (2.20), it is equivalent to show that there exists a unique $u_{\Gamma} \in H_0^1(\Omega)$ such that $\chi_+ B'(u_{\Gamma} + \hat{\phi}_{\Gamma,\infty} - \phi_{\Gamma,\infty}/2) \in L^1(\Omega) \cap H^{-1}(\Omega)$, and

$$\int_{\Omega} \left[\varepsilon_{\Gamma} \nabla u_{\Gamma} \cdot \nabla \eta + \chi_{+} B' \left(u_{\Gamma} + \hat{\phi}_{\Gamma,\infty} - \frac{\phi_{\Gamma,\infty}}{2} \right) \eta \right] dx = 0 \qquad \forall \eta \in H_{0}^{1}(\Omega). \tag{2.23}$$

Define

$$I[u] = \int_{\Omega} \left[\frac{\varepsilon_{\Gamma}}{2} |\nabla u|^2 + \chi_{+} B \left(u + \hat{\phi}_{\Gamma,\infty} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] dx \qquad \forall u \in H_0^1(\Omega).$$

Since $B \geq 0$ and B is convex, we can use the direct method in the calculus of variations to obtain a unique minimizer $u_{\Gamma} \in H_0^1(\Omega)$ of the functional $I: H_0^1(\Omega) \to [0, \infty]$. Moreover, comparing the values $I[u_{\Gamma}]$ and $I[u_{\Gamma,\lambda}]$ for any constant $\lambda > 0$ large enough, where $u_{\Gamma,\lambda} = u_{\Gamma}$ if $|u_{\Gamma}| \leq \lambda$ and $u_{\Gamma,\lambda} = \lambda \operatorname{sign}(u_{\Gamma})$ otherwise, we have by the convexity of B that $u_{\Gamma} = u_{\Gamma,\lambda}$ a.e. Ω for some λ independent on Γ . Hence, $u_{\Gamma} \in L^{\infty}(\Omega)$, and $||u_{\Gamma}||_{L^{\infty}(\Omega)} \leq C$ for some constant C > 0 independent of Γ ; cf. [35]. This allows the use of the Lebesgue Dominated Convergence Theorem in the routine calculations of $(d/dt)|_{t=0}I[u_{\Gamma}+t\eta]=0$ for any $\eta \in C_c^1(\Omega)$ to obtain the equation in (2.23). Since $C_c^1(\Omega)$ is dense in $H_0^1(\Omega)$, (2.23) holds true. The convexity of B now imiplies that u_{Γ} is the unique solution as desired.

The regularity of the solution ψ_{Γ} follows from the elliptic regularity theory [12,21,25,28,29, 32,39], with the same argument above for the regularity of the function $\hat{\phi}_{\Gamma,\infty}$; cf. (2.15) and (2.16). Note that the piecewise C^{∞} smoothness follows from a usual bootstrapping method.

2.3 Electrostatic Free-Energy Functional of Ionic Concentrations

We define

$$\mathcal{X} = \left\{ (c_1, \dots, c_M) \in L^1(\Omega, \mathbb{R}^M) : c_j = 0 \text{ a.e. } \Omega_- \text{ for } j = 1, \dots, M \text{ and } \sum_{j=1}^M q_j c_j \in H^{-1}(\Omega) \right\},$$

$$\mathcal{X}_+ = \left\{ (c_1, \dots, c_M) \in \mathcal{X} : c_j \ge 0 \text{ a.e. } \Omega_+ \text{ for } j = 1, \dots, M \right\}.$$

Here, for any $g \in L^1(\Omega)$, we define $g \in L^1(\Omega) \cap H^{-1}(\Omega)$ by (2.19). The space \mathcal{X} is a Banach space equipped with the norm

$$||c||_{\mathcal{X}} = \sum_{j=1}^{M} ||c_j||_{L^1(\Omega)} + ||\sum_{j=1}^{M} q_j c_j||_{H^{-1}(\Omega)} \quad \forall c = (c_1, \dots, c_M) \in \mathcal{X}.$$

Moreover, \mathcal{X}_+ is a convex and closed subset of \mathcal{X} . For any $c=(c_1,\ldots,c_M)\in\mathcal{X}$, standard arguments (cf. [21, 22, 25, 40]) imply that there exists a unique weak solution ψ to the boundary-value problem (1.4), defined by $\psi\in\hat{\phi}_{\mathrm{C}}+H^1(\Omega)$, $\psi=\phi_{\infty}$ on $\partial\Omega$, and

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla \psi \cdot \nabla \eta \, dx = \sum_{i=1}^{N} Q_{i} \eta(x_{i}) + \int_{\Omega_{+}} \left(\sum_{j=1}^{M} q_{j} c_{j} \right) \eta \, dx \qquad \forall \eta \in C_{c}^{1}(\Omega), \tag{2.24}$$

Equivalently, if $\hat{\phi} \in \hat{\phi}_{\mathrm{C}} + H^1(\Omega)$ satisfies (2.3), then

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla (\psi - \hat{\phi}) \cdot \nabla \eta \, dx = \int_{\Omega_{+}} \left[(\varepsilon_{-} - \varepsilon_{+}) \nabla \hat{\phi} \cdot \nabla \eta + \left(\sum_{j=1}^{M} q_{j} c_{j} \right) \eta \right] dx \qquad \forall \eta \in H_{0}^{1}(\Omega).$$

Clearly, $\psi - \hat{\phi}$ is harmonic in Ω_- . Moreover, it follows from the definition of $\hat{\phi}_{\Gamma,\infty}$ (cf. (2.11)) and L_{Γ} (cf. (2.17)) that

$$\psi = \hat{\phi}_{\Gamma,\infty} + L_{\Gamma} \left(\sum_{j=1}^{M} q_j c_j \right). \tag{2.25}$$

Since the function $s \mapsto s \log s$ $(s \ge 0)$ is bounded below and Ω is bounded, $F_{\Gamma}[c] > -\infty$ for any $c \in \mathcal{X}_+$, where $F_{\Gamma}[c]$ is defined in (1.3).

Theorem 2.2. Let ψ_{Γ} be the unique weak solution to the dielectric-boundary PB equation (1.8). For each $j \in \{1, ..., M\}$, define $c_{\Gamma,j} : \Omega \to [0, \infty)$ by

$$c_{\Gamma,j}(x) = \begin{cases} 0 & \text{if } x \in \overline{\Omega}_{-}, \\ c_{j}^{\infty} e^{-\beta q_{j} \left[\psi_{\Gamma}(x) - \phi_{\Gamma,\infty}(x)/2 \right]} & \text{if } x \in \Omega_{+}. \end{cases}$$
 (2.26)

Then $c_{\Gamma} := (c_{\Gamma,1}, \ldots, c_{\Gamma,M}) \in \mathcal{X}_+$ and ψ_{Γ} is the electrostatic potential corresponding to c_{Γ} , i.e., the unique weak solution to (1.4) with c_j replaced by $c_{\Gamma,j}$ $(j = 1, \ldots, M)$. Moreover, c_{Γ} is the unique minimizer of the functional $F_{\Gamma} : \mathcal{X}_+ \to (-\infty, \infty]$ defined in (1.3), and

$$F_{\Gamma}[c_{\Gamma}] = \frac{1}{2} \sum_{i=1}^{N} Q_{i} (\psi_{\Gamma} - \hat{\phi}_{C})(x_{i})$$

$$+ \int_{\Omega_{+}} \left[\frac{1}{2} (\psi_{\Gamma} - \phi_{\Gamma,\infty}) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) - B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] dx. \tag{2.27}$$

Proof. By the properties of ψ_{Γ} (cf. Theorem 2.1) and $\phi_{\Gamma,\infty}$ (cf. (2.7)), we have $c_{\Gamma} \in \mathcal{X}_{+}$. If we replace c_{j} in (1.4) by $c_{\Gamma,j}$ defined in (2.26) and note the definition of B in (1.2), we get exactly the PB equation (1.8). Therefore, the unique solution ψ_{Γ} to the boundary-value problem of the PB equation (1.8) is also the unique solution to the boundary-value problem of Poisson's equation (1.4) corresponding to c_{Γ} .

We now prove that c_{Γ} is the unique minimizer of $F_{\Gamma}: \mathcal{X}_{+} \to (-\infty, \infty]$. To do so, we first re-write the functional F_{Γ} . Let $c = (c_{1}, \ldots, c_{M}) \in \mathcal{X}_{+}$ and let $\psi \in \hat{\phi}_{\mathbb{C}} + H^{1}(\Omega)$ be the corresponding electrostatic potential, i.e., the weak solution to (1.4) defined in (2.24). Denote $f = \sum_{j=1}^{M} q_{j}c_{j}$. Since f = 0 a.e. in Ω_{-} , we have by the definition of L_{Γ} (cf. (2.17)) that $L_{\Gamma}f$ is harmonic in Ω_{-} . Moreover,

$$\sum_{i=1}^{N} Q_i (L_{\Gamma} f) (x_i) = \int_{\Omega_+} (\hat{\phi}_{\Gamma,\infty} - \phi_{\Gamma,\infty}) f dx;$$

cf. Lemma 3.2 in [34] (where $L/(4\pi)$ and $G/(4\pi)$ are our L_{Γ} and $\hat{\phi}_{\Gamma,\infty} - \phi_{\Gamma,\infty}$ here, respectively). This, together with (2.25) and the fact that all $\psi - \hat{\phi}_{C}$, $\hat{\phi}_{\Gamma,\infty} - \hat{\phi}$, and $L_{\Gamma}f$ are harmonic in Ω_{-} , implies that

$$\sum_{i=1}^{N} Q_i(\psi - \hat{\phi}_{\mathcal{C}})(x_i) = \sum_{i=1}^{N} Q_i(L_{\Gamma}f)(x_i) + \sum_{i=1}^{N} Q_i(\hat{\phi}_{\Gamma,\infty} - \hat{\phi}_{\mathcal{C}})(x_i)$$

$$= \int_{\Omega_+} (\hat{\phi}_{\Gamma,\infty} - \phi_{\Gamma,\infty}) \left(\sum_{i=1}^{M} q_i c_i\right) dx + \sum_{i=1}^{N} Q_i(\hat{\phi}_{\Gamma,\infty} - \hat{\phi}_{\mathcal{C}})(x_i).$$

With this and (2.25), we can rewrite $F_{\Gamma}[c]$ (1.3) as

$$F_{\Gamma}[c] = \int_{\Omega_{+}} \left[\frac{1}{2} \left(\sum_{j=1}^{M} q_{j} c_{j} \right) L_{\Gamma} \left(\sum_{j=1}^{M} q_{j} c_{j} \right) + \sum_{j=1}^{M} \left(\beta^{-1} c_{j} \log c_{j} + \alpha_{j} c_{j} \right) \right] dx + E_{0,\Gamma}, \quad (2.28)$$

where all $\alpha_j = \alpha_j(x)$ (j = 1, ..., M) and $E_{0,\Gamma}$ are independent of c, given by

$$\alpha_{j}(x) = q_{j} \left[\hat{\phi}_{\Gamma,\infty}(x) - \frac{1}{2} \phi_{\Gamma,\infty}(x) \right] + \beta^{-1} \left(3 \log \Lambda - 1 \right) - \mu_{j} \quad \forall x \in \Omega, \ j = 1, \dots, M, \quad (2.29)$$

$$E_{0,\Gamma} = \frac{1}{2} \sum_{i=1}^{N} Q_{i} (\hat{\phi}_{\Gamma,\infty} - \hat{\phi}_{C})(x_{i}) + \beta^{-1} |\Omega_{+}| \sum_{i=1}^{M} c_{j}^{\infty}.$$

Here and below, we denote by |A| the Lebesgue measure of A when no confusion arises.

We now compare $F_{\Gamma}[c]$ and $F_{\Gamma}[c_{\Gamma}]$. By Taylor's expansion, we have for any $s, t \in (0, \infty)$ that

$$s \log s - t \log t = (1 + \log t)(s - t) + \frac{1}{2r}(s - t)^2 \ge (1 + \log t)(s - t),$$

where r is in between s and t. Consequently, by (2.28) and the fact that L_{Γ} is self-adjoint, we have

$$\begin{split} F_{\Gamma}[c] - F_{\Gamma}[c_{\Gamma}] &= \int_{\Omega} \frac{1}{2} \left(\sum_{j=1}^{M} q_{j}(c_{j} - c_{\Gamma,j}) \right) L_{\Gamma} \left(\sum_{j=1}^{M} q_{j}(c_{j} - c_{\Gamma,j}) \right) dx \\ &+ \int_{\Omega} \left(\sum_{j=1}^{M} q_{j}(c_{j} - c_{\Gamma,j}) \right) L_{\Gamma} \left(\sum_{k=1}^{M} q_{k}c_{\Gamma,k} \right) dx \\ &+ \beta^{-1} \sum_{j=1}^{M} \int_{\Omega} \left(c_{j} \log c_{j} - c_{\Gamma,j} \log c_{\Gamma,j} \right) dx + \sum_{j=1}^{M} \int_{\Omega} \left(c_{j} - c_{\Gamma,j} \right) \alpha_{j} dx \\ &\geq \sum_{j=1}^{M} \int_{\Omega} \left(c_{j} - c_{\Gamma,j} \right) \left[q_{j} L_{\Gamma} \left(\sum_{k=1}^{M} q_{k}c_{\Gamma,k} \right) + \beta^{-1} \left(1 + \log c_{\Gamma,j} \right) + \alpha_{j} \right] dx. \end{split}$$

It follows from the fact that $c_j^{\infty} = \Lambda^{-3}e^{\beta\mu_j}$ (cf. the assumption (A2)), (2.25), (2.26), and (2.29) that the quantity inside the brackets in the above integral vanishes. Thus, $F[c] \geq F[c_{\Gamma}]$. Hence, c_{Γ} is a minimizer of $F_{\Gamma} : \mathcal{X}_+ \to (-\infty, \infty]$. Since F_{Γ} is convex, and in particular, $s \mapsto s \log s$ is strictly convex on $(0, \infty)$, the minimizer of F_{Γ} is unique; cf. [34].

Finally, we obtain (2.27) from (1.3) with ψ_{Γ} and c_{Γ} replacing ψ and c, respectively, (1.2), and (2.26).

3 Dielectric Boundary Force

3.1 Electrostatic Free Energy of a Dielectric Boundary

Given any dielectric boundary Γ , we denote by

$$E[\Gamma] = \min_{c \in \mathcal{X}_{\perp}} F_{\Gamma}[c], \tag{3.1}$$

the minimum electrostatic free energy given in Theorem 2.2 (cf. (2.27)). We reformulate $E[\Gamma]$ to convert the discrete part of the energy into volume integrals that will be useful when we calculate the variation of $E[\Gamma]$ with respect to the boundary variation of Γ .

Lemma 3.1. Let Γ be a dielectric boundary satisfying the part of the assumption A1 on Γ in Subsection 2.1. Let $\psi_{\Gamma} \in \hat{\phi}_{\mathbb{C}} + H^1(\Omega)$ be the corresponding solution to the boundary-value problem of PB equation (1.8). We have

$$E[\Gamma] = -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} |\nabla(\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B\left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2}\right) dx + \frac{\varepsilon_{-} - \varepsilon_{+}}{2} \int_{\Omega_{+}} \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \hat{\phi}_{0} dx + \frac{1}{2} \sum_{i=1}^{N} Q_{i} (\hat{\phi}_{\infty} - \hat{\phi}_{C})(x_{i}),$$
(3.2)

where all the functions $\hat{\phi}_{C}$, $\hat{\phi}_{0}$, $\hat{\phi}_{\infty}$, $\phi_{\Gamma,\infty}$, and $\hat{\phi}_{\Gamma,\infty}$ are defined in Subsection 2.1.

Proof. We first prove an elementary identity. Let $u \in C^2(\Omega_-) \cap C^1(\overline{\Omega_-})$ be such that $\Delta u = 0$ in Ω_- . Let $v \in \hat{\phi}_{\mathbb{C}} + H^1(\Omega_-) \cap C(\overline{\Omega_-})$, in particular, $v = \hat{\phi}_{\mathbb{C}}$, $\hat{\phi}_0$, $\hat{\phi}_\infty$, or $\hat{\phi}_{\Gamma,\infty}$ (restricted onto Ω_-). Denote $B_\alpha = \bigcup_{i=1}^N B(x_i, \alpha)$ for $0 < \alpha \ll 1$ and ν the unit normal at $\partial B(\alpha) = \bigcup_{i=1}^N \partial B(x_i, \alpha)$, pointing toward x_i $(i = 1, \ldots, N)$. Since the unit normal n at Γ points from Ω_- to Ω_+ , and since $v = \hat{\phi}_{\mathbb{C}} + \hat{v}$ for some $\hat{v} \in H^1(\Omega_-) \cap C(\overline{\Omega_-})$ and $\hat{\phi}_{\mathbb{C}}$ is given in (1.6), we have

$$\int_{\Omega_{-}} \nabla u \cdot \nabla v \, dx = \lim_{\alpha \to 0^{+}} \int_{\Omega_{-} \setminus B_{\alpha}} \nabla u \cdot \nabla v \, dx$$

$$= \int_{\Gamma} \partial_{n} u \, v \, dS + \lim_{\alpha \to 0^{+}} \sum_{i=1}^{N} \int_{\partial B(x_{i}, \alpha)} \partial_{\nu} u \, v \, dS$$

$$= \int_{\Gamma} \partial_{n} u \, v \, dS. \tag{3.3}$$

Denoting now $W = (1/2) \sum_{i=1}^{N} Q_i(\hat{\phi}_{\infty} - \hat{\phi}_{C})(x_i)$, we have by (3.1) and (2.27) that

$$E[\Gamma] = \frac{1}{2} \sum_{i=1}^{N} Q_i (\hat{\phi}_{\Gamma,\infty} - \hat{\phi}_{\infty})(x_i) + \frac{1}{2} \sum_{i=1}^{N} Q_i (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})(x_i)$$

$$+ \int_{\Omega_+} \left[\frac{1}{2} (\psi_{\Gamma} - \phi_{\Gamma,\infty}) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) - B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] dx + W.$$
 (3.4)

We first consider the first term in (3.4). Note that the unit vector n normal to Γ points from Ω_- to Ω_+ . We have by Green's formula that

$$\begin{split} &\frac{1}{2}\sum_{i=1}^{N}Q_{i}(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})(x_{i})\\ &=\int_{\Omega}\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx \qquad [\text{by (2.3) with }\hat{\phi}=\hat{\phi}_{0} \text{ and }\eta=\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty}]\\ &=\int_{\Omega_{-}}\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx + \int_{\Omega_{+}}\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx\\ &=\int_{\Gamma}\frac{\varepsilon_{-}}{2}\hat{\phi}_{0}\partial_{n}(\hat{\phi}_{\Gamma,\infty}^{-}-\hat{\phi}_{\infty})\,dS + \int_{\Omega_{+}}\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx \qquad [\text{by (3.3)}]\\ &=\int_{\Gamma}\frac{\varepsilon_{+}}{2}\hat{\phi}_{0}\partial_{n}\hat{\phi}_{\Gamma,\infty}^{+}\,dS - \int_{\Gamma}\frac{\varepsilon_{-}}{2}\hat{\phi}_{0}\partial_{n}\hat{\phi}_{\infty}\,dS \qquad [\text{by (2.14)}]\\ &+\int_{\Omega_{+}}\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx\\ &=-\int_{\partial\Omega_{+}}\frac{\varepsilon_{+}}{2}\hat{\phi}_{0}\partial_{n}\hat{\phi}_{\Gamma,\infty}\,dS + \int_{\partial\Omega_{+}}\frac{\varepsilon_{-}}{2}\hat{\phi}_{0}\partial_{n}\hat{\phi}_{\infty}\,dS \qquad [\text{since }\hat{\phi}_{0}=0 \text{ on }\partial\Omega]\\ &+\int_{\Omega_{+}}\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx\\ &=-\int_{\Omega_{+}}\frac{\varepsilon_{+}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx\\ &=-\int_{\Omega_{+}}\frac{\varepsilon_{+}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx\\ &=\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx\\ &=\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx\\ &=\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx\\ &=\frac{\varepsilon_{-}}{2}\nabla\hat{\phi}_{0}\cdot\nabla(\hat{\phi}_{\Gamma,\infty}-\hat{\phi}_{\infty})\,dx. \end{split}$$

Considering now the second and third terms in (3.4), we have

$$\frac{1}{2} \sum_{i=1}^{N} Q_i (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})(x_i)
+ \int_{\Omega_+} \left[\frac{1}{2} (\psi_{\Gamma} - \phi_{\Gamma,\infty}) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) - B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] dx$$

$$\begin{split} &= \sum_{i=1}^{N} Q_{i}(\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})(x_{i}) - \frac{1}{2} \sum_{i=1}^{N} Q_{i}(\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})(x_{i}) \\ &+ \int_{\Omega_{+}} \left[\frac{1}{2}(\psi_{\Gamma} - \phi_{\Gamma,\infty}) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) - B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] dx \\ &= \int_{\Omega} \varepsilon_{\Gamma} \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) dx \quad [by \ (2.11)] \\ &- \frac{1}{2} \int_{\Omega} \left[\varepsilon_{\Gamma} \nabla \psi_{\Gamma} \cdot \nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) + \chi_{+} B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) \right] \quad [by \ (2.20)] \\ &+ \int_{\Omega_{+}} \left[\frac{1}{2} \left(\psi_{\Gamma} - \phi_{\Gamma,\infty} \right) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) - B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] dx \\ &= - \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &+ \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &+ \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &+ \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &+ \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) \cdot \nabla \hat{\phi}_{\Gamma,\infty} dx \\ &+ \int_{\Omega_{+}} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &+ \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) \cdot \nabla (\hat{\phi}_{\Gamma,\infty} - \phi_{\Gamma,\infty}) dx \quad [by \ (2.22) \ and \ (2.13) \] \\ &= - \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &+ \int_{\Omega_{-}} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &+ \int_{\Omega_{-}} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &+ \int_{\Omega_{-}} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &+ \int_{\Omega_{-}} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &- \int_{\Gamma} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &- \int_{\Omega_{+}} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dx \\ &- \int_{\Omega_{+}} \frac{\varepsilon_{\Gamma}}{2} |\nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})|^{2} dx - \int_{\Omega_{+}} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty$$

Now (3.2) follows directly from (3.4) and the above two expressions.

We define $G_{\Gamma}: \hat{\phi}_{\Gamma,\infty} + H_0^1(\Omega) \to \mathbb{R} \cup \{-\infty\}$ by

$$G_{\Gamma}[\psi] = -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} |\nabla(\psi - \hat{\phi}_{\Gamma,\infty})|^2 dx - \int_{\Omega_{+}} B\left(\psi - \frac{\phi_{\Gamma,\infty}}{2}\right) dx + g_{\Gamma,\infty},$$

where

$$g_{\Gamma,\infty} = \frac{\varepsilon_{-} - \varepsilon_{+}}{2} \int_{\Omega_{+}} \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \hat{\phi}_{0} \, dx + \frac{1}{2} \sum_{i=1}^{N} Q_{i} (\hat{\phi}_{\infty} - \hat{\phi}_{C})(x_{i}).$$

We shall call G_{Γ} the PB energy functional. Note that by Lemma 3.1, $E[\Gamma] = G_{\Gamma}[\psi_{\Gamma}]$. In fact, we have the following variational principle for the PB energy functional.

Theorem 3.1. The Euler-Lagrange equation of the PB energy functional $G_{\Gamma}: \hat{\phi}_{\Gamma,\infty} + H_0^1(\Omega) \to \mathbb{R} \cup \{-\infty\}$ is exactly the dielectric-boundary PB equation. Moreover, the functional $G_{\Gamma}[\cdot]$ is uniquely maximized over $\hat{\phi}_{\Gamma,\infty} + H_0^1(\Omega)$ by the solution ψ_{Γ} to the boundary-value problem of the PB equation (1.8), and the maximum value is exactly $E[\Gamma]$.

Proof. Direct calculations verify that the Euler–Lagrange equation for the PB energy functional $G_{\Gamma}[\cdot]$ is indeed the dielectric-boundary PB equation; cf. Definition 2.1. The existence of a unique maximizer can be proved exactly the same way as in the proof of Theorem 2.1. These, together with Lemma 3.1, imply that the maximum value of the free energy is $G_{\Gamma}[\psi_{\Gamma}] = E[\Gamma]$.

We remark that the PB functional $G_{\Gamma}[\cdot]$ is maximized, not minimized, among all the admissible electrostatic potentials. In general, for a charged system occupying a region $D \subseteq \mathbb{R}^3$ with the dielectric coefficient ε and charge density $\rho \in L^2(D)$, the commonly used energy functional of electrostatic potentials ψ is given by

$$\psi \mapsto \int_D \left(-\frac{\varepsilon}{2} |\nabla \psi|^2 + \rho \psi \right) dx.$$

With suitable boundary conditions, this functional is maximized by a unique electrostatic potential. This maximizer is exactly the solution to Poisson's equation, which is the Euler–Lagrange equation of this functional. Moreover, the maximum value of the functional is exactly the electrostatic energy corresponding to the potential determined by Poisson's equation. See [7] for more related discussions.

3.2 Definition and Formula of the Dielectric Boundary Force

Let Γ be a dielectric boundary as given in the assumption A1 in Subsection 2.1. Let $\phi: \mathbb{R}^3 \to \mathbb{R}$ be the signed distance function to Γ , negative in Ω_- (inside Γ) and positive in $\mathbb{R}^3 \setminus \overline{\Omega_-}$ (outside Γ). Then, $n = \nabla \phi$ is exactly the unit normal along Γ , pointing from Ω_- to Ω_+ . Since Γ is assumed to be of the class C^3 , there exists $d_0 > 0$ with

$$d_0 < \frac{1}{2} \min \left(\operatorname{dist} \left(\Gamma, \partial \Omega \right), \min_{1 \le i \le N} \operatorname{dist} \left(x_i, \Gamma \right) \right)$$

such that the signed distance function ϕ is a C^3 -function and $\nabla \phi \neq 0$ in the neighborhood

$$\mathcal{N}_0(\Gamma) = \{ x \in \Omega : \text{dist}(x, \Gamma) < d_0 \}$$
(3.5)

in Ω of Γ ; cf. [25] (Section 14.6) and [31]. Define

$$\mathcal{V} = \{ V \in C_c^2(\mathbb{R}^3, \mathbb{R}^3) : \operatorname{supp}(V) \subset \mathcal{N}_0(\Gamma) \}.$$
(3.6)

Let $V \in \mathcal{V}$. For any $X \in \mathbb{R}^3$, let x = x(t, X) be the unique solution to the initial-value problem

$$\dot{x} = V(x) \quad (t \in \mathbb{R}) \quad \text{and} \quad x(0, X) = X,$$
 (3.7)

where a dot denotes the derivative with respect to t. Define $T_t(X) = x(t, X)$ for any $X \in \mathbb{R}^3$ and any $t \in \mathbb{R}$. Then, $\{T_t\}_{t \in \mathbb{R}}$ is a family of diffeomorphisms and C^2 -maps from \mathbb{R}^3 to \mathbb{R}^3 with $T_0 = I$ the identity map and $T_{-t} = T_t^{-1}$ for any $t \in \mathbb{R}$.

Let $t \in \mathbb{R}$. Since supp $(V) \subseteq \mathcal{N}_0(\Gamma) \subset \Omega$, we have $T_t(\Omega) = \Omega$ and $T_t(\partial\Omega) = \partial\Omega$. Clearly, $T_t(\Omega_-) \subset \Omega$ and $T_t(\Omega_+) = \Omega \setminus \overline{T_t(\Omega_-)}$. Moreover, $\Gamma_t := T_t(\Gamma) = \partial T_t(\Omega_-) = \overline{T_t(\Omega_-)} \cap \overline{T_t(\Omega_+)}$ is of class C^2 . Note that $x_i \in T_t(\Omega_-)$ and $T_t(x_i) = x_i$ for all $i = 1, \ldots, N$. Analogous to (1.5), ε_{Γ_t} is defined correspondingly with respect to $T_t(\Omega_-)$ and $T_t(\Omega_+)$. We shall denote $\Gamma_t = \Gamma_t(V)$ to indicate the dependence of Γ_t on $V \in \mathcal{V}$. For each $t \in \mathbb{R}$, the electrostatic free energy $E[\Gamma_t(V)]$ is defined in (3.1) (cf. also (3.2)) with $\Gamma_t = \Gamma_t(V)$ replacing Γ .

Definition 3.1. Let $V \in \mathcal{V}$. The first variation of $E[\Gamma]$ with respect to the perturbation of Γ defined by V is

$$\delta_{\Gamma,V} E[\Gamma] = \frac{d}{dt} E[\Gamma_t(V)] \bigg|_{t=0} = \lim_{t \to 0^+} \frac{E[\Gamma_t(V)] - E[\Gamma]}{t},$$

if the limit exists.

We recall that the tangential gradient along a dielectric boundary Γ is given by $\nabla_{\Gamma} = (I - n \otimes n)\nabla$, where I is the identity matrix. The following theorem provides an explicit formula of the first variation $\delta_{\Gamma,V}E[\Gamma]$, and its proof is given in Section 5:

Theorem 3.2. Let Γ be a given dielectric boundary as described in the assumption A1 in Subsection 2.1. Let $\psi_{\Gamma} \in \hat{\phi}_{\Gamma,\infty} + H_0^1(\Omega)$ be the unique weak solution to the boundary-value problem of the dielectric-boundary PB equation (1.8). Then, for any $V \in \mathcal{V}$, the first variation $\delta_{\Gamma,V}E[\Gamma]$ exists, and is given by

$$\delta_{\Gamma,V} E[\Gamma] = \int_{\Gamma} q_{\Gamma}(V \cdot n) \, dS,$$

where

$$q_{\Gamma} = -\frac{1}{2} \left(\frac{1}{\varepsilon_{+}} - \frac{1}{\varepsilon_{-}} \right) \left(|\varepsilon_{\Gamma} \partial_{n} \psi_{\Gamma}|^{2} - \varepsilon_{\Gamma} \partial_{n} \psi_{\Gamma} \varepsilon_{\Gamma} \partial_{n} \phi_{\Gamma,\infty} \right) + \frac{\varepsilon_{+} - \varepsilon_{-}}{2} \left(|\nabla_{\Gamma} \psi_{\Gamma}|^{2} - \nabla_{\Gamma} \psi_{\Gamma} \cdot \nabla_{\Gamma} \phi_{\Gamma,\infty} \right) + B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right).$$
 (3.8)

We identify q_{Γ} in (3.8) as the first variation of $E[\Gamma]$ and denote it as $q_{\Gamma} = \delta_{\Gamma} E[\Gamma]$. We call $-\delta_{\Gamma} E[\Gamma]$ the (normal component of the) dielectric boundary force.

4 Some Lemmas: The Calculus of Boundary Variations

4.1 Properties of the Transformation T_t

We first recall some properties of the family of transformations $T_t : \mathbb{R}^3 \to \mathbb{R}^3$ $(t \in \mathbb{R})$ defined by (3.7) in Subsection 3.2 above via a vector field $V \in C_c^2(\mathbb{R}^3, \mathbb{R}^3)$. These properties hold true if we change \mathbb{R}^3 to \mathbb{R}^d with a general dimension $d \geq 2$. They can be proved by direct calculations; cf. [18] (Section 4 of Chapter 9).

(1) Let $X \in \mathbb{R}^3$ and $t \in \mathbb{R}$. Let $\nabla T_t(X)$ be the gradient matrix of T_t at X with its entries $(\nabla T_t(X))_{ij} = \partial_j T_t^i(X)$ (i, j = 1, 2, 3), where T_t^i is the ith component of T_t . Let

$$J_t(X) = \det \nabla T_t(X). \tag{4.1}$$

Then for each $X \in \mathbb{R}^3$ the function $t \mapsto J_t(X)$ is a C^2 -function and

$$\frac{dJ_t}{dt} = ((\nabla \cdot V) \circ T_t)J_t,$$

where \circ denotes the composition of functions or maps. Clearly, $\nabla T_0 = I$, the identity matrix, and $J_0 = 1$. Moreover,

$$J_t(X) = 1 + t(\nabla \cdot V)(X) + H(t, X)t^2 \qquad \forall t \in \mathbb{R} \quad \forall X \in \mathbb{R}^3, \tag{4.2}$$

where H(t, X) satisfies

$$\sup\{|H(t,X)|: t \in \mathbb{R}, X \in \mathbb{R}^3\} < \infty,\tag{4.3}$$

since V is compactly supported.

(2) For each $t \in \mathbb{R}$, we define $A_V(t) : \mathbb{R}^3 \to \mathbb{R}$ by

$$A_V(t)(X) = J_t(X) (\nabla T_t(X))^{-1} (\nabla T_t(X))^{-T},$$
(4.4)

where a superscript T denotes the matrix transpose. Clearly, $A(t) \in C^1(\mathbb{R}^3, \mathbb{R}^{3\times 3})$, and the t-derivative of $A_V(t)$ at each point in \mathbb{R}^3 is

$$A'_{V}(t) = \left[((\nabla \cdot V) \circ T_{t}) - (\nabla T_{t})^{-1} ((\nabla V) \circ T_{t}) \nabla T_{t} - (\nabla T_{t})^{-1} ((\nabla V) \circ T_{t})^{T} (\nabla T_{t}) \right] A_{V}(t).$$

$$(4.5)$$

In particular

$$A_V'(0) = (\nabla \cdot V)I - \nabla V - (\nabla V)^T. \tag{4.6}$$

Moreover,

$$A_V(t)(X) = I + tA_V'(0)(X) + K(t, X)t^2 \qquad \forall t \in \mathbb{R} \quad \forall X \in \mathbb{R}^3, \tag{4.7}$$

where K(t, X) satisfies

$$\sup\{|K(t,X)|: t \in \mathbb{R}, X \in \mathbb{R}^3\} < \infty. \tag{4.8}$$

(3) For any $u \in L^2(\Omega)$ and $t \in \mathbb{R}$, $u \circ T_t \in L^2(\Omega)$ and $u \circ T_t^{-1} \in L^2(\Omega)$. Moreover,

$$\lim_{t \to 0} u \circ T_t = u \quad \text{and} \quad \lim_{t \to 0} u \circ T_t^{-1} = u \quad \text{in } L^2(\Omega). \tag{4.9}$$

For any $u \in H^1(\Omega)$ and $t \in \mathbb{R}$, $u \circ T_t \in H^1(\Omega)$ and $u \circ T_t^{-1} \in H^1(\Omega)$. Moreover,

$$\nabla(u \circ T_t^{-1}) = (\nabla T_t^{-1})^T \left(\nabla u \circ T_t^{-1}\right) \quad \text{and} \quad \nabla(u \circ T_t) = (\nabla T_t)^T \left(\nabla u \circ T_t\right), \quad (4.10)$$

$$\nabla(u \circ T_t^{-1}) = (\nabla T_t^{-1})^T (\nabla u \circ T_t^{-1}) \quad \text{and} \quad \nabla(u \circ T_t) = (\nabla T_t)^T (\nabla u \circ T_t), \quad (4.10)$$

$$\lim_{t \to 0} u \circ T_t = u \quad \text{and} \quad \lim_{t \to 0} u \circ T_t^{-1} = u \quad \text{in } H^1(\Omega). \quad (4.11)$$

If $u \in H^2(\Omega)$, then

$$\lim_{t \to 0} \left\| \frac{u \circ T_t - u}{t} - \nabla u \cdot V \right\|_{H^1(\Omega)} = 0. \tag{4.12}$$

Tangential Force 4.2

This is a geometrical property on the effect of tangential component of a velocity vector field to the motion of an interface. We shall state and prove it for a general d-dimensional space \mathbb{R}^d with $d \geq 2$. We assume that Γ is a C^3 , closed, hypersurface in \mathbb{R}^d . We denote as before the interior and exterior of Γ by Ω_- and Ω_+ , respectively. We also denote by n the unit vector normal to the surface Γ at a point on Γ , pointing from the interior to exterior of Γ . We assume that $V \in C_c^2(\mathbb{R}^d, \mathbb{R}^d)$ and define the transformation $T_t : \mathbb{R}^d \to \mathbb{R}^d$ $(t \in \mathbb{R})$ by $T_t(X) = x(t,X)$ for any $X \in \mathbb{R}^d$ and $t \in \mathbb{R}$, where x = x(t,X) is the unique solution to the initial-value problem (3.7).

Lemma 4.1. If $V \cdot n = 0$ on Γ , then there exist $t_0 > 0$ and C > 0, depending on Γ and V, such that

$$\operatorname{dist}(T_t(X), \Gamma) \le Ct^2 \qquad \forall X \in \Gamma \ \forall t \in \mathbb{R} \ with \ |t| \le t_0, \tag{4.13}$$

$$\left|\left\{x \in \mathbb{R}^d : \chi_{T_t(\Omega_s)}(x) \neq \chi_{\Omega_s}(x)\right\}\right| \le Ct^2 \quad if |t| \le t_0, \quad s = - \text{ or } +.$$

$$(4.14)$$

Proof. We first prove (4.13). Since Γ is of \mathbb{C}^3 , there exist finitely many open balls in \mathbb{R}^d such that their union covers Γ and that the intersection of Γ with each of such open balls is the graph of a C^3 function in a local coordinate system. Let us fix one of such open balls, \mathcal{B} , and assume without loss of generality that the corresponding C^3 -function is given by $h: \prod_{j=1}^{d-1} (a_j - \delta, b_j + \delta) \to \mathbb{R}$ for some $a_j, b_j \in \mathbb{R}$ with $a_j < b_j$ $(j = 1, \dots, d-1)$ and $\delta > 0$, where $\mathcal{B} \cap \Gamma$ is the graph of h on $\prod_{j=1}^{d-1} (a_j - \delta, b_j + \delta)$. Here, we use the local coordinate system depending on \mathcal{B} with the notation

$$X = (X', X_d) \in \mathbb{R}^d, \qquad X' = (X_1, \dots, X_{d-1}) \in \mathbb{R}^{d-1}, \qquad X_d \in \mathbb{R}.$$

So, $X_d = h(X')$ for all $X' \in \prod_{j=1}^{d-1} (a_j - \delta, b_j + \delta)$. We shall assume that $\delta > 0$ is small enough so that the corresponding concentric balls with radius reduced by δ still cover Γ , and that in particular the union of the graphs of h on $\prod_{j=1}^{d-1}(a_j,b_j)$ with all open balls \mathcal{B} is still Γ . Moreover, since all Γ and T_t $(t \in \mathbb{R})$ are smooth, there exists $t'_0 \in (0,1)$ such that, for any $t \in \mathbb{R}$ with $|t| \leq t'_0$ and for any $X = (X', X_d) \in \Gamma$ with $X' \in \prod_{j=1}^{d-1} (a_j, b_j)$, the coordinate $(T_t(X))'$ of $T_t(X) = ((T_t(X))', (T_t(X))_d)$ is still in $\prod_{j=1}^{d-1} (a_j - \delta, b_j + \delta)$, the domain of h. With this setup, we shall prove that there exist $t_0 \in (0, t'_0)$ and C > 0 such that

$$\operatorname{dist}(T_t(X_0), \Gamma) \le Ct^2 \quad \text{if } X_0 = (X_0', X_{0d}) \in \Gamma \text{ with } X_0' \in \prod_{j=1}^{d-1} (a_j, b_j) \text{ and } |t| \le t_0.$$
 (4.15)

This then implies (4.13).

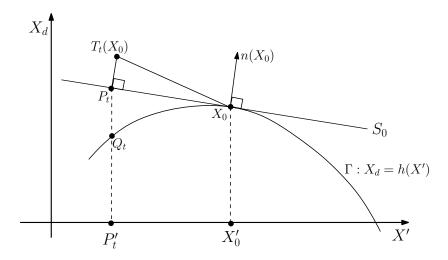


Figure 2: A local graph representation of the surface Γ .

Let us fix an arbitrary point $X_0 = (X_0', X_{0d}) \in \Gamma$ with $X_0' \in \prod_{j=1}^{d-1} (a_j, b_j)$ and $X_{0d} = h(X_0')$; cf. Figure 2. The equation for the plane, S_0 , that is tangent to the surface Γ at $X_0 \in \Gamma$ is given by

$$(X - X_0) \cdot n(X_0) = 0$$
 with $X = (X', X_d) \in \mathbb{R}^d$,

where $n(X_0)$ is the unit vector normal to Γ at X_0 ,

$$n(X_0) = \frac{(-\nabla_{X'}h(X_0'), 1)}{\sqrt{1 + |\nabla_{X'}h(X_0')|^2}}.$$
(4.16)

Let $t \in \mathbb{R}$ with $|t| \leq t'_0$. Denote by $P_t = (P'_t, P_{td}) \in S_0$ the point of the orthogonal projection of the vector $T_t(X_0) - X_0$ on this tangent plane S_0 , given by

$$P_t = -\left[\left(T_t(X_0) - X_0 \right) \cdot n(X_0) \right] n(X_0) + T_t(X_0). \tag{4.17}$$

Denote

$$Q_t = (Q_t', Q_{td}) = (P_t', h(P_t')) \in \Gamma.$$
(4.18)

We show that

$$|T_t(X_0) - Q_t| \le Ct^2$$
 if $|t| \le t_0$ (4.19)

for some constants $t_0 \in (0,1)$ and C > 0 independent of X_0 . This should imply (4.15) as

$$\operatorname{dist}\left(T_{t}(X_{0}),\Gamma\right) \leq |T_{t}(X_{0}) - Q_{t}|.$$

To prove (4.19), it suffices by the triangle inequality to prove

$$|T_t(X_0) - P_t| \le Ct^2,$$
 (4.20)

$$|P_t - Q_t| = |P_{td} - Q_{td}| \le Ct^2, (4.21)$$

for all t with $|t| \leq t_0$. Here and below in the proof, C denotes a generic constant independent of X_0 and $t \in [-t_0, t_0]$. Since $V \in C_c^2(\mathbb{R}^3, \mathbb{R}^3)$, we have by (3.7) that

$$\partial_{tt}T_t(X) = \partial_{tt}x(t,X) = \partial_t(V(x(t,X))) = (\nabla V(x(t,X)))\partial_tx(t,X)$$
$$= (\nabla V(x(t,X)))V(x(t,X)) \le C \qquad \forall t \in \mathbb{R} \ \forall X \in \mathbb{R}^d.$$

Therefore, by Taylor's expansion, (4.17), (3.7), the fact that $|n(X_0)| = 1$, and the assumption that $V(X_0) \cdot n(X_0) = 0$, we have

$$|T_t(X_0) - P_t| = |[x(t, X_0) - X_0] \cdot n(X_0)|$$

$$\leq |x(0, X_0) - X_0| + |t\partial_t x(0, X_0) \cdot n(X_0)| + Ct^2$$

$$= |tV(X_0) \cdot n(X_0)| + Ct^2$$

$$= Ct^2,$$

proving (4.20).

Since V is compactly supported, we have by (3.7) and Taylor's expansion that

$$|T_t(X_0) - X_0| = |x(t, X_0) - X_0| = |t\partial_t x(\xi_t, X_0)| = |t||V(x(\xi_t, X_0))| \le C|t|,$$

where ξ_t is in between 0 and t. This and (4.20) imply

$$|P'_t - X'_0| \le |P_t - X_0| \le |P_t - T_t(X_0)| + |T_t(X_0) - X_0| \le C|t| \quad \text{if } |t| < t_0. \tag{4.22}$$

By (4.18) and Taylor's expansion,

$$Q_{td} = h(P'_t)$$

$$= h(X'_0) + \nabla_{X'}h(X'_0) \cdot (P'_t - X'_0) + \frac{1}{2}\nabla^2_{X'}h(Y'_t)(P'_t - X'_0) \cdot (P'_t - X'_0)$$
(4.23)

for some $Y'_t \in \prod_{j=1}^{d-1} (a_j, b_j)$. Since $(P_t - X_0) \cdot n(X_0) = 0$, $X_{0d} = h(X'_0)$, and $n(X_0)$ is given by (4.16), we have that

$$P_{td} = h(X_0') + \nabla_{X'} h(X_0) \cdot (P_t' - X_0').$$

This, together with (4.23) and (4.22), implies (4.21). The constant C depends on h and V, and hence on Γ and V only.

We now prove (4.14). We only consider the case s = -, as the case s = + can be treated similarly. Moreover, for t = 0, the inequality in (4.14) holds true obviously, since T_0 is the identity map. So, let $t \in \mathbb{R}$ be such that $0 < |t| \le t_0$. We further assume that $0 < t \le t_0$ as the case $-t_0 \le t < 0$ is similar.

We claim that

$$\Omega_{-}\Delta T_{t}(\Omega_{-}) := (\Omega_{-} \setminus T_{t}(\Omega_{-})) \cup (T_{t}(\Omega_{-}) \setminus \Omega_{-}) \subseteq \{X \in \mathbb{R}^{d} : \operatorname{dist}(X, \Gamma) \le Ct^{2}\}, \quad (4.24)$$

where the constant C is exactly the same as in (4.13). In fact, if $X \in \Omega_- \setminus T_t(\Omega_-)$, then $X \in \Omega_-$ and $T_{-t}(X) \in \overline{\Omega_+}$. Hence, $\{T_s(T_{-t}(X))\}_{0 \le s \le t}$ is a C^3 -curve in \mathbb{R}^d , connecting one endpont $T_0(T_{-t}(X)) = T_{-t}(X) \in \overline{\Omega_+}$ to the other $T_t(T_{-t}(X)) = X \in \Omega_-$. Since Γ is a closed hypersurface in \mathbb{R}^d , there must exist $s_0 \in (0,t)$ such that $T_{s_0}(T_{-t}(X)) = T_{s_0-t}(X) \in \Gamma$. Hence, by (4.13) with $t - s_0$ and $T_{s_0-t}(X)$ replacing t and X, respectively,

$$\operatorname{dist}(X,\Gamma) = \operatorname{dist}(T_{t-s_0}(T_{s_0-t}(X)),\Gamma) \le C(t-s_0)^2 \le Ct^2.$$

Similarly, if $X \in T_t(\Omega_-) \setminus \Omega_-$, then dist $(X, \Gamma) \leq Ct^2$. Hence, (4.24) holds true. By (4.24), we have

$$\left| \left\{ X \in \mathbb{R}^d : \chi_{\Omega_-(t)} \neq \chi_{\Omega_-(X)} \right\} \right| = \left| \Omega_- \Delta T_t(\Omega_-) \right| \le \left| \left\{ X \in \mathbb{R}^d : \operatorname{dist}(X, \Gamma) \le Ct^2 \right\} \right|.$$

This implies (4.14) (for s = -), as the right-hand side of the above inequality is bounded by Ct^2 if $|t| \le t_0$ with a possible smaller t_0 (cf. Lemma 2.1 in [33]).

4.3 Continuity and Differentiability

Let Γ be a dielectric boundary satisfying the assumptions in A1 of Subsection 2.1 and $V \in \mathcal{V}$ (cf. (3.6)). Let $\{T_t\}_{t\in\mathbb{R}}$ be the corresponding family of diffeomorphisms defined by (3.7). Let $\hat{\phi} \in W^{1,1}(\Omega)$ satisfy (2.3). We consider the approximations $\hat{\phi} \circ T_t$. Note that $\hat{\phi} \circ T_t - \hat{\phi}$ and $\nabla \hat{\phi} \cdot V$ vanish in any small neighborhood of $\bigcup_{i=1}^N x_i$, as V(X) = 0 and $T_t(X) = X$ for any X in such a neighborhood and any $t \in \mathbb{R}$.

Lemma 4.2. Let $\hat{\phi} \in \hat{\phi}_{C} + H^{1}(\Omega)$ satisfy (2.3). We have

$$\lim_{t \to 0} \|\hat{\phi} \circ T_t - \hat{\phi}\|_{H^1(\Omega)} = 0. \tag{4.25}$$

Moreover, $\nabla \hat{\phi} \cdot V \in H^1(\Omega)$ and

$$\lim_{t \to 0} \left\| \frac{\hat{\phi} \circ T_t - \hat{\phi}}{t} - \nabla \hat{\phi} \cdot V \right\|_{H^1(\Omega)} = 0. \tag{4.26}$$

Proof. Let $\sigma > 0$ be such that $B_{\sigma} := \bigcup_{i=1}^{N} B(x_i, \sigma) \subset \Omega$ and V = 0 on B_{σ} . Then, there exists $\tilde{\phi} \in C^{\infty}(\Omega) \cap H^2(\Omega)$ such that $\tilde{\phi} = 0$ in $B_{\sigma/2}$ and $\tilde{\phi} = \hat{\phi}$ a.e. in $\Omega \setminus B_{\sigma}$. These imply that

 $\tilde{\phi} \circ T_t - \tilde{\phi} = \hat{\phi} \circ T_t - \hat{\phi}$, and $\nabla \tilde{\phi} \cdot V = \nabla \hat{\phi} \cdot V$ a.e. in Ω for all t. This implies that $\nabla \hat{\phi} \cdot V \in H^1(\Omega)$. Moreover, it follows from (4.11) that

$$\lim_{t \to 0} \|\hat{\phi} \circ T_t - \hat{\phi}\|_{H^1(\Omega)} = \lim_{t \to 0} \|\tilde{\phi} \circ T_t - \tilde{\phi}\|_{H^1(\Omega)} = 0,$$

implying (4.25), and from (4.12) that

$$\lim_{t \to 0} \left\| \frac{\hat{\phi} \circ T_t - \hat{\phi}}{t} - \nabla \hat{\phi} \cdot V \right\|_{H^1(\Omega)} = \lim_{t \to 0} \left\| \frac{\tilde{\phi} \circ T_t - \tilde{\phi}}{t} - \nabla \tilde{\phi} \cdot V \right\|_{H^1(\Omega)} = 0,$$

implying (4.26).

We recall that $\phi_{\Gamma,\infty} \in H^1(\Omega) \cap C(\overline{\Omega})$ is the unique weak solution to the boundary-value problem (1.7), defined in (2.5). Similarly, $\phi_{\Gamma_t,\infty} \in H^1(\Omega) \cap C(\overline{\Omega})$ for each $t \in \mathbb{R}$ is the unique weak solution to the same boundary-value problem with $\Gamma_t = T_t(\Gamma)$ replacing Γ .

Lemma 4.3. (1) There exists a unique $\zeta_{\Gamma,V} \in H_0^1(\Omega)$ such that

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla \zeta_{\Gamma,V} \cdot \nabla \eta \, dx = -\int_{\Omega} \varepsilon_{\Gamma} A'_{V}(0) \nabla \phi_{\Gamma,\infty} \cdot \nabla \eta \, dx \qquad \forall \eta \in H_{0}^{1}(\Omega), \tag{4.27}$$

where $A'_{V}(0)$ is defined in (4.6). Moreover, the mapping $V \mapsto \zeta_{\Gamma,V}$ is linear in V, i.e.,

$$\zeta_{\Gamma,c_1V_1+c_2V_2} = c_1\zeta_{\Gamma,V_1} + c_2\zeta_{\Gamma,V_2} \qquad \text{for all } V_1,V_2 \in \mathcal{V} \text{ and } c_1,c_2 \in \mathbb{R}.$$

(2) By modifying the value of $\zeta_{\Gamma,V}$ on a set of zero Lebesgue measure, we have that $\zeta_{\Gamma,V}^{s} \in H^{2}(\Omega_{s}) \cap C^{1}(\Omega_{s})$ for s = - or +. Moreover,

$$\Delta \zeta_{\Gamma,V} = -\nabla \cdot [A_V'(0)\nabla \phi_{\Gamma,\infty}] = \Delta(\nabla \phi_{\Gamma,\infty} \cdot V) \qquad in \ \Omega_- \cup \Omega_+, \tag{4.28}$$

$$[\![\varepsilon_{\Gamma}\partial_{n}\zeta_{\Gamma,V}]\!]_{\Gamma} = -[\![\varepsilon_{\Gamma}A'_{V}(0)\nabla\phi_{\Gamma,\infty}\cdot n]\!]_{\Gamma} \qquad on \ \Gamma.$$

$$(4.29)$$

(3) We have

$$\lim_{t \to 0} \|\phi_{\Gamma_t,\infty} \circ T_t - \phi_{\Gamma,\infty}\|_{H^1(\Omega)} = 0, \tag{4.30}$$

$$\lim_{t \to 0} \left\| \frac{\phi_{\Gamma_t, \infty} \circ T_t - \phi_{\Gamma, \infty}}{t} - \zeta_{\Gamma, V} \right\|_{H^1(\Omega)} = 0. \tag{4.31}$$

(4) If $V \cdot n = 0$ on Γ , then $\zeta_{\Gamma,V} = \nabla \phi_{\Gamma,\infty} \cdot V$ in Ω .

Proof. (1) The existence and uniqueness of $\zeta_{\Gamma,V} \in H_0^1(\Omega)$ that satisfies (4.27) follow from the Lax–Milgram Lemma [22, 25]. By (4.6), $A'_V(0)$ is linear in V. Therefore, by the definition (4.27) of $\zeta_{\Gamma,V} \in H_0^1(\Omega)$, $\zeta_{\Gamma,V}$ is linear in V.

(2) Let s denote - or +. Note by (2.6), (3.6), and (4.6) that $A'_V(0)\nabla\phi_{\Gamma,\infty}\in C^1(\Omega_s)\cap H^1(\Omega_s)$. For any $\eta\in C^1_c(\Omega)$ with supp $(\eta)\subset\Omega_s$, we have by (4.27) and the Divergence Theorem that

$$\int_{\Omega_{\mathbf{s}}} \varepsilon_{\mathbf{s}} \nabla \zeta_{\Gamma,V} \cdot \nabla \eta \, dx = \int_{\Omega_{\mathbf{s}}} \varepsilon_{\mathbf{s}} \nabla \cdot \left[A_V'(0) \nabla \phi_{\Gamma,\infty} \right] \eta \, dx.$$

Hence, $-\Delta \zeta_{\Gamma,V} = \nabla \cdot [A'_V(0)\nabla \phi_{\Gamma,\infty}]$ in Ω_s . Since the right-hand side is in $L^2(\Omega_s) \cap C(\Omega_s)$, it follows from the elliptic regularity theory [25, 32] that $\zeta_{\Gamma,V}^s \in H^2(\Omega_s) \cap C^1(\Omega_s)$, after a possible modification of the value of $\zeta_{\Gamma,V}$ on a set of zero Lebesgue measure. Moreover, the first equality in (4.28) follows.

Let us denote by V^i (i = 1, 2, 3) the components of V. With the conventional summation notation (i.e., repeated indices are summed), we have by (4.6), (2.6), and (2.8) that

$$-\nabla \cdot (A'_{V}(0)\nabla\phi_{\Gamma,\infty})$$

$$= \nabla \cdot \left[\nabla V + (\nabla V)^{T} - (\nabla \cdot V)I\right]\nabla\phi_{\Gamma,\infty}$$

$$= \partial_{i}\left(\partial_{j}V^{i}\partial_{j}\phi_{\Gamma,\infty} + \partial_{i}V^{j}\partial_{j}\phi_{\Gamma,\infty} - \partial_{k}V^{k}\partial_{i}\phi_{\Gamma,\infty}\right)$$

$$= 2\partial_{ij}\phi_{\Gamma,\infty}\partial_{i}V^{j} + \partial_{ii}V^{j}\partial_{j}\phi_{\Gamma,\infty}$$

$$= \partial_{ii}\partial_{j}\phi_{\Gamma,\infty}V^{j} + 2\partial_{ij}\phi_{\Gamma,\infty}\partial_{i}V^{j} + \partial_{ii}V^{j}\partial_{j}\phi_{\Gamma,\infty} \quad [\text{since } \partial_{ii}\phi_{\Gamma,\infty} = 0]$$

$$= \partial_{ii}\left(\partial_{j}\phi_{\Gamma,\infty}V^{j}\right)$$

$$= \Delta(\nabla\phi_{\Gamma,\infty}\cdot V) \quad \text{in } \Omega_{-}\cup\Omega_{+}, \qquad (4.32)$$

implying the second equation in (4.28).

Since $\zeta_{\Gamma,V} \in H_0^1(\Omega)$ and $\Delta \zeta_{\Gamma,V} \in L^2(\Omega_s)$ for s being - or +, and since the unit normal n at the Γ points from Ω_- to Ω_+ , we have by the Divergence Theorem that both sides of the equation in (4.27) are

$$\begin{split} \int_{\Omega} \varepsilon_{\Gamma} \nabla \zeta_{\Gamma,V} \cdot \nabla \eta \, dx &= \int_{\Omega_{-}} \varepsilon_{-} \nabla \zeta_{\Gamma,V} \cdot \nabla \eta \, dx + \int_{\Omega_{+}} \varepsilon_{+} \nabla \zeta_{\Gamma,V} \cdot \nabla \eta \, dx \\ &= -\int_{\Omega_{-}} \varepsilon_{-} \Delta \zeta_{\Gamma,V} \eta \, dx - \int_{\Omega_{+}} \varepsilon_{+} \Delta \zeta_{\Gamma,V} \eta \, dx - \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \partial_{n} \zeta_{\Gamma,V} \rrbracket_{\Gamma} \eta \, dS, \end{split}$$

and

$$\begin{split} &-\int_{\Omega} \varepsilon_{\Gamma} A'_{V}(0) \nabla \phi_{\Gamma,\infty} \cdot \nabla \eta \, dx \\ &= -\int_{\Omega_{-}} \varepsilon_{-} A'_{V}(0) \nabla \phi_{\Gamma,\infty} \cdot \nabla \eta \, dx - \int_{\Omega_{+}} \varepsilon_{+} A'_{V}(0) \nabla \phi_{\Gamma,\infty} \cdot \nabla \eta \, dx \\ &= \int_{\Omega_{-}} \varepsilon_{-} \nabla \cdot (A'_{V}(0) \nabla \phi_{\Gamma,\infty}) \eta \, dx + \int_{\Omega_{+}} \varepsilon_{+} \nabla \cdot (A'_{V}(0) \nabla \phi_{\Gamma,\infty}) \eta \, dx \\ &+ \int_{\Gamma} \llbracket \varepsilon_{\Gamma} A'_{V}(0) \nabla \phi_{\Gamma,\infty} \cdot n \rrbracket_{\Gamma} \eta \, dS, \end{split}$$

respectively. These, together with and (4.28), imply (4.29).

(3) Replacing Γ , $\phi_{\Gamma,\infty}$, and η by Γ_t , $\phi_{\Gamma_t,\infty}$, and $\eta \circ T_t^{-1}$ for $t \in \mathbb{R}$, respectively, in the weak formulation (2.5), we get by the change of variable $x = T_t(X)$ that

$$\int_{\Omega} \varepsilon_{\Gamma} A_V(t) \nabla (\phi_{\Gamma_t,\infty} \circ T_t) \cdot \nabla \eta \, dX = 0 \qquad \forall \eta \in H_0^1(\Omega).$$

This and (2.5) imply for any $\eta \in H_0^1(\Omega)$ that

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla (\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}) \cdot \nabla \eta \, dX = \int_{\Omega} \varepsilon_{\Gamma} [I - A_{V}(t)] \nabla (\phi_{\Gamma_{t},\infty} \circ T_{t}) \cdot \nabla \eta \, dX. \tag{4.33}$$

It follows from a change of variable, (4.2), (4.3), (4.7), and (4.8) that $\|\nabla(\phi_{\Gamma_t,\infty} \circ T_t)\|_{L^2(\Omega)}$ is bounded uniformly in t. Setting $\eta = \phi_{\Gamma_t,\infty} \circ T_t - \phi_{\Gamma,\infty} \in H^1_0(\Omega)$ in (4.33), we then obtain (4.30) by (4.7), (4.8), and the Cauchy–Schwarz and Poincaré inequalities.

Dividing both sides of (4.33) by $t \neq 0$ and setting now $\eta = (\phi_{\Gamma_t,\infty} \circ T_t - \phi_{\Gamma,\infty})/t - \zeta_{\Gamma,V}$ in the resulting equation and also in (4.27), we have by the Cauchy–Schwarz inequality that

$$\begin{split} &\int_{\Omega} \varepsilon_{\Gamma} \left| \nabla \left(\frac{\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}}{t} - \zeta_{\Gamma,V} \right) \right|^{2} dX \\ &= \int_{\Omega} \varepsilon_{\Gamma} \left[\frac{I - A_{V}(t)}{t} + A_{V}'(0) \right] \nabla (\phi_{\Gamma_{t},\infty} \circ T_{t}) \cdot \nabla \left(\frac{\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}}{t} - \zeta_{\Gamma,V} \right) dX \\ &+ \int_{\Omega} \varepsilon_{\Gamma} A_{V}'(0) \nabla \left[\phi_{\Gamma,\infty} - \phi_{\Gamma_{t},\infty} \circ T_{t} \right] \cdot \nabla \left(\frac{\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}}{t} - \zeta_{\Gamma,V} \right) dX \\ &\leq C \left\| \frac{A_{V}(t) - I - t A_{V}'(0)}{t} \right\|_{L^{\infty}(\Omega)} \left\| \phi_{\Gamma_{t},\infty} \circ T_{t} \right\|_{H^{1}(\Omega)} \left\| \frac{\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}}{t} - \zeta_{\Gamma,V} \right\|_{H^{1}(\Omega)} \\ &+ C \|\phi_{\Gamma,\infty} - \phi_{\Gamma_{t},\infty} \circ T_{t} \|_{H^{1}(\Omega)} \left\| \frac{\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}}{t} - \zeta_{\Gamma,V} \right\|_{H^{1}(\Omega)} . \end{split}$$

This, together with Poincaré's inequality, (4.7), (4.8), and (4.30), leads to (4.31).

(4) Assume now $V \cdot n = 0$ on Γ . Recall from subsection 3.2 that the signed distance to Γ , $\phi : \mathbb{R}^3 \to \mathbb{R}$, which is negative in Ω_- and positive outside Γ , is in fact a C^3 -function and also $\nabla \phi \neq 0$ in $\mathcal{N}_0(\Gamma)$, a neighborhood of Γ in Ω ; cf. (3.5). Moreover, $n = \nabla \phi$ on Γ . We define $n = \nabla \phi$ on $\mathcal{N}_0(\Gamma)$. Now, since $V \cdot n = 0$ on Γ , by Lemma 4.1, there exists $t_0 = t_0(V) > 0$ and a constant $C_0 > 0$ which may depend on Γ , such that dist $(x, \Gamma) \leq C_0 t^2$ for all $x \in \Gamma_t$ and all $t \in [-t_0, t_0]$. Let $D(t) = \{x \in \Omega : \text{dist}(x, \Gamma) \leq C_0 t^2\}$. Then $\Gamma_t \subset D(t)$, and hence $\varepsilon_{\Gamma_t} = \varepsilon_{\Gamma}$ on $\Omega \setminus D(t)$, for all $|t| \leq t_0$. Moreover, the measure $|D(t)| = O(t^2)$ as $t \to 0$; cf. Lemma 2.1 in [33].

Let $h_t = (\phi_{\Gamma_t,\infty} - \phi_{\Gamma,\infty})/t$ with $|t| \le t_0$. We have now by (1.7) and that with Γ_t replacing Γ that

$$\int_{\Omega} \varepsilon_{\Gamma_t} \nabla h_t \cdot \nabla \eta \, dx = -\int_{\Omega} \frac{\varepsilon_{\Gamma_t} - \varepsilon_{\Gamma}}{t} \nabla \phi_{\Gamma,\infty} \cdot \nabla \eta \, dx \qquad \forall \eta \in H_0^1(\Omega). \tag{4.34}$$

Setting $\eta=h_t\in H^1_0(\Omega)$, we have by the uniform boundedness of $\nabla\phi_{\Gamma_t,\infty}$ (cf. (2.7)), the Poincaré and Cauchy–Schwarz inequalities, and the fact that $|D(t)|=O(t^2)$ as $t\to 0$ that

$$||h_t||_{H^1(\Omega)} \le C \left(\int_{D(t)} \left| \frac{\varepsilon_{\Gamma_t} - \varepsilon_{\Gamma}}{t} \right|^2 dx \right)^{1/2} \le C,$$

where C > 0 is a generic constant, independent of t. Thus, there exists a subsequence of h_t ($|t| \le t_0$), not relabeled, and some $h \in H_0^1(\Omega)$, such that $h_t \to h$ weakly in $H^1(\Omega)$ as $t \to 0$.

Working on this subsequence, we have by (2.5) (with $\phi_{\Gamma_t,\infty}$ replacing $\phi_{\Gamma,\infty}$), (4.34), (2.7), and the fact that the measure $|D(t)| = O(t^2) \to 0$ as $t \to 0$ that for any $\eta \in H_0^1(\Omega)$

$$\left| \int_{\Omega} \varepsilon_{\Gamma} \nabla h_{t} \cdot \nabla \eta \, dx \right| = \left| \int_{\Omega} (\varepsilon_{\Gamma} - \varepsilon_{\Gamma_{t}}) \nabla h_{t} \cdot \nabla \eta \, dx - \int_{\Omega} \frac{\varepsilon_{\Gamma_{t}} - \varepsilon_{\Gamma}}{t} \nabla \phi_{\Gamma,\infty} \cdot \nabla \eta \, dx \right|$$

$$\leq \left| \int_{D(t)} (\varepsilon_{\Gamma_{t}} - \varepsilon_{\Gamma}) \nabla h_{t} \cdot \nabla \eta \, dx \right| + \left| \int_{D(t)} \frac{\varepsilon_{\Gamma_{t}} - \varepsilon_{\Gamma}}{t} \nabla \phi_{\Gamma,\infty} \cdot \nabla \eta \, dx \right|$$

$$\leq C \left[\|h_{t}\|_{H^{1}(\Omega)} + \frac{1}{|t|} |D(t)|^{1/2} \right] \left(\int_{D(t)} |\nabla \eta|^{2} dx \right)^{1/2}$$

$$\leq C \left(\int_{D(t)} |\nabla \eta|^{2} dx \right)^{1/2}$$

$$\to 0 \quad \text{as } t \to 0.$$

Since $h_t \to h$ weakly in $H^1(\Omega)$, we have

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla h \cdot \nabla \eta \, dx = 0 \qquad \forall \eta \in H_0^1(\Omega).$$

Setting $\eta = h \in H_0^1(\Omega)$, we see that h = 0 in $H_0^1(\Omega)$.

We now show that $\zeta_{\Gamma} = \nabla \phi_{\Gamma,\infty} \cdot V$ in Ω . Let $\eta \in L^2(\Omega)$ and $t \neq 0$. Since $h_t \to h = 0$ weakly in $H^1(\Omega)$, we have by the properties of the transformations T_t $(t \in \mathbb{R})$ (4.9), (4.12), and (4.1)–(4.3) that

$$\begin{split} &\int_{\Omega} \frac{\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}}{t} \eta \, dX \\ &= \int_{\Omega} \frac{\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty} \circ T_{t}}{t} \eta \, dX + \int_{\Omega} \frac{\phi_{\Gamma,\infty} \circ T_{t}}{t} \eta \, dX - \int_{\Omega} \frac{\phi_{\Gamma,\infty} \eta}{t} \, dX \\ &= \int_{\Omega} h_{t} \left(\eta \circ T_{t}^{-1} \right) \det \nabla T_{t}^{-1} dx + \int_{\Omega} \frac{\phi_{\Gamma,\infty}}{t} \left(\eta \circ T_{t}^{-1} \right) \det \nabla T_{t}^{-1} dx - \int_{\Omega} \frac{\phi_{\Gamma,\infty} \eta}{t} \, dx \\ &= \int_{\Omega} h_{t} \left(\eta \circ T_{t}^{-1} \right) \det \nabla T_{t}^{-1} dx \\ &+ \int_{\Omega} \phi_{\Gamma,\infty} \left(\frac{\eta \circ T_{t}^{-1} - \eta}{t} \det \nabla T_{t}^{-1} + \eta \frac{\det \nabla T_{t}^{-1} - 1}{t} \right) dx \\ &\to - \int_{\Omega} \phi_{\Gamma,\infty} \nabla \eta \cdot V \, dx - \int_{\Omega} \phi_{\Gamma,\infty} \eta (\nabla \cdot V) \, dx \\ &= \int_{\Omega} (\nabla \phi_{\Gamma,\infty} \cdot V) \eta \, dx \qquad \text{as } t \to 0. \end{split}$$

This and (4.31), together with the arbitrariness of $\eta \in L^2(\Omega)$, imply that $\zeta_{\Gamma,V} = \nabla \phi_{\Gamma,\infty} \cdot V$ in Ω .

We recall that $\hat{\phi}_{\Gamma,\infty}$ is determined by (2.11) and the boundary condition $\hat{\phi}_{\Gamma,\infty} = \phi_{\infty}$ on $\partial\Omega$. For each $t \in \mathbb{R}$, we denote by $\hat{\phi}_{\Gamma_t,\infty}$ the unique function that is defined by (2.11) with Γ_t replacing Γ and the same boundary condition $\hat{\phi}_{\Gamma_t,\infty} = \phi_{\infty}$ on $\partial\Omega$. Note that all the singularities x_i (i = 1, ..., N) are outside the support of the vector field V.

Lemma 4.4. (1) There exists a unique $\xi_{\Gamma,V} \in H_0^1(\Omega)$ such that

$$\int_{\Omega} \varepsilon_{\Gamma} \nabla \xi_{\Gamma,V} \cdot \nabla \eta \, dx = -\int_{\Omega} \varepsilon_{\Gamma} A'_{V}(0) \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \eta \, dx \qquad \forall \eta \in H_{0}^{1}(\Omega). \tag{4.35}$$

(2) By modifying the value of $\xi_{\Gamma,V}$ on a set of zero Lebesgue measure, we have that $\xi_{\Gamma,V}^{s} \in H^{2}(\Omega_{s}) \cap C^{1}(\Omega_{s})$ for s = - or +. Moreover,

$$\Delta \xi_{\Gamma,V} = -\nabla \cdot A_V'(0) \nabla \hat{\phi}_{\Gamma,\infty} = \Delta(\nabla \hat{\phi}_{\Gamma,\infty} \cdot V) \qquad in \ \Omega_- \cup \Omega_+,$$

$$[\![\varepsilon_\Gamma \partial_n \xi_{\Gamma,V}]\!]_\Gamma = -[\![\varepsilon_\Gamma A_V'(0) \partial_n \hat{\phi}_{\Gamma,\infty}]\!]_\Gamma \qquad on \ \Gamma.$$

$$(4.36)$$

(3) We have

$$\lim_{t \to 0} \|\hat{\phi}_{\Gamma_t,\infty} \circ T_t - \hat{\phi}_{\Gamma,\infty}\|_{H^1(\Omega)} = 0,$$

$$\lim_{t \to 0} \left\| \frac{\hat{\phi}_{\Gamma_t,\infty} \circ T_t - \hat{\phi}_{\Gamma,\infty}}{t} - \xi_{\Gamma,V} \right\|_{H^1(\Omega)} = 0.$$

Proof. The proof is the same as and simpler than that of the next lemma, Lemma 4.5, as there is an extra term B there, which can be set to 0 here. The only exception is the second equality in (4.36) which can be obtained by the calculations same as in (4.32).

We recall that $\psi_{\Gamma} \in \hat{\phi}_{\mathcal{C}} + H^1(\Omega) \cap C(\overline{\Omega}) = \hat{\phi}_{\Gamma,\infty} + H^1(\Omega) \cap C(\overline{\Omega})$ is the unique weak solution to the boundary-value problem of the dielectric-boundary PB equation (1.8); cf. Definition 2.1. For each $t \in \mathbb{R}$, we denote by $\psi_{\Gamma_t} \in \hat{\phi}_{\mathcal{C}} + H^1(\Omega) \cap C(\overline{\Omega})$ the unique solution to the same boundary-value problem with Γ_t replacing Γ .

Lemma 4.5. (1) There exists a unique $\omega_{\Gamma,V} \in H_0^1(\Omega)$ such that

$$\int_{\Omega} \left[\varepsilon_{\Gamma} \nabla \omega_{\Gamma,V} \cdot \nabla \eta + \chi_{+} B'' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \omega_{\Gamma,V} \eta \right] dx$$

$$= -\int_{\Omega} \varepsilon_{\Gamma} A'_{V}(0) \nabla \psi_{\Gamma} \cdot \nabla \eta \, dx$$

$$-\int_{\Omega_{+}} \left[(\nabla \cdot V) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) - \frac{\zeta_{\Gamma,V}}{2} B'' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] \eta \, dx \qquad \forall \eta \in H_{0}^{1}(\Omega). \tag{4.37}$$

(2) By modifying the value of $\omega_{\Gamma,V}$ on a set of zero Lebesgue measure, we have that $\omega_{\Gamma,V}^{s} \in H^{2}(\Omega_{s}) \cap C^{1}(\Omega_{s})$ for s = - or +. Moreover,

$$\Delta\omega_{\Gamma,V} = -\nabla \cdot A_V'(0)\nabla\psi_{\Gamma} = \Delta(\nabla\psi_{\Gamma} \cdot V) \qquad in \ \Omega_-, \tag{4.38}$$

$$\varepsilon_{+} \Delta \omega_{\Gamma,V} - B'' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \omega_{\Gamma,V} = -\varepsilon_{+} \nabla \cdot A'_{V}(0) \nabla \psi_{\Gamma}
+ (\nabla \cdot V) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) - \frac{\zeta_{\Gamma,V}}{2} B'' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \quad in \ \Omega_{+}, \tag{4.39}$$

$$[\![\varepsilon_{\Gamma} \partial_{n} \omega_{\Gamma,V}]\!]_{\Gamma} = -[\![\varepsilon_{\Gamma} A'_{V}(0) \partial_{n} \psi_{\Gamma}]\!]_{\Gamma} \quad on \ \Gamma. \tag{4.40}$$

(3) We have

$$\lim_{t \to 0} \|\psi_{\Gamma_t} \circ T_t - \psi_{\Gamma}\|_{H^1(\Omega)} = 0, \tag{4.41}$$

(4.40)

$$\lim_{t \to 0} \left\| \frac{\psi_{\Gamma_t} \circ T_t - \psi_{\Gamma}}{t} - \omega_{\Gamma, V} \right\|_{H^1(\Omega)} = 0. \tag{4.42}$$

Proof. (1) Since B'' > 0, the support of V does not contain any of the singularities x_i $(i=1,\ldots,N)$, and ψ_{Γ} and $\phi_{\Gamma,\infty}$ are uniformly bounded on the union of the support of V and Ω_+ (cf. (2.16) and (2.21)), the existence and uniqueness of $\omega_{\Gamma,V} \in H_0^1(\Omega)$ that satisfies (4.37) follows from the Lax-Milgram Lemma [22, 25].

- (2) Choosing $\eta \in C^1_c(\Omega)$ in (4.37) with supp $(\eta) \subset \Omega_-$ and applying the Divergence Theorem, we obtain the first equation of (4.38) in a.e. Ω_{-} . Since the right-hand side of this first equation is in $L^2(\Omega_-) \cap C(\Omega_-)$, it follows from the regularity theory [25, 32] that, with a possible modification of the value of $\omega_{\Gamma,V}$ on a set of zero Lebesgue measure, $\omega_{\Gamma,V}^- \in$ $H^2(\Omega_-) \cap C^1(\Omega_-)$. Now, the first equation in (4.38) holds for each point in Ω_- . The second equation is similar to that in (4.28) (cf. (4.32)). By similar arguments, we obtain that $\omega_{\Gamma,V}^+ \in H^2(\Omega_+) \cap C^1(\Omega_+)$ and (4.39). By splitting each of those two integrals in (4.37) that has the term $\nabla \eta$ into integrals over Ω_{-} and Ω_{+} , respectively, using the Divergence Theorem, and using (4.38) and (4.39), we obtain (4.40).
 - (3) Let $\phi_{\mathcal{C}}$ be given as in (1.6) and $t \in \mathbb{R}$. Denote

$$\psi_{\rm r} = \psi_{\Gamma} - \hat{\phi}_{\rm C}$$
 and $\psi_{{\rm r},t} = \psi_{\Gamma_t} - \hat{\phi}_{\rm C}$.

We first prove (4.41). By (4.25) (with $\hat{\phi} = \hat{\phi}_{\rm C}$) in Lemma 4.2, it suffices to prove that

$$\lim_{t \to 0} \|\psi_{\mathbf{r},t} \circ T_t - \psi_{\mathbf{r}}\|_{H^1(\Omega)} = 0. \tag{4.43}$$

By Definition 2.1 and (2.3) (cf. also (2.12)), we have

$$\int_{\Omega} \left[\varepsilon_{\Gamma} \nabla \psi_r \cdot \nabla \eta + \chi_+ B' \left(\psi_r + \hat{\phi}_{\mathcal{C}} - \frac{\phi_{\Gamma, \infty}}{2} \right) \eta \right] dx$$

$$= -(\varepsilon_+ - \varepsilon_-) \int_{\Omega_+} \nabla \hat{\phi}_{\mathcal{C}} \cdot \nabla \eta \, dx \qquad \forall \eta \in H_0^1(\Omega). \tag{4.44}$$

Replacing Γ , Ω_+ , ψ , and η in (4.44) by $\Gamma_t = T_t(\Gamma)$, $T_t(\Omega_+)$, ψ_{Γ_t} , and $\eta = \eta \circ T_t^{-1}$, respectively, we obtain by the change of variable $x = T_t(X)$ and (4.4) that

$$\int_{\Omega} \left[\varepsilon_{\Gamma} A_{V}(t) \nabla (\psi_{r,t} \circ T_{t}) \cdot \nabla \eta + \chi_{+} B' \left(\left(\psi_{r,t} + \hat{\phi}_{C} - \frac{\phi_{\Gamma_{t},\infty}}{2} \right) \circ T_{t} \right) J_{t} \eta \right] dX$$

$$= -(\varepsilon_{+} - \varepsilon_{-}) \int_{\Omega_{+}} A_{V}(t) \nabla(\hat{\phi}_{C} \circ T_{t}) \cdot \nabla \eta \, dX \qquad \forall \eta \in H_{0}^{1}(\Omega). \tag{4.45}$$

Subtracting (4.44) from (4.45) and rearranging terms, we get

$$\int_{\Omega} \varepsilon_{\Gamma} \left[\nabla (\psi_{\mathbf{r},t} \circ T_{t}) - \nabla \psi_{\mathbf{r}} \right] \cdot \nabla \eta \, dX$$

$$= -\int_{\Omega} \varepsilon_{\Gamma} [A_{V}(t) - I] \nabla (\psi_{\mathbf{r},t} \circ T_{t}) \cdot \nabla \eta \, dX$$

$$-\int_{\Omega_{+}} B' \left(\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma_{t},\infty}}{2} \right) \circ T_{t} \right) (J_{t} - 1) \eta \, dX$$

$$-\int_{\Omega_{+}} \left[B' \left(\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma_{t},\infty}}{2} \right) \circ T_{t} \right) - B' \left(\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] \eta \, dX$$

$$- (\varepsilon_{+} - \varepsilon_{-}) \int_{\Omega_{+}} \left[\nabla (\hat{\phi}_{\mathbf{C}} \circ T_{t}) - \nabla \hat{\phi}_{\mathbf{C}} \right] \cdot \nabla \eta \, dX$$

$$- (\varepsilon_{+} - \varepsilon_{-}) \int_{\Omega_{+}} \left[A_{V}(t) - I \right] \nabla (\hat{\phi}_{\mathbf{C}} \circ T_{t}) \cdot \nabla \eta \, dX \qquad \forall \eta \in H_{0}^{1}(\Omega). \tag{4.46}$$

Setting $\eta = \psi_{\mathbf{r},t} \circ T_t - \psi_{\mathbf{r}}$, we have by the uniform bound of all $\psi_{\mathbf{r},t}$ and $\phi_{\Gamma_t,\infty}$ (cf. (2.21) and (2.7)), the Mean-Value Theorem, and the convexity of B that

$$-\left[B'\left(\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma_{t},\infty}}{2}\right) \circ T_{t}\right) - B'\left(\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma,\infty}}{2}\right)\right]\eta$$

$$= -B''(\lambda_{t})\left(\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} \circ T_{t} - \hat{\phi}_{\mathbf{C}} + \frac{1}{2}\phi_{\Gamma_{t},\infty} \circ T_{t} - \frac{1}{2}\phi_{\Gamma,\infty}\right)(\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}})$$

$$= -B''(\lambda_{t})(\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}})^{2}$$

$$-B''(\lambda_{t})\left(\hat{\phi}_{\mathbf{C}} \circ T_{t} - \hat{\phi}_{\mathbf{C}} + \frac{1}{2}\phi_{\Gamma_{t},\infty} \circ T_{t} - \frac{1}{2}\phi_{\Gamma,\infty}\right)(\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}})$$

$$\leq C|(\hat{\phi}_{\mathbf{C}} \circ T_{t} - \hat{\phi}_{\mathbf{C}})(\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}})| + C|(\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty})(\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}})|, \tag{4.47}$$

where λ_t is in between $\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \phi_{\Gamma_t,\infty}/2\right) \circ T_t$ and $\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \phi_{\Gamma,\infty}/2$ at each point in Ω_+ , and the constant C > 0 is independent of t and Γ . Now, the combination of (4.46) with $\eta = \psi_{\mathbf{r},t} \circ T_t - \psi_{\mathbf{r}}$ and (4.47), together with the uniform bounds for $\psi_{\mathbf{r},t}$ and $\phi_{\Gamma_t,\infty}$, and the Cauchy–Schwarz and Poincaré inequalities, leads to

$$\|\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}}\|_{H^{1}(\Omega)} \leq C \|A_{V}(t) - I\|_{L^{\infty}(\Omega)} \|\psi_{\mathbf{r},t} \circ T_{t}\|_{H^{1}(\Omega)} + C \|J_{t} - 1\|_{L^{\infty}(\Omega)}$$

$$+ C \|\hat{\phi}_{\mathbf{C}} \circ T_{t} - \hat{\phi}_{\mathbf{C}}\|_{H^{1}(\Omega_{+})} + C \|\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}\|_{H^{1}(\Omega)}$$

$$+ C \|A_{V}(t) - I\|_{L^{\infty}(\Omega_{+})} \|\hat{\phi}_{\mathbf{C}} \circ T_{t}\|_{H^{1}(\Omega_{+})}.$$

Now the convergence (4.43) follows from (4.2), (4.3), (4.7), (4.8), the uniform bound of $\psi_{r,t}$, Lemma 4.2 (with $\hat{\phi} = \hat{\phi}_C$), and Lemma 4.3.

We now prove (4.42). Let us denote $\hat{\omega}_{\Gamma,V} = \omega_{\Gamma,V} - \nabla \hat{\phi}_{C} \cdot V$. By Lemma 4.2 (cf. (4.26) with $\hat{\phi} = \hat{\phi}_{C}$), we need only to prove that

$$\lim_{t \to 0} \left\| \frac{\psi_{\mathbf{r},t} \circ T_t - \psi_{\mathbf{r}}}{t} - \hat{\omega}_{\Gamma,V} \right\|_{H^1(\Omega)} = 0. \tag{4.48}$$

We first note that the Divergence Theorem and the calculations in (4.32) imply that

$$\int_{\Omega} [A'_{V}(0)\nabla\hat{\phi}_{C} + \nabla(\nabla\hat{\phi}_{C} \cdot V)] \cdot \nabla\eta \, dx$$

$$= -\int_{\Omega} [\nabla \cdot (A'_{V}(0)\nabla\hat{\phi}_{C}) + \Delta(\nabla\hat{\phi}_{C} \cdot V)] \, \eta \, dx$$

$$= 0 \qquad \forall \eta \in H_{0}^{1}(\Omega).$$

This allows us to rewrite (4.37) into the following equation for $\hat{\omega}_{\Gamma,V}$:

$$\int_{\Omega} \left[\varepsilon_{\Gamma} \nabla \hat{\omega}_{\Gamma,V} \cdot \nabla \eta + \chi_{+} B'' \left(\psi_{r} + \hat{\phi}_{C} - \frac{\phi_{\Gamma,\infty}}{2} \right) \hat{\omega}_{\Gamma,V} \eta \right] dX$$

$$= -\int_{\Omega} \varepsilon_{\Gamma} A'_{V}(0) \nabla (\psi_{\Gamma} - \hat{\phi}_{C}) \cdot \nabla \eta \, dX$$

$$-\int_{\Omega_{+}} \left[B' \left(\psi_{r} + \hat{\phi}_{C} - \frac{\phi_{\Gamma,\infty}}{2} \right) (\nabla \cdot V) \right]$$

$$+ B'' \left(\psi_{r} + \hat{\phi}_{C} - \frac{\phi_{\Gamma,\infty}}{2} \right) \left(\nabla \hat{\phi}_{C} \cdot V - \frac{\zeta_{\Gamma,V}}{2} \right) \right] \eta \, dX$$

$$- (\varepsilon_{+} - \varepsilon_{-}) \int_{\Omega_{+}} \left[A'_{V}(0) \nabla \hat{\phi}_{C} + \nabla (\nabla \hat{\phi}_{C} \cdot V) \right] \cdot \nabla \eta \, dX \qquad \forall \eta \in H_{0}^{1}(\Omega). \tag{4.49}$$

Multiplying both sides of (4.46) by 1/t and combining the resulting equation with (4.49), we obtain by rearranging terms that

$$\begin{split} &\int_{\Omega} \varepsilon_{\Gamma} \nabla \left(\frac{\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}}}{t} - \hat{\omega}_{\Gamma,V} \right) \cdot \nabla \eta \, dX \\ &= -\int_{\Omega} \varepsilon_{\Gamma} \left[\left(\frac{A_{V}(t) - I}{t} \right) \nabla (\psi_{\mathbf{r},t} \circ T_{t}) - A'_{V}(0) \nabla \psi_{\mathbf{r}} \right] \cdot \nabla \eta \, dX \\ &- \int_{\Omega_{+}} \left[B' \left(\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma_{t},\infty}}{2} \right) \circ T_{t} \right) \left(\frac{J_{t} - 1}{t} \right) \right. \\ &- B' \left(\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma,\infty}}{2} \right) (\nabla \cdot V) \right] \eta \, dX \\ &- \int_{\Omega_{+}} \left\{ \frac{1}{t} \left[B' \left(\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma_{t},\infty}}{2} \right) \circ T_{t} \right) - B' \left(\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] \right. \\ &- B'' \left(\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma,\infty}}{2} \right) \left(\hat{\omega}_{\Gamma,V} + \nabla \hat{\phi}_{\mathbf{C}} \cdot V - \frac{\zeta_{\Gamma,V}}{2} \right) \right\} \eta \, dX \end{split}$$

$$-(\varepsilon_{+} - \varepsilon_{-}) \int_{\Omega_{+}} \left[\left(\frac{A_{V}(t) - I}{t} \right) \nabla (\hat{\phi}_{C} \circ T_{t}) - A'_{V}(0) \nabla \hat{\phi}_{C} \right] \cdot \nabla \eta \, dX$$

$$-(\varepsilon_{+} - \varepsilon_{-}) \int_{\Omega_{+}} \nabla \left(\frac{\hat{\phi}_{C} \circ T_{t} - \hat{\phi}_{C}}{t} - \nabla \hat{\phi}_{C} \cdot V \right) \cdot \nabla \eta \, dX \qquad \forall \eta \in H_{0}^{1}(\Omega). \tag{4.50}$$

Specifying $\eta = (\psi_{\mathbf{r},t} \circ T_t - \psi_{\mathbf{r}})/t - \hat{\omega}_{\Gamma,V} \in H^1_0(\Omega)$, we have by the fact that B'' > 0, the Mean-Value Theorem, the uniform bound for all the functions $\psi_{\mathbf{r},t}$, $\zeta_{\Gamma,V}$, and $\omega_{\Gamma,V}$ (cf. (2.7), (2.16), (2.21)) that in Ω_+

$$\begin{split} &-\left\{\frac{1}{t}\left[B'\left(\left(\psi_{\mathsf{r},t}+\hat{\phi}_{\mathsf{C}}-\frac{\phi_{\Gamma,\infty}}{2}\right)\circ T_{t}\right)-B'\left(\psi_{\mathsf{r}}+\hat{\phi}_{\mathsf{C}}-\frac{\phi_{\Gamma,\infty}}{2}\right)\right]\\ &-B''\left(\psi_{\mathsf{r}}+\hat{\phi}_{\mathsf{C}}-\frac{\phi_{\Gamma,\infty}}{2}\right)\left(\hat{\omega}_{\Gamma,V}+\nabla\hat{\phi}_{\mathsf{C}}\cdot V-\frac{\zeta_{\Gamma,V}}{2}\right)\right\}\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right)\\ &=-B''\left(\xi_{t}\right)\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}+\frac{\hat{\phi}_{\mathsf{C}}\circ T_{t}-\hat{\phi}_{\mathsf{C}}}{t}-\frac{\phi_{\Gamma,\infty}\circ T_{t}-\phi_{\Gamma,\infty}}{2t}\right)\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right)\\ &+B''\left(\psi_{\mathsf{r}}+\hat{\phi}_{\mathsf{C}}-\frac{\phi_{\Gamma,\infty}}{2}\right)\left(\hat{\omega}_{\Gamma,V}+\nabla\hat{\phi}_{\mathsf{C}}\cdot V-\frac{\zeta_{\Gamma,V}}{2}\right)\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right)\\ &=-B''\left(\xi_{t}\right)\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right)^{2}\\ &-B''\left(\xi_{t}\right)\left(\hat{\omega}_{\Gamma,V}+\frac{\hat{\phi}_{\mathsf{C}}\circ T_{t}-\hat{\phi}_{\mathsf{C}}}{t}-\frac{\phi_{\Gamma,\infty}\circ T_{t}-\phi_{\Gamma,\infty}}{2t}\right)\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right)\\ &+\left[B''\left(\psi_{\mathsf{r}}+\hat{\phi}_{\mathsf{C}}-\frac{\phi_{\Gamma,\infty}}{2}\right)-B''(\xi_{t})\right]\left(\hat{\omega}_{\Gamma,V}+\nabla\hat{\phi}_{\mathsf{C}}\cdot V-\frac{\zeta_{\Gamma,V}}{2}\right)\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right)\\ &+B'''(\xi_{t})\left(\hat{\omega}_{\Gamma,V}+\nabla\hat{\phi}_{\mathsf{C}}\cdot V-\frac{\zeta_{\Gamma,V}}{2}\right)\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right)\\ &\leq -B''\left(\xi_{t}\right)\left(\frac{\hat{\phi}_{\mathsf{C}}\circ T_{t}-\hat{\phi}_{\mathsf{C}}}{t}-\nabla\hat{\phi}_{\mathsf{C}}\cdot V-\frac{\phi_{\Gamma,\infty}\circ T_{t}-\phi_{\Gamma,\infty}}{2t}+\frac{\zeta_{\Gamma,V}}{2}\right)\\ &\cdot\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right)\\ &+B'''(\sigma_{t})\left(\psi_{\mathsf{r}}+\hat{\phi}_{\mathsf{C}}-\frac{\phi_{\Gamma,\infty}}{2}-\xi_{t}\right)\left(\hat{\omega}_{\Gamma,V}+\nabla\hat{\phi}_{\mathsf{C}}\cdot V-\frac{\zeta_{\Gamma,V}}{2}\right)\left(\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right)\\ &\leq C\left(\left|\frac{\hat{\phi}_{\mathsf{C}}\circ T_{t}-\hat{\phi}_{\mathsf{C}}}{t}-\nabla\hat{\phi}_{\mathsf{C}}\cdot V\right|+\left|\frac{\phi_{\Gamma,\infty}\circ T_{t}-\phi_{\Gamma,\infty}}{t}-\zeta_{\Gamma,V}\right|\right)\left|\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right|,\\ &+C\left(|\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}|+\left|\hat{\phi}_{\mathsf{C}}\circ T_{t}-\hat{\phi}_{\mathsf{C}}\right|+|\phi_{\Gamma,\infty}\circ T_{t}-\phi_{\Gamma,\infty}|\right)\right|\frac{\psi_{\mathsf{r},t}\circ T_{t}-\psi_{\mathsf{r}}}{t}-\hat{\omega}_{\Gamma,V}\right|, \end{aligned}$$

where ξ_t and σ_t are in between $(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \phi_{\Gamma_t,\infty}/2) \circ T_t$ and $\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \phi_{\Gamma,\infty}/2$ at each point in Ω_+ . Now, combining this inequality and the identity (4.50) with $\eta = (\psi_{\mathbf{r},t} \circ T_t - \psi_{\mathbf{r}})/t - \hat{\omega}_{\Gamma,V} \in$

 $H_0^1(\Omega)$, we obtain by the Poincaré and Cauchy–Schwarz inequalities and rearranging terms that

$$\begin{split} &\left\| \frac{\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}}}{t} - \hat{\omega}_{\Gamma,V} \right\|_{H^{1}(\Omega)}^{2} \\ &\leq C \int_{\Omega} \left| \left(\frac{A_{V}(t) - I}{t} \right) \nabla(\psi_{\mathbf{r},t} \circ T_{t}) - A_{V}'(0) \nabla \psi_{\mathbf{r}} \right|^{2} dX \\ &+ C \int_{\Omega_{+}} \left| B' \left(\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma,\infty}}{2} \right) \circ T_{t} \right) \left(\frac{J_{t} - 1}{t} \right) - B' \left(\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma,\infty}}{2} \right) (\nabla \cdot V) \right|^{2} dX \\ &+ C \left(\left\| \frac{\hat{\phi}_{\mathbf{C}} \circ T_{t} - \hat{\phi}_{\mathbf{C}}}{t} - \nabla \hat{\phi}_{\mathbf{C}} \cdot V \right\|_{H^{1}(\Omega_{+})}^{2} + \left\| \frac{\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}}{t} - \zeta_{\Gamma,V} \right\|_{L^{2}(\Omega_{+})}^{2} \\ &+ \left\| \psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}} \right\|_{L^{2}(\Omega_{+})}^{2} + \left\| \hat{\phi}_{\mathbf{C}} \circ T_{t} - \hat{\phi}_{\mathbf{C}} \right\|_{L^{2}(\Omega_{+})}^{2} + \left\| \phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty} \right\|_{L^{2}(\Omega_{+})}^{2} \\ &+ C \int_{\Omega_{+}} \left| \left(\frac{A_{V}(t) - I}{t} \right) \nabla(\hat{\phi}_{\mathbf{C}} \circ T_{t}) - A_{V}'(0) \nabla \hat{\phi}_{\mathbf{C}} \right|^{2} dX \\ &= C \left[S_{1}(t) + S_{2}(t) + S_{3}(t) + S_{4}(t) \right]. \end{split} \tag{4.51}$$

It follows from (4.6)–(4.8), Lemma 4.2 (with $\hat{\phi} = \hat{\phi}_C$), and (4.41) that

$$S_{1}(t) = \int_{\Omega} \left| \left[\frac{A_{V}(t) - I}{t} \right] \nabla(\psi_{r,t} \circ T_{t}) - A'_{V}(0) \nabla \psi_{r} \right|^{2} dX$$

$$\leq 2 \int_{\Omega} \left| \left[\frac{A_{V}(t) - I}{t} - A'_{V}(0) \right] \nabla(\psi_{r,t} \circ T_{t}) \right|^{2} dX + 2 \int_{\Omega} \left| A'_{V}(0) \nabla(\psi_{r,t} \circ T_{t} - \psi_{r}) \right|^{2} dX$$

$$\to 0 \quad \text{as } t \to 0.$$

$$(4.52)$$

By the uniform boundedness of $\psi_{r,t}$ and $\phi_{\Gamma_t,\infty}$ (cf. (2.7), (2.16), (2.21)) the Mean-Value Theorem, (4.2) and (4.3), Lemmas 4.2 and 4.3, and (4.41), we have

$$S_{2}(t) = \int_{\Omega_{+}} \left| B' \left(\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma_{t},\infty}}{2} \right) \circ T_{t} \right) \left(\frac{J_{t} - 1}{t} \right) - B' \left(\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma,\infty}}{2} \right) (\nabla \cdot V) \right|^{2} dX$$

$$\leq 2 \int_{\Omega_{+}} \left| B' \left(\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma_{t},\infty}}{2} \right) \circ T_{t} \right) \left(\frac{J_{t} - 1}{t} - \nabla \cdot V \right) \right|^{2} dX$$

$$+ 2 \int_{\Omega_{+}} \left| B' \left(\left(\psi_{\mathbf{r},t} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma_{t},\infty}}{2} \right) \circ T_{t} \right) - B' \left(\psi_{\mathbf{r}} + \hat{\phi}_{\mathbf{C}} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right|^{2} |\nabla \cdot V|^{2} dX$$

$$\leq C \int_{\Omega_{+}} \left| \frac{J_{t} - 1}{t} - \nabla \cdot V \right|^{2} dX$$

$$+ C \int_{\Omega_{+}} (|\psi_{\mathbf{r},t} \circ T_{t} - \psi_{\mathbf{r}}|^{2} + |\hat{\phi}_{\mathbf{C}} \circ T_{t} - \hat{\phi}_{\mathbf{C}}|^{2} + |\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}|^{2}) dX$$

$$\to 0 \quad \text{as } t \to 0.$$

$$(4.53)$$

By Lemma 4.2 (with $\hat{\phi} = \hat{\phi}_{\rm C}$), Lemma 4.3, and (4.41), we have

$$S_{3}(t) = \left\| \frac{\hat{\phi}_{C} \circ T_{t} - \hat{\phi}_{C}}{t} - \nabla \hat{\phi}_{C} \cdot V \right\|_{H^{1}(\Omega_{+})}^{2} + \left\| \frac{\phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty}}{t} - \zeta_{\Gamma,V} \right\|_{L^{2}(\Omega_{+})} + \left\| \psi_{r,t} \circ T_{t} - \psi_{r} \right\|_{L^{2}(\Omega_{+})} + \left\| \hat{\phi}_{C} \circ T_{t} - \hat{\phi}_{C} \right\|_{L^{2}(\Omega_{+})}^{2} + \left\| \phi_{\Gamma_{t},\infty} \circ T_{t} - \phi_{\Gamma,\infty} \right\|_{L^{2}(\Omega_{+})}^{2} + 0 \quad \text{as } t \to 0.$$

$$(4.54)$$

It follows from (4.6)–(4.8) and Lemma 4.2 (with $\hat{\phi} = \hat{\phi}_{\rm C}$) that

$$S_{4}(t) = \int_{\Omega_{+}} \left| \left[\frac{A_{V}(t) - I}{t} \right] \nabla(\hat{\phi}_{C} \circ T_{t}) - A'_{V}(0) \nabla\hat{\phi}_{C} \right|^{2} dX$$

$$\leq C \int_{\Omega_{+}} \left| \left[\frac{A_{V}(t) - I}{t} - A'_{V}(0) \right] \nabla(\hat{\phi}_{C} \circ T_{t}) \right|^{2} + C \int_{\Omega_{+}} |\nabla(\hat{\phi}_{C} \circ T_{t} - \hat{\phi}_{C})|^{2} dX$$

$$\to 0 \quad \text{as } t \to 0.$$

$$(4.55)$$

Now the desired convergence (4.48) follows from (4.51)–(4.55).

5 Proof of Theorem 3.2

Proof of Theorem 3.2. Fix $V \in \mathcal{V}$ (cf. (3.6)). Let $\{T_t\}_{t \in \mathbb{R}}$ be the family of diffeomorphisms from \mathbb{R}^3 to \mathbb{R}^3 defined by $T_t(X) = x(t,X)$ as the solution to the initial-value problem (3.7). We proceed in five steps. In Step 1, we calculate the limit as $t \to 0$ that defines the variation $\delta_{\Gamma,V} E[\Gamma]$; cf. Definition 3.1. In Step 2, we simplify the expression of $\delta_{\Gamma,V} E[\Gamma]$. In Step 3, we convert all the volume integrals in $\delta_{\Gamma,V} E[\Gamma]$ into surface integrals on the boundary Γ , except one volume integral that involves the B' term. In Step 4, we rewrite the surface integrals to have the desired form (i.e., with a factor $V \cdot n$ in the integrand). Finally, in Step 5, we treat the only volume integral term that involves B' to get the desired formula.

Step 1. Let $t \in \mathbb{R}$. We recall that $\phi_{\Gamma_t,\infty}$, $\hat{\phi}_{\Gamma_t,\infty}$, and ψ_{Γ_t} are the solutions to (2.5), (2.11), and (2.20) with $\Gamma_t = T_t(\Gamma)$ replacing Γ , respectively, and that all these functions have the boundary value ϕ_{∞} on $\partial\Omega$. Recall that $\hat{\phi}_0$ and $\hat{\phi}_{\infty}$ are defined by (2.3) and (2.4). We denote in this proof

$$\psi_{\mathbf{r}} = \psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty} \quad \text{and} \quad \psi_{\mathbf{r},t} = \psi_{\Gamma_t} - \hat{\phi}_{\Gamma_t,\infty}.$$
 (5.1)

By (3.1) and (3.2) with Γ_t replacing Γ , the definition of $A_V(t)$ (4.4) and J_t (4.1), and the change of variable $x = T_t(X)$, we have

$$E[\Gamma_t] = -\int_{\Omega} \frac{\varepsilon_{\Gamma_t}}{2} |\nabla \psi_{\mathbf{r},t}|^2 dx - \int_{T_t(\Omega_+)} B\left(\psi_{\Gamma_t} - \frac{\phi_{\Gamma_t,\infty}}{2}\right) dx$$

$$\begin{split} &+\frac{\varepsilon_{-}-\varepsilon_{+}}{2}\int_{T_{t}(\Omega_{+})}\nabla\hat{\phi}_{\Gamma_{t},\infty}\cdot\nabla\hat{\phi}_{0}\,dx+W\\ &=-\int_{\Omega}\frac{\varepsilon_{\Gamma}}{2}\left[A_{V}(t)\nabla(\psi_{r,t}\circ T_{t})\cdot\nabla(\psi_{r,t}\circ T_{t})\right]dX\\ &-\int_{\Omega_{+}}B\left(\left(\psi_{\Gamma_{t}}-\frac{\phi_{\Gamma_{t},\infty}}{2}\right)\circ T_{t}\right)J_{t}\,dX\\ &+\frac{\varepsilon_{-}-\varepsilon_{+}}{2}\int_{\Omega_{+}}A_{V}(t)\nabla(\hat{\phi}_{\Gamma_{t},\infty}\circ T_{t})\cdot\nabla(\hat{\phi}_{0}\circ T_{t})\,dX+W, \end{split}$$

where $W = (1/2) \sum_{i=1}^{N} Q_i (\hat{\phi}_{\infty} - \hat{\phi}_0)(x_i)$ is independent of Γ . Consequently,

$$\frac{E[\Gamma_{t}] - E[\Gamma]}{t} = -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2t} \left[A_{V}(t) \nabla (\psi_{r,t} \circ T_{t}) \cdot \nabla (\psi_{r,t} \circ T_{t}) - \nabla \psi_{r} \cdot \nabla \psi_{r} \right] dX
- \int_{\Omega_{+}} \frac{1}{t} \left[B\left(\left(\psi_{\Gamma_{t}} - \frac{\phi_{\Gamma_{t},\infty}}{2} \right) \circ T_{t} \right) J_{t} - B\left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] dX
+ \frac{\varepsilon_{-} - \varepsilon_{+}}{2} \int_{\Omega_{+}} \frac{1}{t} \left[A_{V}(t) \nabla (\hat{\phi}_{\Gamma_{t},\infty} \circ T_{t}) \cdot \nabla (\hat{\phi}_{0} \circ T_{t}) - \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \hat{\phi}_{0} \right] dX
= -\delta_{1}(t) - \delta_{2}(t) + \frac{\varepsilon_{-} - \varepsilon_{+}}{2} \delta_{3}(t).$$
(5.2)

By rearranging the terms, we obtain that

$$\delta_{1}(t) = \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} \left[\frac{A_{V}(t) - I - tA'_{V}(0)}{t} \right] \nabla(\psi_{r,t} \circ T_{t}) \cdot \nabla(\psi_{r,t} \circ T_{t}) dX$$

$$+ \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} A'_{V}(0) \nabla(\psi_{r,t} \circ T_{t}) \cdot \nabla(\psi_{r,t} \circ T_{t}) dX$$

$$+ \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} \left[\nabla(\psi_{r,t} \circ T_{t}) + \nabla\psi_{r} \right] \cdot \nabla\left(\frac{\psi_{r,t} \circ T_{t} - \psi_{r}}{t}\right) dX.$$

It thus follows from (4.7), (4.8), Lemma 4.4, and Lemma 4.5 that

$$\lim_{t \to 0} \delta_1(t) = \int_{\Omega} \varepsilon_{\Gamma} \left[\frac{1}{2} A_V'(0) \nabla \psi_{\mathbf{r}} \cdot \nabla \psi_{\mathbf{r}} + \nabla \psi_{\mathbf{r}} \cdot \nabla (\omega_{\Gamma,V} - \xi_{\Gamma,V}) \right] dX, \tag{5.3}$$

where $\xi_{\Gamma,V}$ and $\omega_{\Gamma,V}$ are defined in (4.35) in Lemma 4.4 and (4.37) in Lemma 4.5, respectively. Denote $q = \psi_{\Gamma} - \phi_{\Gamma,\infty}/2$ and $q_t = (\psi_{\Gamma_t} - \phi_{\Gamma_t,\infty}/2) \circ T_t$. The second term $\delta_2(t)$ in (5.2) can be written as

$$\delta_2(t) = \int_{\Omega_+} \frac{J_t - 1}{t} B(q_t) \, dX + \int_{\Omega_+} \frac{B(q_t) - B(q)}{t} \, dX,\tag{5.4}$$

Since the $L^{\infty}(\Omega)$ -norm of q_t is bounded uniformly in $t \in \mathbb{R}$ (cf. (2.15) and (2.21)), it follows from Lemma 4.3 and Lemma 4.5 that $q_t \to q$ in $L^2(\Omega)$. Hence, $B(q_t) \to B(q)$ in $L^2(\Omega_+)$ as

 $t \to 0$. This, together with (4.2) and (4.3), implies that

$$\lim_{t \to 0} \int_{\Omega_{+}} \frac{J_{t} - 1}{t} B(q_{t}) dX = \int_{\Omega_{+}} (\nabla \cdot V) B(q) dX.$$
 (5.5)

Now Taylor's expansion implies that

$$\frac{B(q_t(X)) - B(q(X))}{t}$$

$$= B'(q(X)) \frac{q_t(X) - q(X)}{t} + \frac{1}{2} B''(\eta_t(X)) [q_t(X) - q(X)] \frac{q_t(X) - q(X)}{t}, \text{ a.e. } X \in \Omega_+,$$

where $\eta_t(X)$ is in between q(X) and $q_t(X)$, and its $L^{\infty}(\Omega)$ -norm is bounded uniformly in t. It then follows from Lemma 4.3 and Lemma 4.5 that

$$\left| \int_{\Omega_+} B''(\eta_t) (q_t - q) \frac{q_t - q}{t} dX \right| \le C \|q_t - q\|_{L^2(\Omega_+)} \left\| \frac{q_t - q}{t} \right\|_{L^2(\Omega_+)} \to 0 \quad \text{as } t \to 0,$$

where C is a constant independent of t. Consequently, by Lemma 4.3 and Lemma 4.5 that

$$\lim_{t\to 0} \int_{\Omega_+} \frac{B(q_t) - B(q)}{t} dX = \lim_{t\to 0} \int_{\Omega_+} B'(q) \frac{q_t - q}{t} dX = \int_{\Omega_+} B'(q) \left(\omega_{\Gamma,V} - \frac{\zeta_{\Gamma,V}}{2}\right) dX,$$

where $\omega_{\Gamma,V}$ and $\zeta_{\Gamma,V}$ are given in (4.37) and (4.27), respectively. This, together with (5.4) and (5.5), and our definition of q and q_t , implies that

$$\lim_{t \to 0} \delta_2(t) = \int_{\Omega_+} \left[(\nabla \cdot V) B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma, \infty}}{2} \right) + B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma, \infty}}{2} \right) \left(\omega_{\Gamma, V} - \frac{\zeta_{\Gamma, V}}{2} \right) \right] dX. \tag{5.6}$$

Rearranging the terms, we have

$$\delta_{3}(t) = \int_{\Omega_{+}} \frac{A_{V}(t) - I - tA'_{V}(0)}{t} \nabla(\hat{\phi}_{\Gamma_{t},\infty} \circ T_{t}) \cdot \nabla(\hat{\phi}_{0} \circ T_{t}) dX$$

$$+ \int_{\Omega_{+}} \frac{\nabla(\hat{\phi}_{\Gamma_{t},\infty} \circ T_{t}) - \nabla\hat{\phi}_{\Gamma,\infty}}{t} \cdot \nabla(\hat{\phi}_{0} \circ T_{t}) dx$$

$$+ \int_{\Omega_{+}} \nabla\hat{\phi}_{\Gamma,\infty} \cdot \frac{\nabla(\hat{\phi}_{0} \circ T_{t}) - \nabla\hat{\phi}_{0}}{t} dX$$

$$+ \int_{\Omega_{+}} A'_{V}(0) \nabla(\hat{\phi}_{\Gamma_{t},\infty} \circ T_{t}) \cdot \nabla(\hat{\phi}_{0} \circ T_{t}) dX.$$

Therefore, we have by (4.7), (4.8), Lemma 4.2 (with $\hat{\phi} = \hat{\phi}_{\rm C}$), and Lemma 4.4 that

$$\lim_{t \to 0} \delta_3(t) = \int_{\Omega_+} \left[\nabla \xi_{\Gamma,V} \cdot \nabla \hat{\phi}_0 + \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla (\nabla \hat{\phi}_0 \cdot V) + A_V'(0) \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \hat{\phi}_0 \right] dX. \tag{5.7}$$

It now follows from Definition 3.1, (5.2), (5.3), (5.6), and (5.7) that the first variation $\delta_{\Gamma} E[\Gamma]$ exists and is given by

$$\delta_{\Gamma,V} E[\Gamma] = -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} A'_{V}(0) \nabla \psi_{r} \cdot \nabla \psi_{r} \, dX + \int_{\Omega} \varepsilon_{\Gamma} \nabla \psi_{r} \cdot \nabla \xi_{\Gamma,V} \, dX - \int_{\Omega} \varepsilon_{\Gamma} \nabla \psi_{r} \cdot \nabla \omega_{\Gamma,V} \, dX$$

$$-\int_{\Omega_{+}} \left[(\nabla \cdot V) B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) + B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \left(\omega_{\Gamma,V} - \frac{\zeta_{\Gamma,V}}{2} \right) \right] dX$$

$$+ \frac{\varepsilon_{-} - \varepsilon_{+}}{2} \int_{\Omega_{+}} \nabla \xi_{\Gamma,V} \cdot \nabla \hat{\phi}_{0} \, dX$$

$$+ \frac{\varepsilon_{-} - \varepsilon_{+}}{2} \int_{\Omega_{+}} \left[\nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla (\nabla \hat{\phi}_{0} \cdot V) + A'_{V}(0) \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \hat{\phi}_{0} \right] dX$$

$$= M_{1} + M_{2} + M_{3} + M_{4} + M_{5} + M_{6}. \tag{5.8}$$

Step 2. We now simplify this expression. By Lemma 4.4 and our notation $\psi_{\rm r} = \psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}$, we can express the sum of the first two integrals above as

$$M_{1} + M_{2} = -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} A'_{V}(0) \nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) \cdot \nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) dX$$
$$-\int_{\Omega} \varepsilon_{\Gamma} A'_{V}(0) \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) dX$$
$$= -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} A'_{V}(0) \nabla \psi_{\Gamma} \cdot \nabla \psi_{\Gamma} dX + \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} A'_{V}(0) \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \hat{\phi}_{\Gamma,\infty} dX.$$
(5.9)

Note that the last two integrals exist as the singularities x_i $(1 \le i \le N)$ of ψ_{Γ} and $\hat{\phi}_{\Gamma,\infty}$ are outside the support of V and $A'_V(0)$ is given in (4.6). By (2.20) in Definition 2.1 and (2.11) we have

$$\int_{\Omega} \left[\varepsilon_{\Gamma} \nabla \psi_r \cdot \nabla \eta + \chi_+ B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma, \infty}}{2} \right) \eta \right] dX = 0$$

for all $\eta \in C_c^1(\Omega)$ and hence all $\eta \in H_0^1(\Omega)$. Setting $\eta = \omega_{\Gamma,V}$, we get the two- $\omega_{\Gamma,V}$ terms in (5.8) (one is M_3 and the other is part of M_4) cancelled:

$$\int_{\Omega} \left[\varepsilon_{\Gamma} \nabla \psi_{\mathbf{r}} \cdot \nabla \omega_{\Gamma,V} + \chi_{+} B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \omega_{\Gamma,V} \right] dX = 0.$$
 (5.10)

To simplify M_5 , we note that we can replace η in (2.3) (with $\hat{\phi} = \hat{\phi}_0$) and (2.11) by $\xi_{\Gamma,V} \in H_0^1(\Omega)$, as $\xi_{\Gamma,V}|_{\Omega_-} \in C^2(\Omega_-)$; cf. the remark below (2.4) and that below (2.12). It then follows that

$$M_{5} = \frac{\varepsilon_{-}}{2} \int_{\Omega_{+}} \nabla \xi_{\Gamma,V} \cdot \nabla \hat{\phi}_{0} \, dX - \frac{\varepsilon_{+}}{2} \int_{\Omega_{+}} \nabla \xi_{\Gamma,V} \cdot \nabla \hat{\phi}_{0} \, dX$$
$$= -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} \nabla \xi_{\Gamma,V} \cdot \nabla \hat{\phi}_{0} \, dX + \frac{1}{2} \sum_{i=1}^{N} Q_{i} \xi_{\Gamma,V}(x_{i}) \quad [\text{by (2.3) with } \hat{\phi} = \hat{\phi}_{0}]$$

$$= -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} \nabla \xi_{\Gamma,V} \cdot \nabla \hat{\phi}_{0} dX + \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \xi_{\Gamma,V} dX \quad [by (2.11)]$$

$$= \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} \nabla \xi_{\Gamma,V} \cdot \nabla (\hat{\phi}_{\Gamma,\infty} - \hat{\phi}_{0} - \phi_{\Gamma,\infty}) dX \quad [by (2.5)]$$

$$= -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} A'_{V}(0) \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla (\hat{\phi}_{\Gamma,\infty} - \hat{\phi}_{0} - \phi_{\Gamma,\infty}) dX. \quad [by Lemma 4.4]$$
(5.11)

Since $\hat{\phi}_0$ is harmonic in the support of V that excludes all x_i (i = 1, ..., N), we have by the same calculations as in (4.32) that

$$\nabla \cdot \left[\nabla (\nabla \hat{\phi}_0 \cdot V) + A'_V(0) \nabla \hat{\phi}_0 \right] = 0 \text{ in } \Omega.$$

Thus, since the normal n along Γ points from Ω_- to Ω_+ , we have by the Divergence Theorem that

$$\frac{\varepsilon_{-}}{2} \int_{\Omega_{+}} \nabla \hat{\phi}_{\Gamma,\infty} \cdot \left[\nabla (\nabla \hat{\phi}_{0} \cdot V) + A'_{V}(0) \nabla \hat{\phi}_{0} \right] dX$$

$$= -\frac{\varepsilon_{-}}{2} \int_{\Gamma} \hat{\phi}_{\Gamma,\infty} \left[\nabla (\nabla \hat{\phi}_{0} \cdot V) + A'_{V}(0) \nabla \hat{\phi}_{0} \right] \cdot n \, dS$$

$$= -\frac{\varepsilon_{-}}{2} \int_{\Omega_{-}} \nabla \hat{\phi}_{\Gamma,\infty} \cdot \left[\nabla (\nabla \hat{\phi}_{0} \cdot V) + A'_{V}(0) \nabla \hat{\phi}_{0} \right] dX.$$

Therefore, since $A'_{V}(0)$ (cf. (4.6)) is symmetric,

$$M_{6} = \frac{\varepsilon_{-} - \varepsilon_{+}}{2} \int_{\Omega_{+}} \nabla \hat{\phi}_{\Gamma,\infty} \cdot \left[\nabla (\nabla \hat{\phi}_{0} \cdot V) + A'_{V}(0) \nabla \hat{\phi}_{0} \right] dX$$

$$= -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} \left[\nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla (\nabla \hat{\phi}_{0} \cdot V) + A'_{V}(0) \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \hat{\phi}_{0} \right] dX$$

$$= -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} A'_{V}(0) \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \hat{\phi}_{0} dX. \quad [by (2.11)]$$
(5.12)

It now follows from (5.8)–(5.12) that

$$\delta_{\Gamma,V} E[\Gamma] = -\int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} A'_{V}(0) \nabla \psi_{\Gamma} \cdot \nabla \psi_{\Gamma} \, dX + \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} A'_{V}(0) \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \phi_{\Gamma,\infty} \, dX$$

$$+ \int_{\Omega_{+}} \left[\frac{\zeta_{\Gamma,V}}{2} B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) - (\nabla \cdot V) B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \right] dX$$

$$= P_{1} + P_{2} + P_{3}. \tag{5.13}$$

Step 3. We convert most of these volume integrals into surface integrals on Γ . We shall use the following identities that can be verified by using the Divergence Theorem and approximations by smooth functions:

$$\int_{D} (\nabla \cdot U) \nabla a \cdot \nabla b \, dx = -\int_{D} U \cdot (\nabla^{2} a \nabla b + \nabla^{2} b \nabla a) \, dx + \int_{\partial D} (\nabla a \cdot \nabla b) (U \cdot \nu) \, dx, \quad (5.14)$$

$$\int_{D} (\nabla U) \nabla a \cdot \nabla b \, dx = -\int_{D} U \cdot (\Delta a \nabla b + \nabla^{2} b \nabla a) \, dx + \int_{\partial D} (\nabla a \cdot \nu) (\nabla b \cdot U) \, dx. \tag{5.15}$$

Here, $D \subset \mathbb{R}^3$ is a bounded open set with a C^1 boundary ∂D , $U \in H^1(D, \mathbb{R}^3)$, $a, b \in H^2(D)$, $\nabla^2 a$ is the Hessian matrix of a, and ν is the unit exterior normal at the boundary ∂D . If in addition $\Delta a = \Delta b = 0$ in D, then we have by (5.14) and (5.15) that

$$\int_{D} (\nabla U + (\nabla U)^{T} - (\nabla \cdot U)I)\nabla a \cdot \nabla b \, dx$$

$$= \int_{\partial D} [(\nabla a \cdot U) \cdot (\nabla b \cdot \nu) + (\nabla b \cdot U) \cdot (\nabla a \cdot \nu) - (\nabla a \cdot \nabla b) \cdot (U \cdot \nu)] \, dS. \tag{5.16}$$

Note that V=0 in a neighborhood of all x_i $(1 \le i \le N)$ and V=0 on $\partial\Omega$ and that the unit normal vector n on Γ points from Ω_- to Ω_+ . By Theorem 2.1, $\Delta\psi_{\Gamma}=0$ on $\Omega_-\cap \operatorname{supp}(V)$ and $\varepsilon_+\Delta\psi_{\Gamma}=B'(\psi_{\Gamma}-\phi_{\Gamma,\infty}/2)$ on Ω_+ . Therefore, we have by (4.6), (5.14), and (5.15) that

$$\begin{split} P_{1} &= \int_{\Omega} \frac{\varepsilon_{\Gamma}}{2} [\nabla V + (\nabla V)^{T} - (\nabla \cdot V)I] \nabla \psi_{\Gamma} \cdot \nabla \psi_{\Gamma} \, dX \\ &= \int_{\Omega_{-}} \varepsilon_{-} (\nabla V) \nabla \psi_{\Gamma} \cdot \nabla \psi_{\Gamma} \, dX + \int_{\Omega_{+}} \varepsilon_{+} (\nabla V) \nabla \psi_{\Gamma} \cdot \nabla \psi_{\Gamma} \, dX \\ &- \int_{\Omega_{-}} \frac{\varepsilon_{-}}{2} (\nabla \cdot V) \nabla \psi_{\Gamma} \cdot \nabla \psi_{\Gamma} \, dX - \int_{\Omega_{+}} \frac{\varepsilon_{+}}{2} (\nabla \cdot V) \nabla \psi_{\Gamma} \cdot \nabla \psi_{\Gamma} \, dX \\ &= -\int_{\Omega_{-}} \varepsilon_{-} V \cdot (\Delta \psi_{\Gamma} \nabla \psi_{\Gamma} + \nabla^{2} \psi_{\Gamma} \nabla \psi_{\Gamma}) \, dX + \int_{\Gamma} \varepsilon_{-} (\nabla \psi_{\Gamma}^{-} \cdot V) (\nabla \psi_{\Gamma}^{-} \cdot n) \, dS \\ &- \int_{\Omega_{+}} \varepsilon_{+} V \cdot (\Delta \psi_{\Gamma} \nabla \psi_{\Gamma} + \nabla^{2} \psi_{\Gamma} \nabla \psi_{\Gamma}) \, dX - \int_{\Gamma} \varepsilon_{+} (\nabla \psi_{\Gamma}^{+} \cdot V) (\psi_{\Gamma}^{+} \cdot n) \, dS \\ &+ \int_{\Omega_{-}} \varepsilon_{-} V \cdot \nabla^{2} \psi_{\Gamma} \nabla \psi_{\Gamma} \, dX - \int_{\Gamma} \frac{\varepsilon_{-}}{2} |\nabla \psi_{\Gamma}^{-}|^{2} (V \cdot n) \, dS \\ &+ \int_{\Omega_{+}} \varepsilon_{+} V \cdot \nabla^{2} \psi_{\Gamma} \nabla \psi_{\Gamma} \, dX + \int_{\Gamma} \frac{\varepsilon_{+}}{2} |\nabla \psi_{\Gamma}^{+}|^{2} (V \cdot n) \, dS \\ &= -\int_{\Omega_{-}} \varepsilon_{-} \Delta \psi_{\Gamma} (\nabla \psi_{\Gamma} \cdot V) \, dX + \int_{\Gamma} \varepsilon_{-} (\nabla \psi_{\Gamma}^{-} \cdot V) (\nabla \psi_{\Gamma}^{-} \cdot n) \, dS - \int_{\Gamma} \frac{\varepsilon_{-}}{2} |\nabla \psi_{\Gamma}^{-}|^{2} (V \cdot n) \, dS \\ &= \int_{\Gamma} \varepsilon_{-} (\nabla \psi_{\Gamma}^{-} \cdot V) (\nabla \psi_{\Gamma}^{-} \cdot n) \, dS - \int_{\Gamma} \varepsilon_{+} (\nabla \psi_{\Gamma}^{+} \cdot V) (\nabla \psi_{\Gamma}^{+} \cdot n) \, dS \\ &= \int_{\Gamma} \varepsilon_{-} (\nabla \psi_{\Gamma}^{-} \cdot V) (\nabla \psi_{\Gamma}^{-} \cdot n) \, dS + \int_{\Gamma} \frac{\varepsilon_{+}}{2} |\nabla \psi_{\Gamma}^{+}|^{2} (V \cdot n) \, dS \\ &- \int_{\Gamma} \frac{\varepsilon_{-}}{2} |\nabla \psi_{\Gamma}^{-}|^{2} (V \cdot n) \, dS + \int_{\Gamma} \frac{\varepsilon_{+}}{2} |\nabla \psi_{\Gamma}^{+}|^{2} (V \cdot n) \, dS \\ &- \int_{\Omega_{+}} B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) (\nabla \psi_{\Gamma} \cdot V) \, dX, \end{split}$$

$$(5.17)$$

where a superscript - or + denotes the restriction from Ω_- or Ω_+ , respectively.

Since $\hat{\phi}_{\Gamma,\infty}$ and $\phi_{\Gamma,\infty}$ are harmonic in $\Omega_- \cap \text{supp}(V)$ and Ω_+ , and since the normal n points from Ω_- to Ω_+ , we have by (4.6), (5.16), and the notation of jumps (2.10) that

$$P_{2} = \int_{\Omega_{-}} \frac{\varepsilon_{-}}{2} [(\nabla \cdot V)I - \nabla V - (\nabla V)^{T}] \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \phi_{\Gamma,\infty} dX$$

$$+ \int_{\Omega_{+}} \frac{\varepsilon_{+}}{2} [(\nabla \cdot V)I - \nabla V - (\nabla V)^{T}] \nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \phi_{\Gamma,\infty} dX$$

$$= \frac{1}{2} \int_{\Gamma} [\![\varepsilon_{\Gamma} (\nabla \hat{\phi}_{\Gamma,\infty} \cdot V) (\nabla \phi_{\Gamma,\infty} \cdot n) + \varepsilon_{\Gamma} (\nabla \hat{\phi}_{\Gamma,\infty} \cdot n) (\nabla \phi_{\Gamma,\infty} \cdot V) - \varepsilon_{\Gamma} (\nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \phi_{\Gamma,\infty}) (V \cdot n)]\!]_{\Gamma} dS.$$
(5.18)

Using the Divergence Theorem and noting again that the normal n at Γ points from Ω_{-} to Ω_{+} , we obtain

$$P_{3} = \int_{\Omega_{+}} \frac{\zeta_{\Gamma,V}}{2} B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dX + \int_{\Omega_{+}} V \cdot B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) \left(\nabla \psi_{\Gamma} - \frac{\nabla \phi_{\Gamma,\infty}}{2} \right) dX$$

$$+ \int_{\Gamma} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) (V \cdot n) dS$$

$$= \int_{\Omega_{+}} \left[\frac{1}{2} \left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) + \nabla \psi_{\Gamma} \cdot V \right] B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dX$$

$$+ \int_{\Gamma} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) (V \cdot n) dS. \tag{5.19}$$

It now follows from (5.13) and (5.17)–(5.19) that

$$\delta_{\Gamma,V} E[\Gamma] = \int_{\Gamma} \varepsilon_{-}(\nabla \psi_{\Gamma}^{-} \cdot V)(\nabla \psi_{\Gamma}^{-} \cdot n) \, dS - \int_{\Gamma} \varepsilon_{+}(\nabla \psi_{\Gamma}^{+} \cdot V)(\nabla \psi_{\Gamma}^{+} \cdot n) \, dS$$

$$- \int_{\Gamma} \frac{\varepsilon_{-}}{2} |\nabla \psi_{\Gamma}^{-}|^{2} (V \cdot n) \, dS + \int_{\Gamma} \frac{\varepsilon_{+}}{2} |\nabla \psi_{\Gamma}^{+}|^{2} (V \cdot n) \, dS$$

$$+ \frac{1}{2} \int_{\Gamma} [\![\varepsilon_{\Gamma}(\nabla \hat{\phi}_{\Gamma,\infty} \cdot V)(\nabla \phi_{\Gamma,\infty} \cdot n)]\!]_{\Gamma} \, dS$$

$$+ \frac{1}{2} \int_{\Gamma} [\![\varepsilon_{\Gamma}(\nabla \hat{\phi}_{\Gamma,\infty} \cdot n)(\nabla \phi_{\Gamma,\infty} \cdot V)]\!]_{\Gamma} \, dS$$

$$- \frac{1}{2} \int_{\Gamma} [\![\varepsilon_{\Gamma}(\nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \phi_{\Gamma,\infty})(V \cdot n)]\!]_{\Gamma} \, dS$$

$$+ \int_{\Omega_{+}} \frac{1}{2} (\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V) \, B'\left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2}\right) dX$$

$$+ \int_{\Gamma} B\left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2}\right) (V \cdot n) \, dS. \tag{5.20}$$

Step 4. We express the surface integrals into those with the factor $V \cdot n$ in the integrand. Note that on each side of Γ , we can write

$$\nabla \psi_{\Gamma} = (\nabla \psi_{\Gamma} \cdot n) n + \nabla_{\Gamma} \psi_{\Gamma} = \partial_n \psi_{\Gamma} n + \nabla_{\Gamma} \psi_{\Gamma} \quad \text{on } \Gamma,$$

where $\nabla_{\Gamma}\psi_{\Gamma} = (I - n \otimes n)\nabla\psi_{\Gamma}$ is the tangential derivative. Clearly $n \cdot \nabla_{\Gamma}\psi_{\Gamma} = 0$. Moreover, $\nabla_{\Gamma}\psi_{\Gamma}^{+} = \nabla_{\Gamma}\psi_{\Gamma}^{-}$ on Γ . Thus,

$$\nabla \psi_{\Gamma}^{+} - \nabla \psi_{\Gamma}^{-} = (\partial_{n} \psi_{\Gamma}^{+} - \partial_{n} \psi_{\Gamma}^{-})n \quad \text{on } \Gamma.$$

By Theorem 2.1, we have also $\varepsilon_+ \nabla \psi_{\Gamma}^+ \cdot n = \varepsilon_- \nabla \psi_{\Gamma}^- \cdot n = \varepsilon_\Gamma \nabla \psi_{\Gamma} \cdot n$ on Γ . Therefore, the first four terms in (5.20) are

$$\int_{\Gamma} \varepsilon_{-}(\nabla \psi_{\Gamma}^{-} \cdot V)(\nabla \psi_{\Gamma}^{-} \cdot n) \, dS - \int_{\Gamma} \varepsilon_{+}(\nabla \psi_{\Gamma}^{+} \cdot V)(\nabla \psi_{\Gamma}^{+} \cdot n) \, dS \\
- \int_{\Gamma} \frac{\varepsilon_{-}}{2} |\nabla \psi_{\Gamma}^{-}|^{2} (V \cdot n) \, dS + \int_{\Gamma} \frac{\varepsilon_{+}}{2} |\nabla \psi_{\Gamma}^{+}|^{2} (V \cdot n) \, dS \\
= - \int_{\Gamma} \varepsilon_{\Gamma} \partial_{n} \psi_{\Gamma} (\partial_{n} \psi_{\Gamma}^{+} - \partial_{n} \psi_{\Gamma}^{-})(V \cdot n) \, dS \\
+ \int_{\Gamma} \frac{\varepsilon_{+}}{2} |\partial_{n} \psi_{\Gamma}^{+}|^{2} (V \cdot n) \, dS + \int_{\Gamma} \frac{\varepsilon_{+}}{2} |\nabla_{\Gamma} \psi_{\Gamma}|^{2} (V \cdot n) \, dS \\
- \int_{\Gamma} \frac{\varepsilon_{-}}{2} |\partial_{n} \psi_{\Gamma}^{-}|^{2} (V \cdot n) \, dS - \int_{\Gamma} \frac{\varepsilon_{-}}{2} |\nabla_{\Gamma} \psi_{\Gamma}|^{2} (V \cdot n) \, dS \\
= - \int_{\Gamma} \varepsilon_{+} |\partial_{n} \psi_{\Gamma}^{+}|^{2} (V \cdot n) \, dS + \int_{\Gamma} \varepsilon_{-} |\partial_{n} \psi_{\Gamma}^{-}|^{2} (V \cdot n) \, dS \\
+ \int_{\Gamma} \frac{\varepsilon_{+}}{2} |\partial_{n} \psi_{\Gamma}^{+}|^{2} (V \cdot n) \, dS + \int_{\Gamma} \frac{\varepsilon_{+}}{2} |\nabla_{\Gamma} \psi_{\Gamma}|^{2} (V \cdot n) \, dS \\
- \int_{\Gamma} \frac{\varepsilon_{-}}{2} |\partial_{n} \psi_{\Gamma}^{-}|^{2} (V \cdot n) \, dS - \int_{\Gamma} \frac{\varepsilon_{-}}{2} |\nabla_{\Gamma} \psi_{\Gamma}|^{2} (V \cdot n) \, dS \\
= - \frac{1}{2} \left(\frac{1}{\varepsilon_{+}} - \frac{1}{\varepsilon_{-}} \right) \int_{\Gamma} |\varepsilon_{\Gamma} \partial_{n} \psi_{\Gamma}|^{2} (V \cdot n) \, dS + \frac{\varepsilon_{+} - \varepsilon_{-}}{2} \int_{\Gamma} |\nabla_{\Gamma} \psi_{\Gamma}|^{2} (V \cdot n) \, dS. \quad (5.21)$$

Similarly, on each side of Γ , we have with $u_{\Gamma} = \phi_{\Gamma,\infty}$ or $\hat{\phi}_{\Gamma,\infty}$ that

$$\nabla u_{\Gamma} \cdot V = (\partial_n u_{\Gamma} n + \nabla_{\Gamma} u_{\Gamma}) \cdot ((V \cdot n) n + (I - n \otimes n) V)$$
$$= \partial_n u_{\Gamma} (V \cdot n) + \nabla_{\Gamma} u_{\Gamma} (I - n \otimes n) V.$$

Moreover, $\varepsilon_+ \partial_n u_{\Gamma}^+ = \varepsilon_- \partial_n u_{\Gamma}^-$ and $\partial_{\Gamma} u_{\Gamma}^+ = \partial_{\Gamma} u_{\Gamma}^-$ on Γ . Therefore, the next three terms in (5.20) become

$$\begin{split} &\frac{1}{2} \int_{\Gamma} \llbracket \varepsilon_{\Gamma} (\nabla \hat{\phi}_{\Gamma,\infty} \cdot V) (\nabla \phi_{\Gamma,\infty} \cdot n) \rrbracket_{\Gamma} \, dS + \frac{1}{2} \int_{\Gamma} \llbracket \varepsilon_{\Gamma} (\nabla \hat{\phi}_{\Gamma,\infty} \cdot n) (\nabla \phi_{\Gamma,\infty} \cdot V) \rrbracket_{\Gamma} \, dS \\ &- \frac{1}{2} \int_{\Gamma} \llbracket \varepsilon_{\Gamma} (\nabla \hat{\phi}_{\Gamma,\infty} \cdot \nabla \phi_{\Gamma,\infty}) (V \cdot n) \rrbracket_{\Gamma} \, dS \end{split}$$

$$\begin{split}
&= \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \partial_{n} \hat{\phi}_{\Gamma,\infty} \partial_{n} \phi_{\Gamma,\infty} \rrbracket_{\Gamma}(V \cdot n) \, dS \\
&- \frac{1}{2} \int_{\Gamma} \llbracket \varepsilon_{\Gamma} (\partial_{n} \hat{\phi}_{\Gamma,\infty} \partial_{n} \phi_{\Gamma,\infty} + \nabla_{\Gamma} \hat{\phi}_{\Gamma,\infty} \cdot \nabla_{\Gamma} \phi_{\Gamma,\infty}) \rrbracket_{\Gamma}(V \cdot n) \, dS \\
&= \frac{1}{2} \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \partial_{n} \hat{\phi}_{\Gamma,\infty} \partial_{n} \phi_{\Gamma,\infty} \rrbracket_{\Gamma}(V \cdot n) \, dS - \frac{1}{2} \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \nabla_{\Gamma} \hat{\phi}_{\Gamma,\infty} \cdot \nabla_{\Gamma} \phi_{\Gamma,\infty} \rrbracket_{\Gamma}(V \cdot n) \, dS.
\end{split} (5.22)$$

It now follows from (5.20)–(5.22) that

$$\delta_{\Gamma,V} E[\Gamma] = -\frac{1}{2} \left(\frac{1}{\varepsilon_{+}} - \frac{1}{\varepsilon_{-}} \right) \int_{\Gamma} |\varepsilon_{\Gamma} \partial_{n} \psi_{\Gamma}|^{2} (V \cdot n) \, dS + \frac{\varepsilon_{+} - \varepsilon_{-}}{2} \int_{\Gamma} |\nabla_{\Gamma} \psi_{\Gamma}|^{2} (V \cdot n) \, dS$$

$$+ \frac{1}{2} \int_{\Gamma} [\![\varepsilon_{\Gamma} \partial_{n} \hat{\phi}_{\Gamma,\infty} \partial_{n} \phi_{\Gamma,\infty}]\!]_{\Gamma} (V \cdot n) \, dS - \frac{1}{2} \int_{\Gamma} [\![\varepsilon_{\Gamma} \nabla_{\Gamma} \hat{\phi}_{\Gamma,\infty} \cdot \nabla_{\Gamma} \phi_{\Gamma,\infty}]\!]_{\Gamma} (V \cdot n) \, dS$$

$$+ \int_{\Omega_{+}} \frac{1}{2} \left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dX$$

$$+ \int_{\Gamma} B \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) (V \cdot n) \, dS.$$

$$(5.23)$$

Step 5. We finally rewrite the volume integral above into a surface integral on the boundary Γ . Recall from the beginning of Subsection 3.2 that the signed distance function $\phi: \mathbb{R}^3 \to \mathbb{R}$ with respect to Γ is a C^3 -function and $\nabla \phi \neq 0$ in the neighborhood $\mathcal{N}_0(\Gamma)$ of Γ . We extend $n = \nabla \phi$ on Γ to $\mathcal{N}_0(\Gamma)$, i.e., we define $n = \nabla \phi$ at every point in $\mathcal{N}_0(\Gamma)$. Note that $n \in C^2(\mathcal{N}_0(\Gamma))$. Since $V \in \mathcal{V}$ vanishes outside $\mathcal{N}_0(\Gamma)$, both the normal component $(V \cdot n)n$ and the tangential component $V - (V \cdot n)n = (I - n \otimes n)V$ of V are in the class of vector fields V; cf. (3.6). Since

$$V = (V \cdot n)n + (I - n \otimes n)V$$
 and $(I - n \otimes n)V \cdot n = 0$,

we have by Lemma 4.3 that

$$\begin{split} \zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V &= \zeta_{\Gamma,(V \cdot n)n + (I - n \otimes n)V} - \nabla \phi_{\Gamma,\infty} \cdot [(V \cdot n)n + (I - n \otimes n)V] \\ &= \zeta_{\Gamma,(V \cdot n)n} - \nabla \phi_{\Gamma,\infty} \cdot (V \cdot n)n + \zeta_{\Gamma,(I - n \otimes n)V} - \nabla \phi_{\Gamma,\infty} \cdot (I - n \otimes n)V \\ &= \zeta_{\Gamma,(V \cdot n)n} - \nabla \phi_{\Gamma,\infty} \cdot (V \cdot n)n \quad \text{in } \Omega. \end{split}$$

Therefore, we may assume that

$$V = (V \cdot n)n$$
 in $\mathcal{N}_0(\Gamma)$. (5.24)

By Lemma 4.3, $\zeta_{\Gamma,V}^s \in H^2(\Omega_s)$ for s = - or +. Thus, by (4.28), $\Delta(\nabla \phi_{\Gamma,\infty} \cdot V) \in L^2(\Omega_s)$ for s = - or +. Therefore,

$$\nabla \phi_{\Gamma,\infty} \cdot V \in H^2(\Omega_s) \quad \text{for } s = - \text{ or } +.$$
 (5.25)

Recall from (5.1) that $\psi_{\rm r} = \psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty} \in H^1_0(\Omega)$. Note by Theorem 2.1 that $\Delta \psi_{\rm r} = 0$ in Ω_- and $\varepsilon_+ \Delta \psi_{\rm r} = B'(\psi_{\Gamma} - \phi_{\Gamma,\infty}/2)$ in Ω_+ . Note also by (4.28) in Lemma 4.3 that $\Delta(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V) = 0$

0 in $\Omega_- \cup \Omega_+$. We then obtain by Green's second identity with our convention that the normal n at Γ pointing from Ω_- to Ω_+ and the fact that $[\![\varepsilon_\Gamma \zeta_{\Gamma,V} \partial_n \psi_r]\!]_{\Gamma} = 0$ which follows from the third equation in (2.22) that twice of the volume term in (5.23) is

$$Q := \int_{\Omega_{+}} \left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dX$$

$$= \int_{\Omega_{+}} \varepsilon_{+} \left[\left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) \Delta \psi_{r} - \psi_{r} \Delta \left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) \right] dX$$

$$+ \int_{\Omega_{-}} \varepsilon_{-} \left[\left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) \Delta \psi_{r} - \psi_{r} \Delta \left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) \right] dX$$

$$= - \int_{\Gamma} \left[\varepsilon_{\Gamma} \left[\left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) \partial_{n} \psi_{r} - \psi_{r} \partial_{n} \left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) \right] \right]_{\Gamma} dS$$

$$= \int_{\Gamma} \left[\varepsilon_{\Gamma} \left[\nabla \phi_{\Gamma,\infty} \cdot V \right] \partial_{n} \psi_{r} \right]_{\Gamma} dS + \int_{\Gamma} \left[\varepsilon_{\Gamma} \psi_{r} \partial_{n} \zeta_{\Gamma,V} \right]_{\Gamma} dS - \int_{\Gamma} \left[\varepsilon_{\Gamma} \psi_{r} \partial_{n} \left(\nabla \phi_{\Gamma,\infty} \cdot V \right) \right]_{\Gamma} dS$$

$$= Q_{1} + Q_{2} - Q_{3}. \tag{5.26}$$

It follows from (5.24) that

$$Q_1 = \int_{\Gamma} \llbracket \varepsilon_{\Gamma} (\nabla \phi_{\Gamma,\infty} \cdot V) \partial_n \psi_{\Gamma} \rrbracket_{\Gamma} dS = \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \partial_n \phi_{\Gamma,\infty} \partial_n \psi_{\Gamma} \rrbracket_{\Gamma} (V \cdot n) dS.$$
 (5.27)

Since $\llbracket \phi_r \rrbracket_{\Gamma} = 0$ and $\llbracket \varepsilon_{\Gamma} \partial_n \phi_{\Gamma,\infty} \rrbracket_{\Gamma} = 0$, we have by Lemma 4.3 (cf. (4.29)) that

$$Q_{2} = \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \psi_{r} \partial_{n} \zeta_{\Gamma, V} \rrbracket_{\Gamma} dS$$

$$= -\int_{\Gamma} \llbracket \varepsilon_{\Gamma} \psi_{r} A'_{V}(0) \nabla \phi_{\Gamma, \infty} \cdot n \rrbracket_{\Gamma} dS$$

$$= \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \psi_{r} \left[\nabla V + (\nabla V)^{T} - (\nabla \cdot V) I \right] \nabla \phi_{\Gamma, \infty} \cdot n \rrbracket_{\Gamma} dS$$

$$= \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \psi_{r} \left[\nabla V + (\nabla V)^{T} \right] \nabla \phi_{\Gamma, \infty} \cdot n \rrbracket_{\Gamma} dS$$

$$= \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \psi_{r} \nabla \phi_{\Gamma, \infty} \cdot \left[\nabla V + (\nabla V)^{T} \right] n \rrbracket_{\Gamma} dS. \tag{5.28}$$

Denoting by n^j the jth component of n and noting that $\partial_i n^j n^j = (1/2)\partial_i ||n||^2 = 0$, we obtain on each side of Γ (i.e., on $\mathcal{N}_0(\Gamma) \cup \Omega_-$ and $\mathcal{N}_0(\Gamma) \cup \Omega_+$) that

$$\nabla \phi_{\Gamma,\infty} \cdot (\nabla V + (\nabla V)^T) n$$

$$= \partial_i \phi_{\Gamma,\infty} \left(\partial_j V^i + \partial_i V^j \right) n^j$$

$$= \partial_i \phi_{\Gamma,\infty} \partial_j ((V \cdot n) n^i) n^j + \partial_i \phi_{\Gamma,\infty} \partial_i ((V \cdot n) n^j) n^j \qquad [by (5.24)]$$

$$= \partial_i \phi_{\Gamma,\infty} \partial_i (V \cdot n) n^i n^j + \partial_i \phi_{\Gamma,\infty} (V \cdot n) \partial_j n^i n^j$$

$$+ \partial_i \phi_{\Gamma,\infty} \partial_i (V \cdot n) n^j n^j + \partial_i \phi_{\Gamma,\infty} (V \cdot n) \partial_i n^j n^j$$

= $(\nabla \phi_{\Gamma,\infty} \cdot n) \nabla (V \cdot n) \cdot n + \nabla \phi_{\Gamma,\infty} \cdot ((\nabla n) n) (V \cdot n) + \nabla \phi_{\Gamma,\infty} \cdot \nabla (V \cdot n).$

This and (5.28), together with the fact that $[\![\varepsilon_{\Gamma}\nabla\phi_{\Gamma,\infty}\cdot n]\!]_{\Gamma}=0$ on Γ , lead to

$$Q_{2} = \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \psi_{\mathbf{r}} \nabla \phi_{\Gamma,\infty} \cdot (\nabla n) n \rrbracket_{\Gamma} (V \cdot n) dS + \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \psi_{\mathbf{r}} \nabla \phi_{\Gamma,\infty} \cdot \nabla (V \cdot n) \rrbracket_{\Gamma} dS$$

$$= Q_{2,1} + Q_{2,2}. \tag{5.29}$$

To further simplify these terms, let us recall the surface divergence $\nabla_{\Gamma}v$ for a vector field v along the boundary Γ and its integral on Γ

$$\nabla_{\Gamma} \cdot v = \nabla \cdot v - (\nabla v) n \cdot n, \tag{5.30}$$

$$\int_{\Gamma} \nabla_{\Gamma} \cdot v \, dS = 2 \int_{\Gamma} H(v \cdot n) \, dS,\tag{5.31}$$

where H is the mean curvature; cf. [18] (Section 5 of Chapter 9).

Consider the term $Q_{2,1}$ in (5.29). Since $n = \nabla \phi$ is a unit vector field, we have $n \cdot (\nabla n)n = n^i \partial_j n^i n^j = (1/2)n^j \partial_j (n^i n^i) = 0$. Hence, on each side of Γ , we have

$$\nabla \phi_{\Gamma,\infty} \cdot (\nabla n) n = \nabla_{\Gamma} \phi_{\Gamma,\infty} \cdot (\nabla n) n. \tag{5.32}$$

Let us denote $\alpha_{\Gamma} = \psi_{r} \nabla_{\Gamma} \phi_{\Gamma,\infty}$ and note that $[\![\alpha_{\Gamma}]\!]_{\Gamma} = 0$. Hence $\alpha_{\Gamma} \in H^{1}(\mathcal{N}_{0}(\Gamma), \mathbb{R}^{3})$. Note also that $\alpha_{\Gamma} \cdot n = 0$. Thus,

$$(\nabla \alpha_{\Gamma})n \cdot n + \alpha_{\Gamma} \cdot (\nabla n)n = [(\nabla \alpha_{\Gamma})^{T} n + (\nabla n)^{T} \alpha_{\Gamma}] \cdot n$$

$$= \nabla (\alpha_{\Gamma} \cdot n) \cdot n$$

$$= 0 \quad \text{in } \mathcal{N}_{0}(\Gamma). \tag{5.33}$$

This implies that

$$(\nabla \alpha_{\Gamma} n) \cdot n = -\alpha_{\Gamma} \cdot (\nabla n) n \in H^{1}(\mathcal{N}_{0}(\Gamma)). \tag{5.34}$$

By (5.24), we have for s = - or + that

$$\nabla(\nabla\phi_{\Gamma,\infty}\cdot V)\cdot n = \nabla((\nabla\phi_{\Gamma,\infty}\cdot n)(V\cdot n))\cdot n$$

= $(\nabla(\nabla\phi_{\Gamma,\infty}\cdot n)\cdot n)(V\cdot n) + (\nabla\phi_{\Gamma,\infty}\cdot n)\nabla(V\cdot n)\cdot n$ in $\Omega_{\rm s}\cap\mathcal{N}_0(\Gamma)$.

This, together with (2.6) and (5.25), implies for s = - or + that

$$(\nabla(\nabla\phi_{\Gamma,\infty}\cdot n)\cdot n)(V\cdot n)\in H^1(\Omega_s\cap\mathcal{N}_0(\Gamma)). \tag{5.35}$$

Therefore, since $\nabla_{\Gamma}\phi_{\Gamma,\infty} = \nabla\phi_{\Gamma,\infty} - (\nabla\phi_{\Gamma,\infty} \cdot n)n$, $\Delta\phi_{\Gamma,\infty} = 0$ in Ω_- and Ω_+ , and ψ_r and $\phi_{\Gamma,\infty}$ are in $W^{1,\infty}$ on each side of Γ , we can verify that for s = - or +

$$(\nabla \cdot \alpha_{\Gamma})(V \cdot n) = (\nabla \psi_{\mathbf{r}} \cdot \nabla \phi_{\Gamma,\infty})(V \cdot n) - (\nabla \psi_{\mathbf{r}} \cdot n)(\nabla \phi_{\Gamma,\infty} \cdot n)(V \cdot n)$$

$$-\psi_{\mathbf{r}}(\nabla(\nabla\phi_{\Gamma,\infty}\cdot n)\cdot n)(V\cdot n) - \psi_{\mathbf{r}}(\nabla\phi_{\Gamma,\infty}\cdot n)(\nabla\cdot n)(V\cdot n) \in H^{1}(\Omega_{\mathbf{s}}\cap\mathcal{N}_{0}(\Gamma)). \tag{5.36}$$

By (5.34), (5.36), and (5.30) (with α_{Γ} replacing v), we have for s = - or + that

$$(\nabla_{\Gamma} \cdot \alpha_{\Gamma})(V \cdot n) = (\nabla \cdot \alpha_{\Gamma})(V \cdot n) - (\nabla \alpha_{\Gamma} n \cdot n)(V \cdot n) \in H^{1}(\Omega_{s} \cap \mathcal{N}_{0}(\Gamma)). \tag{5.37}$$

With all the regularity results (5.34), (5.36), and (5.37), we have now by (5.32), (5.33), and (5.30) (with α_{Γ} replacing v) that

$$Q_{2,1} = \int_{\Gamma} [\![\varepsilon_{\Gamma}\alpha_{\Gamma} \cdot (\nabla n)n]\!]_{\Gamma}(V \cdot n) dS$$

$$= -\int_{\Gamma} [\![\varepsilon_{\Gamma}(\nabla \alpha_{\Gamma})n \cdot n]\!]_{\Gamma}(V \cdot n) dS$$

$$= \int_{\Gamma} [\![\varepsilon_{\Gamma}(\nabla_{\Gamma} \cdot \alpha_{\Gamma} - \nabla \cdot \alpha_{\Gamma})]\!]_{\Gamma}(V \cdot n) dS.$$
(5.38)

Consider now the term $Q_{2,2}$ in (5.29). On each side of Γ ,

$$\nabla \phi_{\Gamma,\infty} \cdot \nabla (V \cdot n) = [(\nabla \phi_{\Gamma,\infty} \cdot n) n + \nabla_{\Gamma} \phi_{\Gamma,\infty}] \cdot [(\nabla (V \cdot n) \cdot n) n + \nabla_{\Gamma} (V \cdot n)]$$
$$= (\nabla \phi_{\Gamma,\infty} \cdot n) (\nabla (V \cdot n) \cdot n) + \nabla_{\Gamma} \phi_{\Gamma,\infty} \cdot \nabla_{\Gamma} (V \cdot n).$$

Since $\llbracket \psi_r \rrbracket_{\Gamma} = 0$ and $\llbracket \varepsilon_{\Gamma} \nabla \phi_{\Gamma,\infty} \cdot n \rrbracket_{\Gamma} = 0$, we thus have

$$\begin{split}
& [\![\varepsilon_{\Gamma}\psi_{\mathbf{r}}\nabla\phi_{\Gamma,\infty}\cdot\nabla(V\cdot n)]\!]_{\Gamma} \\
&= [\![\varepsilon_{\Gamma}\psi_{\mathbf{r}}(\nabla\phi_{\Gamma,\infty}\cdot n)(\nabla(V\cdot n)\cdot n)]\!]_{\Gamma} + [\![\varepsilon_{\Gamma}\psi_{\mathbf{r}}\nabla_{\Gamma}\phi_{\Gamma,\infty}\cdot\nabla_{\Gamma}(V\cdot n)]\!]_{\Gamma} \\
&= [\![\varepsilon_{\Gamma}\alpha_{\Gamma}\cdot\nabla_{\Gamma}(V\cdot n)]\!]_{\Gamma}.
\end{split} (5.39)$$

One can verify that on both side of Γ

$$\nabla_{\Gamma} \cdot ((V \cdot n)\alpha_{\Gamma}) = (V \cdot n)\nabla_{\Gamma} \cdot \alpha_{\Gamma} + \alpha_{\Gamma} \cdot \nabla_{\Gamma}(V \cdot n).$$

Consequently, we have by (5.29), (5.39), (5.31), and the fact that $\nabla_{\Gamma}\phi_{\Gamma,\infty} \cdot n = 0$ on each side of Γ that

$$\begin{split} Q_{2,2} &= \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \alpha_{\Gamma} \cdot \nabla_{\Gamma} (V \cdot n) \rrbracket_{\Gamma} \, dS \\ &= \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \nabla_{\Gamma} \cdot ((V \cdot n) \alpha_{\Gamma}) \rrbracket_{\Gamma} \, dS - \int_{\Gamma} \llbracket \varepsilon_{\Gamma} (V \cdot n) \nabla_{\Gamma} \cdot \alpha_{\Gamma} \rrbracket_{\Gamma} \, dS \\ &= \int_{\Gamma} \llbracket 2\varepsilon_{\Gamma} H((V \cdot n) \alpha_{\Gamma} \cdot n) \rrbracket_{\Gamma} \, dS - \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \nabla_{\Gamma} \cdot \alpha_{\Gamma} \rrbracket_{\Gamma} (V \cdot n) \, dS \\ &= - \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \nabla_{\Gamma} \cdot \alpha_{\Gamma} \rrbracket_{\Gamma} (V \cdot n) \, dS. \end{split}$$

This, together with (5.29), (5.38), and the notation $\alpha_{\Gamma} = \psi_{r} \nabla_{\Gamma} \phi_{\Gamma,\infty}$, implies that

$$Q_2 = -\int_{\Gamma} \llbracket \varepsilon_{\Gamma} \nabla \cdot \alpha_{\Gamma} \rrbracket_{\Gamma}(V \cdot n) \, dS = -\int_{\Gamma} \llbracket \varepsilon_{\Gamma} \nabla \cdot (\psi_{r} \nabla_{\Gamma} \phi_{\Gamma, \infty}) \rrbracket_{\Gamma}(V \cdot n) \, dS. \tag{5.40}$$

Now, let us calculate the term Q_3 in (5.26). Since $V = (V \cdot n)n$ (cf. (5.24)), we have from both sides of Γ that

$$\nabla(\nabla\phi_{\Gamma,\infty}\cdot V)\cdot n = \nabla\left((\nabla\phi_{\Gamma,\infty}\cdot n)(V\cdot n)\right)\cdot n$$
$$= \nabla(\nabla\phi_{\Gamma,\infty}\cdot n)\cdot n(V\cdot n) + (\nabla\phi_{\Gamma,\infty}\cdot n)\nabla(V\cdot n)\cdot n.$$

Since $[\![\varepsilon_{\Gamma}\nabla\phi_{\Gamma,\infty}\cdot n]\!]_{\Gamma}=0$, we have by (5.26) and (5.35) that

$$Q_3 = \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \psi_{\Gamma} \nabla (\nabla \phi_{\Gamma,\infty} \cdot V) \cdot n \rrbracket_{\Gamma} dS = \int_{\Gamma} \llbracket \varepsilon_{\Gamma} \psi_{\Gamma} \nabla (\nabla \phi_{\Gamma,\infty} \cdot n) \cdot n \rrbracket_{\Gamma} (V \cdot n) dS.$$
 (5.41)

It now follows from (5.26), (5.27), (5.40), and (5.41) that

$$Q = \int_{\Gamma} \llbracket \varepsilon_{\Gamma} [\partial_n \phi_{\Gamma,\infty} \partial_n \psi_{\Gamma} - \nabla \cdot (\psi_{\Gamma} \nabla_{\Gamma} \phi_{\Gamma,\infty}) - \psi_{\Gamma} \nabla (\nabla \phi_{\Gamma,\infty} \cdot n) \cdot n] \rrbracket_{\Gamma} (V \cdot n) \, dS. \tag{5.42}$$

By the definition of the tangential gradient, the fact that $\Delta \phi_{\Gamma,\infty} = 0$ on both sides of Γ (cf. (2.8)), and $\nabla \cdot n = 2H$ on Γ , we can simplify the terms inside the pair of brackets in (5.42). On both sides of Γ , we have

$$\begin{split} \partial_n \phi_{\Gamma,\infty} \partial_n \psi_{\mathbf{r}} - \nabla \cdot (\psi_{\mathbf{r}} \nabla_{\Gamma} \phi_{\Gamma,\infty}) - \psi_{\mathbf{r}} \nabla (\nabla \phi_{\Gamma,\infty} \cdot n) \cdot n \\ &= \partial_n \phi_{\Gamma,\infty} \partial_n \psi_{\mathbf{r}} - \nabla \cdot [\psi_{\mathbf{r}} \nabla \phi_{\Gamma,\infty} - \psi_{\mathbf{r}} (\nabla \phi_{\Gamma,\infty} \cdot n) n] - \psi_{\mathbf{r}} \nabla (\nabla \phi_{\Gamma,\infty} \cdot n) \cdot n \\ &= \partial_n \phi_{\Gamma,\infty} \partial_n \psi_{\mathbf{r}} - \nabla \psi_{\mathbf{r}} \cdot \nabla \phi_{\Gamma,\infty} - \psi_{\mathbf{r}} \Delta \phi_{\Gamma,\infty} \\ &+ \nabla (\psi_{\mathbf{r}} (\nabla \phi_{\Gamma,\infty} \cdot n)) \cdot n + \psi_{\mathbf{r}} (\nabla \phi_{\Gamma,\infty} \cdot n) (\nabla \cdot n) - \psi_{\mathbf{r}} \nabla (\nabla \phi_{\Gamma,\infty} \cdot n) \cdot n \\ &= \partial_n \phi_{\Gamma,\infty} \partial_n \psi_{\mathbf{r}} - \nabla \psi_{\mathbf{r}} \cdot \nabla \phi_{\Gamma,\infty} + (\nabla \phi_{\Gamma,\infty} \cdot n) (\nabla \psi_{\mathbf{r}} \cdot n) + \psi_{\mathbf{r}} (\nabla \phi_{\Gamma,\infty} \cdot n) (\nabla \cdot n) \\ &= 2\partial_n \phi_{\Gamma,\infty} \partial_n \psi_{\mathbf{r}} - [(\nabla \psi_{\mathbf{r}} \cdot n) n + \nabla_{\Gamma} \psi_{\mathbf{r}}] [(\nabla \phi_{\Gamma,\infty} \cdot n) n + \nabla_{\Gamma} \phi_{\Gamma,\infty}] + 2H \psi_{\mathbf{r}} \partial_n \phi_{\Gamma,\infty} \\ &= \partial_n \phi_{\Gamma,\infty} \partial_n \psi_{\mathbf{r}} - \nabla_{\Gamma} \phi_{\Gamma,\infty} \cdot \nabla_{\Gamma} \psi_{\mathbf{r}} + 2H \psi_{\mathbf{r}} \partial_n \phi_{\Gamma,\infty}. \end{split}$$

Plug this into (5.42). Noting that $\psi_{\rm r} = \psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}$ and that all $\nabla_{\Gamma}\psi_{\rm r}$, $\nabla_{\Gamma}\phi_{\Gamma,\infty}$, $\varepsilon_{\Gamma}\partial_n(\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty})$, and $\varepsilon_{\Gamma}\partial_n\phi_{\Gamma,\infty}$ are continuous across the boundary Γ , we obtain that

$$Q = \int_{\Gamma} \llbracket \varepsilon_{\Gamma} (\partial_{n} \psi_{\Gamma} \partial_{n} \phi_{\Gamma,\infty} - \nabla_{\Gamma} \psi_{\Gamma} \cdot \nabla_{\Gamma} \phi_{\Gamma,\infty}) \rrbracket_{\Gamma} (V \cdot n) \, dS$$

$$= \int_{\Gamma} \llbracket \varepsilon_{\Gamma} [\partial_{n} (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) \partial_{n} \phi_{\Gamma,\infty} - \nabla_{\Gamma} (\psi_{\Gamma} - \hat{\phi}_{\Gamma,\infty}) \cdot \nabla_{\Gamma} \phi_{\Gamma,\infty}] \rrbracket_{\Gamma} (V \cdot n) \, dS. \tag{5.43}$$

Finally, we obtain by (5.23), (5.26), and (5.43) that some of the terms in $\delta_{\Gamma,V}E[\Gamma]$ (5.23) are simplified into

$$\begin{split} &\frac{1}{2} \int_{\Gamma} [\![\varepsilon_{\Gamma} \partial_{n} \hat{\phi}_{\Gamma,\infty} \partial_{n} \phi_{\Gamma,\infty}]\!]_{\Gamma}(V \cdot n) \, dS - \frac{1}{2} \int_{\Gamma} [\![\varepsilon_{\Gamma} \nabla_{\Gamma} \hat{\phi}_{\Gamma,\infty} \cdot \nabla_{\Gamma} \phi_{\Gamma,\infty}]\!]_{\Gamma}(V \cdot n) \, dS \\ &+ \int_{\Omega_{+}} \frac{1}{2} \left(\zeta_{\Gamma,V} - \nabla \phi_{\Gamma,\infty} \cdot V \right) B' \left(\psi_{\Gamma} - \frac{\phi_{\Gamma,\infty}}{2} \right) dX \end{split}$$

$$\begin{split} &=\frac{1}{2}\int_{\Gamma}[\![\varepsilon_{\Gamma}\partial_{n}\hat{\phi}_{\Gamma,\infty}\partial_{n}\phi_{\Gamma,\infty}]\!]_{\Gamma}(V\cdot n)\,dS - \frac{1}{2}\int_{\Gamma}[\![\varepsilon_{\Gamma}\nabla_{\Gamma}\hat{\phi}_{\Gamma,\infty}\cdot\nabla_{\Gamma}\phi_{\Gamma,\infty}]\!]_{\Gamma}(V\cdot n)\,dS + \frac{1}{2}Q\\ &=\frac{1}{2}\int_{\Gamma}[\![\varepsilon_{\Gamma}(\partial_{n}\psi_{\Gamma}\partial_{n}\phi_{\Gamma,\infty}-\nabla_{\Gamma}\psi_{\Gamma}\cdot\nabla_{\Gamma}\phi_{\Gamma,\infty})]\!]_{\Gamma}(V\cdot n)\,dS\\ &=\frac{1}{2}\int_{\Gamma}\varepsilon_{+}\partial_{n}\psi_{\Gamma}^{+}\partial_{n}\phi_{\Gamma,\infty}^{+}(V\cdot n)dS - \frac{1}{2}\int_{\Gamma}\varepsilon_{-}\partial_{n}\psi_{\Gamma}^{-}\partial_{n}\phi_{\Gamma,\infty}^{-}(V\cdot n)dS\\ &-\frac{\varepsilon_{+}}{2}\int_{\Gamma}\nabla_{\Gamma}\psi_{\Gamma}\cdot\nabla_{\Gamma}\phi_{\Gamma,\infty}(V\cdot n)\,dS + \frac{\varepsilon_{-}}{2}\int_{\Gamma}\nabla_{\Gamma}\psi_{\Gamma}\cdot\nabla_{\Gamma}\phi_{\Gamma,\infty}(V\cdot n)\,dS\\ &=\frac{1}{2}\left(\frac{1}{\varepsilon_{+}}-\frac{1}{\varepsilon_{-}}\right)\int_{\Gamma}\varepsilon_{\Gamma}\partial_{n}\psi_{\Gamma}\varepsilon_{\Gamma}\partial_{n}\phi_{\Gamma,\infty}(V\cdot n)dS - \frac{\varepsilon_{+}-\varepsilon_{-}}{2}\int_{\Gamma}\nabla_{\Gamma}\psi_{\Gamma}\cdot\nabla_{\Gamma}\phi_{\Gamma,\infty}(V\cdot n)\,dS. \end{split}$$

This and (5.23) imply the desired formula (3.8). The proof is complete.

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