RENORMALIZED ENERGY AND PEACH-KÖHLER FORCES FOR SCREW DISLOCATIONS WITH ANTIPLANE SHEAR

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Abstract. We present a variational framework for studying screw dislocations subject to antiplane shear. Using a classical model developed by Cermelli & Gurtin [CG99], methods of Calculus of Variations are exploited to prove existence of solutions, and to derive a useful expression of the Peach-Köhler forces acting on a system of dislocation. This provides a setting for studying the dynamics of the dislocations, which is done in [BFLM14].

1. Introduction

Dislocations are one-dimensional defects in crystalline materials [Nab67]. Their modeling is of great interest in materials science because important material properties, such as rigidity and conductivity, can be strongly affected by the presence of dislocations. For example, large collections of dislocations can result in plastic deformations in solids under applied loads.

In this note, we derive an expression for the renormalized energy associated to a system screw dislocations in cylindrical crystalline materials using a continuum model introduced by Cermelli and Gurtin [CG99]. We use the renormalized energy to derive an expression for the forces on the dislocations, called Peach-Köhler forces. These forces drive the dynamics of the system, which is studied in [BFLM14]. The proofs of some results that are used in [BFLM14] are contained in this note.

Following [CG99], we consider here an elastic body $B \subset \mathbb{R}^3$ undergoing *antiplane shear* in the x_3 direction, with $B = \Omega \times \mathbb{R}$, where $\Omega \subset \mathbb{R}^2$ is a bounded simply connected open set with Lipschitz boundary. The deformations $\Phi : B \to B$ are of the form

$$\Phi(x_1, x_2, x_3) := (x_1, x_2, x_3 + u(x_1, x_2)),$$

with $u : \Omega \to \mathbb{R}$, and the deformation gradient $\mathbf{F}$ is given by

$$\mathbf{F} = \nabla\Phi := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \partial_1 u & \partial_2 u & 1 \end{pmatrix} = \mathbf{I} + \mathbf{e}_3 \otimes \begin{pmatrix} \nabla u \\ 0 \end{pmatrix}. \tag{1.1}$$

The assumption of antiplane shear allows us to reduce the three-dimensional problem to a two-dimensional problem. We will consider strain fields $\mathbf{h}$ that are defined on the cross-section Ω, taking values in $\mathbb{R}^2$. When no dislocations are present, in this setting it turns out that $\mathbf{h} = \nabla u$; however, the presence of dislocations causes the strain field to be singular at the sites of the dislocations.

A screw dislocation is a line singularity in the strain field for the body B. In the antiplane shear setting, this line is parallel to the x_3 axis; in the cross-section Ω a screw dislocation is represented as a point singularity. A screw dislocation is characterized by a position $\mathbf{z} \in \Omega$ and a vector $\mathbf{b} \in \mathbb{R}^3$, called the *Burgers* vector. The position $\mathbf{z} \in \Omega$ is a point where the strain field fails to be the gradient of a smooth function; the Burgers vector measures the severity of this failure. More specifically, a strain field associated with a system of N screw dislocations at the positions

$$\mathcal{Z} := \{\mathbf{z}_1, \dots, \mathbf{z}_N\},$$

with corresponding Burgers vectors

$$\mathcal{B} := \{\mathbf{b}_1, \dots, \mathbf{b}_N\}$$

satisfies the relation

$$\operatorname{curl} \mathbf{h} = \sum_{i=1}^{N} b_i \delta_{\mathbf{z}_i} \quad \text{in } \Omega \tag{1.2}$$

in the sense of distributions. The notation $\operatorname{curl}\mathbf{h}$ denotes the scalar curl, $\partial_1 h_2 - \partial_2 h_1$. Thus, in the antiplane shear setting, the Burgers vectors can be written as $\mathbf{b}_i = b_i\mathbf{e}_3$, the scalar b_i is called the *Burgers modulus* for the dislocation at $\mathbf{z}_i$, and it is given by

$$b_i = \int_{\ell_i} \mathbf{h}\cdot\mathbf{t}\,\mathrm{d}s,$$

where ℓ_i is any counterclockwise loop surrounding the dislocation point $\mathbf{z}_i$ and no other dislocation points, $\mathbf{t}$ is the tangent to ℓ_i, and $\mathrm{d}s$ is the line element. Since $\mathbf{b}_i = b_i\mathbf{e}_3$ for all $i \in \{1,\dots,N\}$, by abuse of notation from now on we will use the symbol $\mathcal{B}$ both for the set of Burgers vectors and for the set of Burgers moduli. When dislocations are present, the deformation gradient $\mathbf{F}$ cannot be any longer represented by the last expression in (1.1), which needs to be replaced with

$$\mathbf{F} = \mathbf{I} + \mathbf{e}_3 \otimes \begin{pmatrix} \mathbf{h} \\ 0 \end{pmatrix}.$$

Our goal is to derive an energy associated to systems of screw dislocation and obtain an expression for the forces on the dislocations (Peach-Köhler forces [PK50]). This lays the foundation needed to study the dynamics of the dislocations, which is investigated in [BFLM14], where the expression for the Peach-Köhler force is used along with an energy-dissipation criterion described in [CG99] to obtain an evolution equation for the system of dislocations.

Our investigation of the energy associated to a system of dislocations will be undertaken in the context of linear elasticity for singular strains $\mathbf{h}$. The energy density W is given by

$$W(\mathbf{h}) := \frac{1}{2}\mathbf{h}\cdot\mathbf{L}\mathbf{h}$$

as functions of the strain $\mathbf{h}$, where the elasticity tensor $\mathbf{L}$ is a symmetric, positive-definite matrix. In suitable coordinates, $\mathbf{L}$ is written in terms of the Lamé moduli λ, μ of the material

$$\mathbf{L} := \begin{pmatrix} \mu & 0 \\ 0 & \mu\lambda^2 \end{pmatrix}. \tag{1.3}$$

We require $\mu > 0$, and the energy is isotropic if and only if $\lambda = 1$. The energy of a strain field $\mathbf{h}$ is given by

$$J(\mathbf{h}) := \int_\Omega W(\mathbf{h}(\mathbf{x}))\,\mathrm{d}\mathbf{x},$$

and the equilibrium equation is

$$\operatorname{div}\mathbf{L}\mathbf{h} = 0 \quad \text{in } \Omega. \tag{1.4}$$

Equations (1.2) and (1.4) provide a characterization of strain fields describing screw dislocation systems in linearly elastic materials.

To be precise, we say that a strain field $\mathbf{h} \in L^2(\Omega;\mathbb{R}^2)$ corresponds to a *system of dislocations* at the positions $\mathcal{Z}$ with Burgers vectors $\mathcal{B}$ if $\mathbf{h}$ satisfies

$$\begin{cases} \operatorname{curl}\mathbf{h} = \sum_{i=1}^N b_i\delta_{\mathbf{z}_i} \\ \operatorname{div}\mathbf{L}\mathbf{h} = 0 \end{cases} \quad \text{in } \Omega, \tag{1.5}$$

in the sense of distributions.

In analogy to the theory of Ginzburg-Landau vortices [BBH94], no variational principle can be associated with (1.5) because the elastic energy of a system of screw dislocations is not finite (see, e.g., [CL05, CG99, Nab67]), so we cannot study (1.5) directly in terms of energy minimization. Indeed, the simultaneous requirements of finite energy and (1.2) are incompatible, since, if $\operatorname{curl}\mathbf{h} = \delta_{\mathbf{z}_0}$, $\mathbf{z}_0 \in \Omega$, and if $B_\varepsilon(\mathbf{z}_0) \subset\subset \Omega$, then

$$\int_{\Omega\setminus B_\varepsilon(\mathbf{z}_0)} |\mathbf{h}|^2 \mathrm{d}\mathbf{x} = O(|\log\varepsilon|).$$

In the engineering literature (see, e.g., [CG99, Nab67]), this problem is usually overcome by regularizing the energy. By removing small cores of size $\varepsilon > 0$ centered at the dislocations, we will replace J by J_ε (cf. Section 2) and obtain finite-energy strains, $\mathbf{h}_\varepsilon$, as minimizers of J_ε. Upon taking $\varepsilon \to 0$ we will recover a unique limiting strain $\mathbf{h}_0 = \lim_{\varepsilon\to 0} \mathbf{h}_\varepsilon$, satisfying (1.5). From this, we can compute a renormalized energy U associated with the limiting strain. In Section 3, we show that

$$J_\varepsilon(\mathbf{h}_\varepsilon) = C \log \varepsilon + U(\mathbf{z}_1, \ldots, \mathbf{z}_N) + O(\varepsilon). \tag{1.6}$$

This type of asymptotic expansion was first proved by Bethuel, Brezis, and Hélein in [BBH93] for Ginzburg-Landau vortices, while the case of edge dislocations was studied in [CL05]. Note that (1.6) can also be obtained as a consequence of Γ-convergence, see, e.g., [AP14, SS03] and the references therein for Ginzburg-Landau vortices, [DLGP12, GPPS13, GLP10] for edge dislocations, and [ACP11, CG09, CGM11, FG07, GM05, GM06, SZ12] for other dislocations models. Finally, it is important to mention that we ignore here the core energy. We refer to [Nab67, TOP96, VKHLLO12] for more details.

The renormalized energy U is a function only of the positions $\{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$, and its gradient with respect to $\mathbf{z}_i$ gives the opposite of the Peach-Köhler force on $\mathbf{z}_i$, denoted $\mathbf{j}_i$. In Section 4 (see Theorem. 4.1), we show that

$$\mathbf{j}_i = -\nabla_{\mathbf{z}_i} U = \int_{\ell_i} \{W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)\}\, \mathbf{n}\, \mathrm{d}s,$$

where ℓ_i is a suitably chosen loop around $\mathbf{z}_i$ and $\mathbf{n}$ is the outer unit normal to the set bounded by ℓ_i containing $\mathbf{z}_i$. The quantity $W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)$ is the Eshelby stress tensor, see [Esh51, Gur95].

There are two different kinds of forces acting on a dislocation when other dislocations are present: the interactions with the other dislocations and the interactions with $\partial\Omega$. Therefore, the expression of $\mathbf{j}_i$ contains two contributions, where the one coming from the boundary balances the tractions of the forces generated by all the dislocations. It is the gradient of the solution u_0 to an elliptic problem with Neumann boundary conditions (2.19). Precisely, we show that $\mathbf{j}_i$ has the form

$$\mathbf{j}_i(\mathbf{z}_1, \ldots, \mathbf{z}_N) = b_i \mathbf{J}\mathbf{L}\Big[\sum_{j\neq i} \mathbf{k}_j(\mathbf{z}_i; \mathbf{z}_j) + \nabla u_0(\mathbf{z}_i; \mathbf{z}_1, \ldots, \mathbf{z}_N)\Big],$$

where $\mathbf{J}$ is the rotation matrix of an angle $\pi/2$, and $\mathbf{k}_j(\cdot; \mathbf{z}_j)$ is the fundamental singular strain generated by the dislocation $\mathbf{z}_j$, see (2.4). It is important to notice that the force on the i-th dislocation is a function of the positions *all* the dislocations. This explicit formula is useful for computing $\mathbf{j}_i$, and is employed in [BFLM14] to study the motion of the dislocations.

In Section 2 we show how to regularize the energy to use variational techniques to study the problem. In Section 3 we derive the renormalized energy, which we will use in Section 4 to derive the Peach-Köhler force.

2. REGULARIZED ENERGIES AND SINGULAR STRAINS

We consider a system of dislocations at the positions $\mathcal{Z} = \{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$ with Burgers vectors $\mathcal{B} = \{\mathbf{b}_1, \ldots, \mathbf{b}_N\}$. We regularize the energy J by removing the singular points from the domain Ω. We define the sets $E_{\varepsilon,i} := E_\varepsilon(\mathbf{z}_i)$, where

$$E_r(\mathbf{z}) = \left\{ (x_1, x_2) \in \mathbb{R}^2 : (x_1 - z_1)^2 + \left(\frac{x_2 - z_2}{\lambda}\right)^2 < r^2 \right\}$$

is an ellipse centered at $\mathbf{z}$ for $r > 0$; the parameter λ is one of the the Lamé moduli of the material (cf. (1.3)). Let $\varepsilon_0 > 0$ be fixed (depending on Ω, $\mathcal{Z}$, and λ) such that for all $\varepsilon \in (0, \varepsilon_0)$ we have $E_{\varepsilon,i} \subset\subset \Omega$, and $\overline{E}_{\varepsilon,i} \cap \overline{E}_{\varepsilon,j} = \emptyset$ for all $i \neq j$. We define the sets

$$\Omega_\varepsilon := \Omega \setminus \left(\bigcup_{i=1}^N \overline{E}_{\varepsilon,i} \right) \quad \text{for} \quad \varepsilon \in (0, \varepsilon_0). \tag{2.1}$$

The shape of the cores $E_{\varepsilon,i}$ is not crucial, but in the sequel we will find the ellipses $E_{\varepsilon,i}$ centered at $\mathbf{z}_i$ to be useful for computations.

We now define the energy functional at the level ε by setting

$$J_\varepsilon(\mathbf{h}) := \int_{\Omega_\varepsilon} W(\mathbf{h})\, \mathrm{d}\mathbf{x}.$$

By removing cores around the singular set $\mathcal{Z}$, we have regularized the energy, in the sense that it will not necessarily be infinite on strains satisfying (1.5). However, since we have effectively removed the dislocations from the problem, we account for their presence by a judicious choice of function space. We define

$$H^{\mathrm{curl}}(\Omega_\varepsilon) := \{\mathbf{h} \in L^2(\Omega_\varepsilon, \mathbb{R}^2) : \mathrm{curl}\,\mathbf{h} \in L^2(\Omega_\varepsilon)\}$$

and

$$H_0^{\mathrm{curl}}(\Omega_\varepsilon, \mathcal{Z}, \mathcal{B}) := \left\{ \mathbf{h} \in H^{\mathrm{curl}}(\Omega_\varepsilon),\ \mathrm{curl}\,\mathbf{h} = 0,\ \int_{\partial E_{\varepsilon,i}} \mathbf{h}\cdot\mathbf{t}\,\mathrm{d}s = b_i,\ i = 1, \ldots, N \right\}, \tag{2.2}$$

where $\mathbf{t}$ is the unit tangent vector to $\partial E_{\varepsilon,i}$. The condition on $\mathbf{h}$ involving the Burgers moduli b_i in (2.2) reintroduces the dislocations into the regularized problem, and it prevents the minimizers of J_ε from being gradients of H^1 functions. In order to keep the notation shorter, we will write only $H_0^{\mathrm{curl}}(\Omega_\varepsilon)$ whenever it is possible to do so without confusion. We will denote by $\mathbf{n}$ the unit outward normal on $\partial\Omega_\varepsilon$.

Lemma 2.1. *Let $\mathbf{h}_\varepsilon$ be a minimizer of J_ε in $H_0^{\mathrm{curl}}(\Omega_\varepsilon)$. Then it satisfies the Euler equations*

$$\begin{cases} \mathrm{div}(\mathbf{L}\mathbf{h}_\varepsilon) = 0 & \text{in } \Omega_\varepsilon\,, \\ \mathbf{L}\mathbf{h}_\varepsilon \cdot \mathbf{n} = 0 & \text{on } \partial\Omega_\varepsilon\,. \end{cases} \tag{2.3}$$

Moreover, the solution to (2.3) *is unique.*

Proof. Given that the functional J_ε is quadratic, the result is achieved by computing the vanishing of its first variation. Let $w \in H^1(\Omega_\varepsilon)$; then

$$\begin{aligned} \delta J_\varepsilon(\mathbf{h}_\varepsilon)[w] &= \lim_{t\to 0} \frac{J_\varepsilon(\mathbf{h}_\varepsilon + t\nabla w) - J_\varepsilon(\mathbf{h}_\varepsilon)}{t} \\ &= \lim_{t\to 0} \frac{1}{t} \left(\int_{\Omega_\varepsilon} t\nabla w \cdot \mathbf{L}\mathbf{h}_\varepsilon + \frac{1}{2} t^2 \nabla w \cdot \mathbf{L}\nabla w \,\mathrm{d}\mathbf{x} \right) \\ &= \int_{\Omega_\varepsilon} \nabla w \cdot \mathbf{L}\mathbf{h}_\varepsilon \,\mathrm{d}\mathbf{x} = -\int_{\Omega_\varepsilon} w\,\mathrm{div}(\mathbf{L}\mathbf{h}_\varepsilon)\,\mathrm{d}\mathbf{x} + \int_{\partial\Omega_\varepsilon} w\,\mathbf{L}\mathbf{h}_\varepsilon \cdot \mathbf{n}\,\mathrm{d}s(\mathbf{x}). \end{aligned}$$

By setting $\delta J_\varepsilon(\mathbf{h}_\varepsilon)[w] = 0$ for all $w \in H^1(\Omega_\varepsilon)$, we get (2.3).

To prove uniqueness, assume that $\mathbf{h}_\varepsilon$ and $\widetilde{\mathbf{h}}_\varepsilon$ both solve system (2.3). Then the path integral of the difference $\mathbf{h}_\varepsilon - \widetilde{\mathbf{h}}_\varepsilon$ over any loop in Ω_ε must vanish, and so $\mathbf{h}_\varepsilon - \widetilde{\mathbf{h}}_\varepsilon = \nabla u$ for some function $u \in H^1(\Omega_\varepsilon)$. Since u solves the weak Euler equation

$$\int_{\Omega_\varepsilon} \nabla w \cdot \mathbf{L}\nabla u \,\mathrm{d}\mathbf{x} = 0, \qquad \text{for all } w \in H^1(\Omega_\varepsilon),$$

taking $w = u$ we obtain $J_\varepsilon(\nabla u) = 0$, and as $\mathbf{L}$ is positive definite, we conclude that $\nabla u = 0$. ☐

2.1. Singular Strains and the Limit $\varepsilon \to 0$.

We introduce the singular strains $\mathbf{k}_i(\cdot;\mathbf{z}_i) : \mathbb{R}^2 \setminus \{\mathbf{z}_i\} \to \mathbb{R}^2$, $i = 1, \ldots, N$, as

$$\mathbf{k}_i(\mathbf{x};\mathbf{z}_i) = \frac{b_i\lambda}{2\pi(\lambda^2(x_1 - z_{i,1})^2 + (x_2 - z_{i,2})^2)} \begin{pmatrix} -(x_2 - z_{i,2}) \\ x_1 - z_{i,1} \end{pmatrix}. \tag{2.4}$$

We will often abbreviate $\mathbf{k}_i(\cdot;\mathbf{z}_i)$ as $\mathbf{k}_i$. Each $\mathbf{k}_i$ enjoys several nice properties; in particular, each can be written as the gradient of a multi-valued function, precisely

$$\mathbf{k}_i(\mathbf{x};\mathbf{z}_i) = \frac{b_i}{2\pi} \nabla_{\mathbf{x}} \arctan\left(\frac{x_2 - z_{i,2}}{\lambda(x_1 - z_{i,1})} \right),$$

and it is straightforward to compute directly that

$$\mathrm{curl}_{\mathbf{x}}\, \mathbf{k}_i(\mathbf{x};\mathbf{z}_i) = \mathbf{b}_i \delta_{\mathbf{z}_i}(\mathbf{x}) \quad \text{in } \mathbb{R}^2, \tag{2.5a}$$

$$\mathrm{div}_{\mathbf{x}}\, (\mathbf{L}\mathbf{k}_i(\mathbf{x};\mathbf{z}_i)) = 0 \quad \text{in } \mathbb{R}^2 \setminus \{\mathbf{z}_i\}, \tag{2.5b}$$

$$\mathbf{L}\mathbf{k}_i(\mathbf{x};\mathbf{z}_i) \cdot \mathbf{n} = 0 \quad \text{on } \partial E_{\varepsilon,i}. \tag{2.5c}$$

In particular, by (2.5c) and (2.5b),

$$\int_{\partial\Omega} \mathbf{L} \sum_{i=1}^N \mathbf{k}_i(\mathbf{y};\mathbf{z}_i) \cdot \mathbf{n}(\mathbf{y})\,\mathrm{d}s(\mathbf{y}) = \int_{\partial\Omega_\varepsilon} \mathbf{L} \sum_{i=1}^N \mathbf{k}_i(\mathbf{y};\mathbf{z}_i) \cdot \mathbf{n}(\mathbf{y})\,\mathrm{d}s(\mathbf{y}) = 0. \tag{2.6}$$

However, it is important to note that the integral in (2.6) is only well-defined when the dislocations are away from the boundary ($\varepsilon_0 > 0$). Indeed, the integral is divergent when $\mathbf{z}_i \in \partial\Omega$, which would require $\varepsilon_0 = 0$.

These singular strains $\mathbf{k}_i$ are "fundamental" to the problem of screw dislocations in the sense that they are the building blocks of the singular part of the strain field $\mathbf{h}$ that represents the system of dislocations.

Lemma 2.2. *Let* $\mathbf{h} \in H_0^{\mathrm{curl}}(\Omega_\varepsilon,\, \mathcal{Z},\, \mathcal{B})$*. Then*

$$\mathbf{h} = \sum_{i=1}^{N} \mathbf{k}_i + \nabla u$$

for some $u \in H^1(\Omega_\varepsilon)$*. Moreover, the minimization problem*

$$\min\left\{ J_\varepsilon(\mathbf{h}) \;\middle|\; \mathbf{h} \in H_0^{\mathrm{curl}}(\Omega_\varepsilon,\, \mathcal{Z},\, \mathcal{B}) \right\} \tag{2.7}$$

is equivalent to the minimization problem

$$\min\left\{ I_\varepsilon(u) \;\middle|\; u \in H^1(\Omega_\varepsilon) \right\}, \tag{2.8}$$

where

$$I_\varepsilon(u) = \int_{\Omega_\varepsilon} W(\nabla u) \mathrm{d}\mathbf{x} + \sum_{i=1}^{N} \int_{\partial\Omega} u \mathbf{L}\mathbf{k}_i \cdot \mathbf{n}\, \mathrm{d}s - \sum_{i=1}^{N} \sum_{j \neq i} \int_{\partial E_{\varepsilon,i}} u \mathbf{L}\mathbf{k}_j \cdot \mathbf{n}\, \mathrm{d}s \tag{2.9}$$

(here the last integral comes with a minus sign because $\mathbf{n}$ *points outside* $E_{\varepsilon,i}$*, by definition of outer normal). Minimizers* u_ε *of* (2.8) *exist and are solutions of the Neumann problem*

$$\begin{cases} \operatorname{div}(\mathbf{L}\nabla u) = 0 & \text{in } \Omega_\varepsilon, \\ \mathbf{L}\Big(\nabla u + \sum_{i=1}^{N} \mathbf{k}_i\Big) \cdot \mathbf{n} \;= 0 & \text{on } \partial\Omega, \\ \mathbf{L}\Big(\nabla u + \sum_{j \neq i} \mathbf{k}_j\Big) \cdot \mathbf{n} \;= 0 & \text{on } \partial E_{\varepsilon,i},\; i = 1, 2, \ldots, N. \end{cases} \tag{2.10}$$

Proof. Let $\mathbf{h} \in H_0^{\mathrm{curl}}(\Omega_\varepsilon, \mathcal{Z}, \mathcal{B})$. By (2.5a), $\int_\ell (\mathbf{h} - \sum_{i=1}^{N} \mathbf{k}_i) \cdot \mathrm{d}\mathbf{x} = 0$ for any loop $\ell \subset \Omega_\varepsilon$ and thus, $\mathbf{h} - \sum_{i=1}^{N} \mathbf{k}_i = \nabla u$ for some $u \in H^1(\Omega_\varepsilon)$. In turn

$$J_\varepsilon(\mathbf{h}) = \sum_{i=1}^{N} J_\varepsilon(\mathbf{k}_i) + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \int_{\Omega_\varepsilon} \mathbf{L}\mathbf{k}_i \cdot \mathbf{k}_j \mathrm{d}\mathbf{x} + I_\varepsilon(u) \tag{2.11}$$

where $I_\varepsilon(u)$ is given by (2.9) and where in the last sum in the expression for I_ε we omit the terms with $i = j$ because $\mathbf{L}\mathbf{k}_i \cdot \mathbf{n} = 0$ on each $\partial E_{\varepsilon,i}$ (see (2.5c)). Hence, the minimization of J_ε over $\mathbf{h} \in H_0^{\mathrm{curl}}(\Omega_\varepsilon,\, \mathcal{Z},\, \mathcal{B})$ is achieved by minimizing I_ε over $u \in H^1(\Omega_\varepsilon)$.

To show that minimizers solve the Neumann problem (2.10), we compute the first variation of I_ε and apply Stokes's theorem to find that, given $\varphi \in H^1(\Omega_\varepsilon)$,

$$\delta I_\varepsilon(u)[\varphi] = -\int_{\Omega_\varepsilon} \varphi \operatorname{div}(\mathbf{L}\nabla u)\, \mathrm{d}x + \int_{\partial\Omega} \varphi \mathbf{L}\left(\nabla u + \sum_{i=1}^{N} \mathbf{k}_i\right) \cdot \mathbf{n}\, \mathrm{d}s - \sum_{i=1}^{N} \int_{\partial E_{\varepsilon,i}} \varphi \mathbf{L}\left(\nabla u + \sum_{j \neq i} \mathbf{k}_j\right) \cdot \mathbf{n}\, \mathrm{d}s.$$

By requiring that $\delta I_\varepsilon(u)[\varphi] = 0$ for all $\varphi \in H^1(\Omega_\varepsilon)$, we obtain that (2.10) is satisfied. ☐

The following two lemmas are slight adaptations of [CL05, Lemmas 4.2, 4.3], so we do not present the full proofs here. The key tool is an ε-independent Poincaré inequality for Ω_ε, [CL05, Proposition A.2].

Lemma 2.3. *Let* $\varepsilon_0 > 0$ *be fixed as in* (2.1)*. Assume that* $\mathbf{L}$ *is positive definite. Then there exist positive constants* c_1 *and* c_2*, depending only on* $\mathbf{L}$ *and* ε_0 *(in particular, independent of* ε*), such that*

$$I_\varepsilon(u) \geqslant c_1 \|u\|^2_{H^1(\Omega_\varepsilon)} - c_2 \|u\|_{H^1(\Omega_\varepsilon)}. \tag{2.12}$$

for all $u \in H^1(\Omega_\varepsilon)$ *subject to the constraint*

$$\int_{\Omega_{\varepsilon_0}} u(\mathbf{x})\, \mathrm{d}\mathbf{x} = 0. \tag{2.13}$$

Moreover, for every $\varepsilon \in (0, \varepsilon_0)$ the minimization problem (2.8) *admits a unique solution $u_\varepsilon \in H^1(\Omega_\varepsilon)$ satisfying* (2.13)*. Each u_ε satisfies*

$$\|u\|_{H^1(\Omega_\varepsilon)} \leqslant M, \tag{2.14}$$

where $M > 0$ is a constant independent of ε.

Sketch of Proof. Since $\mathbf{L}$ is positive definite, we have

$$I_\varepsilon(u) \geqslant C \int_{\Omega_\varepsilon} |\nabla u|^2 \,\mathrm{d}\mathbf{x} - \sum_{i=1}^{N} \sup_{\mathbf{x}\in\partial\Omega} |\mathbf{L}\mathbf{k}_i(\mathbf{x}, \mathbf{z}_i)| \int_{\partial\Omega} |u_\varepsilon| \,\mathrm{d}s - \sum_{i=1}^{N} \sum_{j\neq i} \sup_{\mathbf{x}\in\partial E_{\varepsilon,i}} |\mathbf{L}\mathbf{k}_j(\mathbf{x}, \mathbf{z}_j)| \int_{\partial E_{\varepsilon,i}} |u_\varepsilon| \,\mathrm{d}s$$

Adapting the proof of [CL05, Proposition A.2], for which (2.13) is crucial, we can find a constant $c_1 = c_1(\lambda, \varepsilon_0)$ such that

$$\int_{\Omega_\varepsilon} |\nabla u|^2 \,\mathrm{d}\mathbf{x} \geqslant c_1 \|u\|^2_{H^1(\Omega_\varepsilon)}. \tag{2.15}$$

Moreover, in [CL05] it is proved that there exist constants C_1, C_2 independent of ε such that

$$\int_{\partial\Omega} |u_\varepsilon| \,\mathrm{d}s \leqslant C_1 \|u_\varepsilon\|_{H^1(\Omega_\varepsilon)}, \quad \text{and} \quad \int_{\partial E_{\varepsilon,i}} |u_\varepsilon| \,\mathrm{d}s \leqslant C_2 \|u_\varepsilon\|_{H^1(\Omega_\varepsilon)}. \tag{2.16}$$

From the definition of $\mathbf{k}_i(\mathbf{x}, \mathbf{z}_i)$ (see (2.4)), it is easy to see that there exist constants $c' = c'(\lambda, \varepsilon_0)$ and $c'' = c''(\lambda, \varepsilon_0)$ such that

$$\sup_{\mathbf{x}\in\partial\Omega} |\mathbf{L}\mathbf{k}_i(\mathbf{x}, \mathbf{z}_i)| < c', \quad \text{and} \quad \sup_{\mathbf{x}\in\partial E_{\varepsilon,i}} |\mathbf{L}\mathbf{k}_j(\mathbf{x}, \mathbf{z}_j)| < c'', \; i \neq j. \tag{2.17}$$

Estimates (2.15), (2.16), and (2.17) prove (2.12). The uniqueness of the solution and the bound (2.14) are straightforward conclusions from the convexity of the functional I_ε and the fact that $I_\varepsilon(0) = 0$. □

Lemma 2.4. *Assume that $\mathbf{L}$ is positive definite, and let u_ε be the unique solution to* (2.8) *that satisfies* (2.13)*. Then, as $\varepsilon \to 0$, the sequence $\{u_\varepsilon\}$ converges strongly in $H^1_{\mathrm{loc}}(\Omega \setminus \mathcal{Z})$ to a solution u_0 of the problem*

$$\min\left\{ I_0(u) \;\middle|\; u \in H^1(\Omega) \right\}, \tag{2.18}$$

where

$$I_0(u) := \int_\Omega W(\nabla u) \,\mathrm{d}\mathbf{x} + \sum_{i=1}^{N} \int_{\partial\Omega} u \, \mathbf{L}\mathbf{k}_i \cdot \mathbf{n} \,\mathrm{d}s.$$

Moreover, $I_\varepsilon(u_\varepsilon) \to I_0(u_0)$.

Sketch of Proof. One can extend u_ε to Ω and obtain an inequality $\|u_\varepsilon\|_{H^1(\Omega)} \leqslant cM$, with M as in (2.14) [CL05, Prop. A.7], which leads to $\int_{\partial E_{\varepsilon,i}} u_\varepsilon \mathbf{L}\mathbf{k}_k \cdot \mathbf{n} \,\mathrm{d}s \to 0$ as $\varepsilon \to 0$. Also, a subsequence (not relabeled) of $\{u_\varepsilon\}$ converges $u_\varepsilon \rightharpoonup u_0$ weakly in $H^1(\Omega)$. Now, if we fix $\delta \in (0, \varepsilon_0)$ and consider $\varepsilon < \delta$, from (2.9) we have

$$I_\varepsilon(u_\varepsilon) \geqslant \int_{\Omega_\delta} W(\nabla u_\varepsilon) \mathrm{d}\mathbf{x} + \sum_{i=1}^{N} \int_{\partial\Omega} u_\varepsilon \mathbf{L}\mathbf{k}_i \cdot \mathbf{n} \,\mathrm{d}s - \sum_{i=1}^{N} \sum_{j\neq i} \int_{\partial E_{\varepsilon,i}} u_\varepsilon \mathbf{L}\mathbf{k}_j \cdot \mathbf{n} \,\mathrm{d}s.$$

Taking $\varepsilon \to 0$ gives $\liminf_{\varepsilon\to 0} I_\varepsilon(u_\varepsilon) \geqslant \int_{\Omega_\delta} W(\nabla u_0) \mathrm{d}\mathbf{x} + \sum_{i=1}^{N} \int_{\partial\Omega} u_0 \mathbf{L}\mathbf{k}_i \cdot \mathbf{n} \,\mathrm{d}s$. Taking $\delta \to 0$ gives $\liminf_{\varepsilon\to 0} I_\varepsilon(u_\varepsilon) \geqslant I_0(u_0)$. But $I_\varepsilon(u_\varepsilon) \leqslant I_\varepsilon(u_0)$, so $\limsup_{\varepsilon\to 0} I_\varepsilon(u_\varepsilon) \leqslant I_0(u_0)$, and $I_\varepsilon(u_\varepsilon) \to I_0(u_0)$. Strong convergence of $u_\varepsilon \to u_0$ in $H^1(\Omega \setminus \mathcal{Z})$ follows from convergence of the energies, see [Eva90]. □

Remark 2.5. The solutions u_0 to (2.18) are also solutions of the Neumann problem

$$\begin{cases} \operatorname{div}(\mathbf{L}\nabla u) = 0 & \text{in } \Omega, \\ \mathbf{L}\Big(\nabla u + \sum_{i=1}^{N} \mathbf{k}_i\Big) \cdot \mathbf{n} \; = 0 & \text{on } \partial\Omega, \end{cases} \tag{2.19}$$

and therefore u_0 can be represented in terms of a Green's function

$$u_0(\mathbf{x}; \mathbf{z}_1, \ldots, \mathbf{z}_N) = \int_{\partial\Omega} G(\mathbf{x}, \mathbf{y}) \mathbf{L} \sum_{i=1}^{N} \mathbf{k}_i(\mathbf{y}; \mathbf{z}_i) \cdot \mathbf{n}(\mathbf{y}) \,\mathrm{d}s(\mathbf{y}), \tag{2.20}$$

exhibiting the explicit dependence on the parameters $\mathbf{z}_1, \ldots, \mathbf{z}_N$. The function $\nabla u_0(\mathbf{x}; \mathbf{z}_1, \ldots, \mathbf{z}_N)$ represents the elastic strain at the point $\mathbf{x} \in \Omega$ due to the presence of $\partial\Omega$ and the dislocations at $\mathbf{z}_i$ with Burgers moduli b_i. For this reason, we refer to $\nabla u_0(\mathbf{x}; \mathbf{z}_1, \ldots, \mathbf{z}_N)$ as the boundary-response strain at $\mathbf{x}$ due to $\mathcal{Z}$.

Combining the results of Lemmas 2.2, 2.3, and 2.4, we conclude the following theorem, which characterizes the strain field associated to a system of dislocations.

Theorem 2.6. *Let $\mathcal{Z}$ and $\mathcal{B}$ be given, and let $\Omega \in \mathbb{R}^2$ be a bounded domain with $\partial\Omega \in C^2$. Then the minimization problem*

$$\min_{\mathbf{h} \in H_0^{\mathrm{curl}}(\Omega_\varepsilon, \mathcal{Z}, \mathcal{B})} \int_{\Omega_\varepsilon} W(\mathbf{h}) \mathrm{d}\mathbf{x}$$

admits a unique solution, $\mathbf{h}_\varepsilon$. Moreover, $\mathbf{h}_\varepsilon \to \mathbf{h}_0$ strongly in $L^2_{\mathrm{loc}}(\Omega \setminus \mathcal{Z})$, where

$$\mathbf{h}_0(\mathbf{x}) = \sum_{i=1}^{N} \mathbf{k}_i(\mathbf{x}; \mathbf{z}_i) + \nabla u_0(\mathbf{x}; \mathbf{z}_1, \ldots, \mathbf{z}_N) \tag{2.21}$$

is a solution of

$$\begin{cases} \operatorname{curl} \mathbf{h} = \sum_{i=1}^{N} \mathbf{b}_i \delta_{\mathbf{z}_i} \\ \operatorname{div} \mathbf{L}\mathbf{h} = 0 \end{cases} \quad \text{in } \Omega,$$

in the sense of distributions, and u_0 is a minimizer of (2.18) *and solves the Neumann problem* (2.19)*.*

2.2. **Alternative form of the fundamental singular strains.** When computing integrals over the cores $E_{R,i}$, we find some computations later in the paper are simplified by using eccentric anomaly centered at $\mathbf{z}_i$

$$\tau_i := \arctan\left(\frac{\tan\theta_i}{\lambda}\right).$$

Using τ, the ellipse $\partial E_{i,R}$ is parametrized by the curve $\rho(\tau_i) = \mathbf{z}_i + (R\cos\tau_i, \lambda R \sin\tau_i)$, so

$$\mathbf{n} = \frac{1}{\sqrt{\lambda^2\cos^2\tau_i + \sin^2\tau_i}} \begin{pmatrix} \lambda\cos\tau_i \\ \sin\tau_i \end{pmatrix}, \quad \mathbf{k}_i(R, \tau_i; \mathbf{z}_i) = \frac{b_\ell}{2\pi\lambda R} \begin{pmatrix} -\lambda\sin\tau_i \\ \cos\tau_i \end{pmatrix}. \tag{2.22}$$

3. The Renormalized Energy

Recall the definition of ε_0 from the beginning of Section 2.

Theorem 3.1. *Let $0 < \varepsilon < \varepsilon_0$ and let $\mathbf{h}_\varepsilon$ be a solution of* (2.7)*. Then*

$$J_\varepsilon(\mathbf{h}_\varepsilon) = \int_{\Omega_\varepsilon} \frac{1}{2}\mathbf{h}_\varepsilon \cdot \mathbf{L}\mathbf{h}_\varepsilon \,\mathrm{d}\mathbf{x} = \sum_{i=1}^{N} \frac{\mu\lambda b_i^2}{4\pi} \log\frac{1}{\varepsilon} + U(\mathbf{z}_1, \ldots, \mathbf{z}_N) + O(\varepsilon), \tag{3.1}$$

where

$$U(\mathbf{z}_1, \ldots, \mathbf{z}_N) := U_S(\mathbf{z}_1, \ldots, \mathbf{z}_N) + U_I(\mathbf{z}_1, \ldots, \mathbf{z}_N) + U_E(\mathbf{z}_1, \ldots, \mathbf{z}_N) \tag{3.2}$$

and, using (2.21)*, for any $\varepsilon < R < \varepsilon_0$*

$$U_S(\mathbf{z}_1, \ldots, \mathbf{z}_N) := \sum_{i=1}^{N} \frac{\mu\lambda b_i^2}{4\pi} \log R + \sum_{i=1}^{N} \int_{\Omega \setminus E_{R,i}} W(\mathbf{k}_i) \,\mathrm{d}\mathbf{x}, \tag{3.3}$$

$$U_I(\mathbf{z}_1, \ldots, \mathbf{z}_N) := \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \int_{\Omega} \mathbf{k}_j \cdot \mathbf{L}\mathbf{k}_i \,\mathrm{d}\mathbf{x},$$

$$U_E(\mathbf{z}_1, \ldots, \mathbf{z}_N) := \int_{\Omega} W(\nabla u_0) \,\mathrm{d}\mathbf{x} + \sum_{i=1}^{N} \int_{\partial\Omega} u_0 \mathbf{L}\mathbf{k}_i \cdot \mathbf{n} \,\mathrm{d}s. \tag{3.4}$$

Remark 3.2. We refer to the energy U in (3.2) as the *renormalized energy.* U_S is the "self" energy associated to the presence of a dislocation, U_I is the energy associated to the interaction between dislocations, and U_E is the energy associated to the elastic medium. Note that Theorem 3.1 asserts that the renormalized energy is independent of ε, and we will show that it can be written in terms of the limit shear $\mathbf{h}_0$ as in Theorem 2.6. This fact will be used in identifying the force on a dislocation in Section 4.

Proof. If we expand $J_\varepsilon(\mathbf{h}_\varepsilon)$ as in (2.11), we see that the three terms on the right side of (2.11) correspond to the terms U_S, U_I, U_E. We begin with $\sum_{i=1}^N J_\varepsilon(\mathbf{k}_i)$ and fix $R \in (\varepsilon, \varepsilon_0)$. Each term in this sum can be written as

$$J_\varepsilon(\mathbf{k}_i) = \int_{\Omega_\varepsilon \setminus E_{R,i}} W(\mathbf{k}_i)\,\mathrm{d}\mathbf{x} \; + \int_{A_{i,R,\varepsilon}} W(\mathbf{k}_i)\,\mathrm{d}\mathbf{x},$$

where $A_{i,R,\varepsilon} := E_{R,i} \setminus E_{\varepsilon,i}$. Using the representation for $\mathbf{k}_i$ in (2.22), we have

$$\int_{A_{i,R,\varepsilon}} \frac{1}{2}\mathbf{k}_i \cdot \mathbf{L}\mathbf{k}_i \,\mathrm{d}\mathbf{x} = \frac{\mu\lambda b_i^2}{4\pi} \log\left(\frac{R}{\varepsilon}\right), \tag{3.5}$$

and this accounts for the $\log \frac{1}{\varepsilon}$ term in the energy (3.1) and the $\log R$ term in (3.3).

To show that

$$\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \int_{\Omega_\varepsilon} \mathbf{k}_j \cdot \mathbf{L}\mathbf{k}_i \,\mathrm{d}\mathbf{x} \longrightarrow \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \int_{\Omega} \mathbf{k}_j \cdot \mathbf{L}\mathbf{k}_i \,\mathrm{d}\mathbf{x} \qquad \text{as} \quad \varepsilon \to 0, \tag{3.6}$$

we note that $\mathbf{k}_i$ is integrable in $E_{R,i}$ (it grows like r_i^{-1}) and $\mathbf{L}\mathbf{k}_j$ is bounded on $E_{R,i}$ for $j \neq i$, hence (3.6) holds by Lebesgue Dominated Convergence Theorem. From Lemma 2.4, we have that $I_\varepsilon(u_\varepsilon) \to I_0(u_0)$ as $\varepsilon \to 0$, whence (3.4) follows.

To show that U is independent of R, we need only show that U_S is independent of R. If we take $R' \neq R$, without loss of generality we can assume $R' < R$, then by (3.5)

$$\int_{\Omega \setminus E_{R',i}} W(\mathbf{k}_i)\,\mathrm{d}\mathbf{x} - \int_{\Omega \setminus E_{R,i}} W(\mathbf{k}_i)\,\mathrm{d}\mathbf{x} = \int_{A_{i,R,R'}} W(\mathbf{k}_i)\,\mathrm{d}\mathbf{x} = \frac{\mu\lambda b_i^2}{4\pi} \log \frac{R}{R'},$$

so that

$$\int_{\Omega \setminus E_{R',i}} W(\mathbf{k}_i)\,\mathrm{d}\mathbf{x} + \frac{\mu\lambda b_i^2}{4\pi} \log R' = \int_{\Omega \setminus E_{R,i}} W(\mathbf{k}_i)\,\mathrm{d}\mathbf{x} + \frac{\mu\lambda b_i^2}{4\pi} \log R,$$

which shows that (3.3) is independent of the choice of $R < \varepsilon_0$. ☐

The renormalized energy U will blow up like the log of the distance between dislocations, i.e. $U \sim -\log|\mathbf{z}_i - \mathbf{z}_j|$. This is made precise in [BFLM14].

4. The Force on a Dislocation

In this section we determine the force $\mathbf{j}_i$ on the dislocation at $\mathbf{z}_i$ for a given a system of dislocations $\mathcal{Z}$ with Burgers vectors $\mathcal{B}$, and show that $\mathbf{j}_i = -\nabla_{\mathbf{z}_i} U$. Following [CG99], the Peach-Köhler force on the dislocation at $\mathbf{z}_i$ (also called the net configurational traction) is given by

$$\mathbf{j}_i := \lim_{R \to 0} \int_{\partial E_{R,i}} \mathbf{C}\mathbf{n}\,\mathrm{d}s, \tag{4.1}$$

where the stress tensor is the Eshelby stress ([Esh51, Gur95])

$$\mathbf{C} := W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0). \tag{4.2}$$

Here $\mathbf{I}$ is the identity matrix and $\mathbf{h}_0$ is defined in (2.21).

Theorem 4.1. *Let $\mathbf{h}_0$ be the limiting singular strain defined by* (2.21) *and let U the associated renormalized energy given in* (3.2). *Then for $\ell \in \{1, \ldots, N\}$ and any $R \in (0, \varepsilon_0)$*

$$\nabla_{\mathbf{z}_\ell} U(\mathbf{z}_1, \ldots, \mathbf{z}_N) = -\int_{\partial E_{R,\ell}} \{W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)\}\,\mathbf{n}\,\mathrm{d}s, \tag{4.3}$$

and so the force on the dislocation at $\mathbf{z}_\ell$ is given by

$$\mathbf{j}_\ell = -\nabla_{\mathbf{z}_\ell} U. \tag{4.4}$$

Moreover,

$$\mathbf{j}_\ell(\mathbf{z}_1, \ldots, \mathbf{z}_N) = b_\ell \mathbf{J}\mathbf{L}\left(\nabla u_0(\mathbf{z}_\ell; \mathbf{z}_1, \ldots, \mathbf{z}_N) + \sum_{i \neq \ell} \mathbf{k}_i(\mathbf{z}_\ell; \mathbf{z}_i)\right), \quad \text{where} \quad \mathbf{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{4.5}$$

and u_0 is the solution to (2.19).

Proof. Formula (4.3) is proved in the Appendix. From (4.3), we show (4.4) and (4.5) as follows. Recall that the renormalized energy is independent of $R < \varepsilon_0$ (see the proof of Theorem 3.1), so

$$-\nabla_{\mathbf{z}_\ell} U = \int_{\partial E_{R,\ell}} \mathbf{C}\mathbf{n}\,\mathrm{d}s = \lim_{R\to 0}\int_{\partial E_{R,\ell}} \mathbf{C}\mathbf{n}\,\mathrm{d}s = \mathbf{j}_\ell, \tag{4.6}$$

establishing (4.4) in view of (4.1).

The field $\mathbf{h}_0$ has a singularity at $\mathbf{z}_\ell$ which comes from the term $\mathbf{k}_\ell$ (see (2.21)), and we decompose $\mathbf{h}_0$ into the *singular part at* $\mathbf{z}_\ell$ and the *regular part at* $\mathbf{z}_\ell$,

$$\mathbf{h}_0(\mathbf{x}) = \mathbf{k}_\ell(\mathbf{x};\mathbf{z}_\ell) + \widetilde{\mathbf{h}}(\mathbf{x}), \qquad \text{where } \widetilde{\mathbf{h}}(\mathbf{x}) := \nabla u_0(\mathbf{x}) + \sum_{i\neq\ell}\mathbf{k}_i(\mathbf{x};\mathbf{z}_i). \tag{4.7}$$

Using (4.7), we write the Eshelby stress $\mathbf{C}$ from (4.2) as

$$\mathbf{C} = \left(\frac{1}{2}\mathbf{k}_\ell\cdot\mathbf{L}\mathbf{k}_\ell + \mathbf{k}_\ell\cdot\mathbf{L}\widetilde{\mathbf{h}} + \frac{1}{2}\widetilde{\mathbf{h}}\cdot\mathbf{L}\widetilde{\mathbf{h}}\right)\mathbf{I} - \mathbf{k}_\ell\otimes(\mathbf{L}\mathbf{k}_\ell) - \mathbf{k}_\ell\otimes(\mathbf{L}\widetilde{\mathbf{h}}) - \widetilde{\mathbf{h}}\otimes(\mathbf{L}\mathbf{k}_\ell) - \widetilde{\mathbf{h}}\otimes(\mathbf{L}\widetilde{\mathbf{h}}).$$

Since $\widetilde{\mathbf{h}}$ is smooth and bounded on $\overline{E}_{R,\ell}$ we have

$$\lim_{R\to 0}\int_{\partial E_{R,\ell}}\left(\frac{1}{2}\widetilde{\mathbf{h}}\cdot\mathbf{L}\widetilde{\mathbf{h}}\right)\mathbf{n}\,\mathrm{d}s = 0 \quad \text{and} \quad \lim_{R\to 0}\int_{\partial E_{R,\ell}}\widetilde{\mathbf{h}}\otimes(\mathbf{L}\widetilde{\mathbf{h}})\mathbf{n}\,\mathrm{d}s = 0.$$

Using the fact that $\mathbf{L}\mathbf{k}_\ell\cdot\mathbf{n} = 0$ on $\partial E_{R,\ell}$ (see (2.5c)) we have

$$\int_{\partial E_{R,\ell}}\widetilde{\mathbf{h}}\otimes(\mathbf{L}\mathbf{k}_\ell)\,\mathbf{n}\,\mathrm{d}s = 0, \quad \text{and} \quad \int_{\partial E_{R,\ell}}\mathbf{k}_\ell\otimes(\mathbf{L}\mathbf{k}_\ell)\,\mathbf{n}\,\mathrm{d}s = 0, \quad \forall R < \bar{R}.$$

Using (2.22) we have $\mathbf{k}_\ell\cdot\mathbf{L}\mathbf{k}_\ell = \mu b_\ell^2/(4\pi^2R^2)$ on $\partial E_{R,\ell}$, and so

$$\int_{\partial E_{R,\ell}}\frac{1}{2}(\mathbf{k}_\ell\cdot\mathbf{L}\mathbf{k}_\ell)\mathbf{n}\,\mathrm{d}s = \frac{\mu b_\ell^2}{8\pi^2R^2}\int_{\partial E_{R,\ell}}\mathbf{n}\,\mathrm{d}s = 0,$$

for all $R < \varepsilon_0$. Therefore the only contribution in (4.6) will come from

$$\left(\left(\mathbf{k}_\ell\cdot\mathbf{L}\widetilde{\mathbf{h}}\right)\mathbf{I} - \mathbf{k}_\ell\otimes(\mathbf{L}\widetilde{\mathbf{h}})\right)\mathbf{n} = (\mathbf{n}\otimes\mathbf{k}_\ell)\,\mathbf{L}\widetilde{\mathbf{h}} - (\mathbf{k}_\ell\otimes\mathbf{n})\,\mathbf{L}\widetilde{\mathbf{h}}.$$

Now, using (2.22), it is easy to see that

$$\mathbf{n}\otimes\mathbf{k}_\ell - \mathbf{k}_\ell\otimes\mathbf{n} = \frac{b_\ell}{2\pi\lambda R\sqrt{\lambda^2\cos^2\tau + \sin^2\tau}}\begin{pmatrix} 0 & \lambda \\ -\lambda & 0 \end{pmatrix}$$

and, since $\mathrm{d}s = R\sqrt{\lambda^2\cos^2\tau + \sin^2\tau}\,\mathrm{d}\tau$,

$$\int_{\partial E_{R,\ell}}(\mathbf{n}\otimes\mathbf{k}_\ell - \mathbf{k}_\ell\otimes\mathbf{n})\,\mathbf{L}\widetilde{\mathbf{h}}\,\mathrm{d}s = \frac{b_\ell}{2\pi}\int_0^{2\pi}\mathbf{J}\mathbf{L}\widetilde{\mathbf{h}}\,\mathrm{d}\tau.$$

Since the integrand is smooth on $E_{R,\ell}$, we conclude that

$$\lim_{R\to 0}\int_{\partial E_{R,\ell}}(\mathbf{n}\otimes\mathbf{k}_\ell - \mathbf{k}_\ell\otimes\mathbf{n})\,\mathbf{L}\widetilde{\mathbf{h}}\,\mathrm{d}s = \frac{b_\ell}{2\pi}\int_0^{2\pi}\mathbf{J}\mathbf{L}\widetilde{\mathbf{h}}(\mathbf{z}_\ell)\,\mathrm{d}\tau = b_\ell\mathbf{J}\mathbf{L}\widetilde{\mathbf{h}}(\mathbf{z}_\ell),$$

which, in view of (4.6), establishes (4.5). □

Remark 4.2. The formula (4.5) gives the force on the dislocation at $\mathbf{z}_\ell$, and it shows that, as a function of $\mathbf{z}_\ell$, the force $\mathbf{j}_\ell$ is smooth in the interior of $\Omega\setminus\{\mathbf{z}_1,\ldots,\mathbf{z}_{\ell-1},\mathbf{z}_{\ell+1},\ldots,\mathbf{z}_N\}$. That is, provided $\mathbf{z}_\ell$ is not colliding with another dislocation or with $\partial\Omega$, then the force is given by a smooth function. Of course, $\mathbf{j}_\ell$ depends on the positions of *all* the dislocations, and the same reasoning applies to $\mathbf{j}_\ell$ as a function of any $\mathbf{z}_i$.

Remark 4.3. We find agreement between (4.5) and equation (8.18) from [CG99], where the force on $\mathbf{z}_\ell$ is given by b_ℓ times a $\pi/2$-rotation of the regular part of the strain at $\mathbf{z}_\ell$ (i.e., $\widetilde{\mathbf{h}}$). Since we have a formula for the regular part, we are able to write the Peach-Köhler force more explicitly (in terms of the solution to (2.19)). We have also shown that assumption (A3) from [CG99] holds for screw dislocations, validating the derivation of (8.18) in [CG99].

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5. APPENDIX

We present the proof of (4.3) along with some necessary lemmas. We begin by noting that $U(\mathbf{z}_1,\dots,\mathbf{z}_N) = \widehat{U}(\mathbf{z}_1,\dots,\mathbf{z}_N) + \overline{U}(\mathbf{z}_1,\dots,\mathbf{z}_N)$ where

$$\begin{aligned}\widehat{U}(\mathbf{z}_1,\dots,\mathbf{z}_N) &= \int_{\Omega_\varepsilon} W(\mathbf{h}_0)\,\mathrm{d}\mathbf{x},\\ \overline{U}(\mathbf{z}_1,\dots,\mathbf{z}_N) &= \sum_{i=1}^{N}\sum_{m\neq i}\int_{E_{\varepsilon,m}} W(\mathbf{k}_i)\,\mathrm{d}\mathbf{x} + \sum_{m=1}^{N}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\int_{E_{\varepsilon,m}} \mathbf{k}_j\cdot\mathbf{L}\mathbf{k}_i\,\mathrm{d}\mathbf{x} + \\ &\qquad + \sum_{m=1}^{N}\int_{E_{\varepsilon,m}} W(\nabla u_0)\,\mathrm{d}\mathbf{x} + \sum_{m=1}^{N}\sum_{i=1}^{N}\int_{\partial E_{\varepsilon,m}} u_0\mathbf{L}\mathbf{k}_i\cdot\mathbf{n}\,\mathrm{d}s, \end{aligned} \tag{5.1}$$

which follows from a direct computation and integration by parts to eliminate the integral over $\partial\Omega$ from U_E.

We introduce the notation $D_\ell^{\mathbf{v}}u$ for the derivative of a function $u = u(\mathbf{x};\mathbf{z}_1,\dots,\mathbf{z}_N)$ with respect to the ℓ-th dislocation location in the direction $\mathbf{v}$,

$$D_\ell^{\mathbf{v}}u(\mathbf{x}) := \frac{\mathrm{d}}{\mathrm{d}\xi}u(\mathbf{x};\mathbf{z}_1,\dots,\mathbf{z}_\ell+\xi\mathbf{v},\dots,\mathbf{z}_N)\Big|_{\xi=0}.$$

Lemma 5.1. *The fields* $\mathbf{k}_i(\mathbf{x};\mathbf{z}_i)$, $u_0(\mathbf{x};\mathbf{z}_1,\dots,\mathbf{z}_N)$, *and* $\mathbf{h}_0(\mathbf{x};\mathbf{z}_1,\dots,\mathbf{z}_N)$ *are smooth with respect to* $\mathbf{z}_\ell$ *for every* $\ell\in\{1,\dots,N\}$. *Moreover,* $D_\ell^{\mathbf{v}}\mathbf{k}_i(\mathbf{x}) = 0$ *if* $\ell\neq i$,

$$D_\ell^{\mathbf{v}}\mathbf{k}_\ell(\mathbf{x}) = -D\mathbf{k}_\ell(\mathbf{x})\mathbf{v} = -\nabla\left(\mathbf{k}_\ell(\mathbf{x})\cdot\mathbf{v}\right) \tag{5.2}$$

$$D_\ell^{\mathbf{v}}\mathbf{h}_0(\mathbf{x}) = \nabla w(\mathbf{x}), \quad \text{where} \quad w(\mathbf{x}) = D_\ell^{\mathbf{v}}u_0(\mathbf{x}) - \mathbf{k}_\ell(\mathbf{x})\cdot\mathbf{v} \tag{5.3}$$

Proof. The form of $\mathbf{k}$ in (2.4) shows that $\mathbf{k}_i$ is smooth with respect to $\mathbf{z}_\ell$ for all $i,\ell = 1,\dots,N$, and in particular that $\mathbf{k}_i(\mathbf{x}) = \mathbf{k}(\mathbf{x};\mathbf{z}_i)$ is independent of $\mathbf{z}_\ell$ if $\ell\neq i$ so $D_\ell^{\mathbf{v}}\mathbf{k}_i = 0$. That form also shows that $\mathbf{k}(\mathbf{x};\mathbf{z}_\ell+\xi\mathbf{v}) = \mathbf{k}(\mathbf{x}-\xi\mathbf{v};\mathbf{z}_\ell) = \mathbf{k}_\ell(\mathbf{x}-\xi\mathbf{v})$ so that $D_\ell^{\mathbf{v}}\mathbf{k}_\ell(\mathbf{x}) = -(D\mathbf{k}_\ell)\mathbf{v}$, where $D\mathbf{k}_\ell$ is the derivative of $\mathbf{k}_\ell$ with respect to $\mathbf{x}$. Now because $\operatorname{curl}\mathbf{k}_\ell = 0$, we have $D\mathbf{k}_\ell(\mathbf{x})\mathbf{v} = \nabla\left(\mathbf{k}_\ell(\mathbf{x})\cdot\mathbf{v}\right)$, which establishes (5.2).

Since u_0 solves the elliptic problem (2.19), it can be represented as in (2.20), in terms of the Green's function $G(\mathbf{x},\mathbf{y})$. The smoothness of u_0 in $\mathbf{z}_\ell$ follows from the smoothness of $\mathbf{k}_i$ for each $i,\ell = 1,\dots,N$. Hence, $\mathbf{h}_0$ is smooth in $\mathbf{z}_\ell$ and $D_\ell^{\mathbf{v}}\mathbf{h}_0 = D_\ell^{\mathbf{v}}\nabla u_0 + D_\ell^{\mathbf{v}}\mathbf{k}_\ell = \nabla(D_\ell^{\mathbf{v}}u_0 - \mathbf{k}_\ell\cdot\mathbf{v})$, which establishes (5.3). □

We will take derivatives of the energy with respect to the dislocations positions. This will involve integrals over cores that are centered at $\mathbf{z}_\ell + \xi\mathbf{v}$ whose integrands are evaluated on these shifted cores or on their complements in Ω. Thus, we will need to be able to take derivatives of integrals over sets that depend on ξ and whose integrands are functions that depend on ξ.

Lemma 5.2. *Let* $f = f(\mathbf{x},\xi)$, $g = g(\mathbf{x},\xi)$, *and* $r = r(\mathbf{x},\xi)$ *be defined on* $E_\varepsilon(\mathbf{x}_0+\xi\mathbf{v})$, $\partial E_\varepsilon(\mathbf{x}_0+\xi\mathbf{v})$, *and* $\Omega\setminus E_\varepsilon(\mathbf{x}_0+\xi\mathbf{v})$, *respectively, for* ξ *a real parameter,* $\varepsilon > 0$, $\mathbf{v}\in\mathbb{R}^2$. *Then*

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\xi}\int_{E_\varepsilon(\mathbf{x}_0+\xi\mathbf{v})} f(\mathbf{x},\xi)\,\mathrm{d}\mathbf{x}\bigg|_{\xi=0} &= \int_{E_\varepsilon(\mathbf{x}_0)} D_\xi f(\mathbf{x},0)\,\mathrm{d}\mathbf{x} \\
&= \int_{E_\varepsilon(\mathbf{x}_0)} \partial_\xi f(\mathbf{x},0)\,\mathrm{d}\mathbf{x} + \int_{\partial E_\varepsilon(\mathbf{x}_0)} f(\mathbf{x},0)\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}s, && (5.4) \\
\frac{\mathrm{d}}{\mathrm{d}\xi}\int_{\partial E_\varepsilon(\mathbf{x}_0+\xi\mathbf{v})} g(\mathbf{x},\xi)\,\mathrm{d}s\bigg|_{\xi=0} &= \int_{\partial E_\varepsilon(\mathbf{x}_0)} D_\xi g(\mathbf{x},0)\,\mathrm{d}s, && (5.5) \\
\frac{\mathrm{d}}{\mathrm{d}\xi}\int_{\Omega\setminus E_\varepsilon(\mathbf{x}_0+\xi\mathbf{v})} r(\mathbf{x},\xi)\,\mathrm{d}\mathbf{x}\bigg|_{\xi=0} &= \int_{\Omega\setminus E_\varepsilon(\mathbf{x}_0)} \partial_\xi r(\mathbf{x},0)\,\mathrm{d}\mathbf{x} - \int_{\partial E_\varepsilon(\mathbf{x}_0)} r(\mathbf{x},0)\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}s, && (5.6)
\end{aligned}$$

where $D_\xi f := \partial_\xi f + \nabla f\cdot\mathbf{v}$.

Proof. We compute

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\int_{E_\varepsilon(\mathbf{x}_0+\xi\mathbf{v})} f(\mathbf{x},\xi)\mathrm{d}\mathbf{x} = \frac{\mathrm{d}}{\mathrm{d}\xi}\int_{E_\varepsilon(\mathbf{x}_0)} f(\mathbf{x}+\xi\mathbf{v},\xi)\mathrm{d}\mathbf{x} = \int_{E_\varepsilon(\mathbf{x}_0)} (\partial_\xi f(\mathbf{x}+\xi\mathbf{v},\xi) + \nabla f(\mathbf{x}+\xi\mathbf{v},\xi)\cdot\mathbf{v})\mathrm{d}\mathbf{x}.$$

If we send $\xi\to 0$ and apply the divergence theorem we obtain (5.4). A similar computation gives (5.5) but the divergence theorem is not applied. If $\hat{r}$ is a smooth extension of r to Ω then

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\xi}\int_{\Omega\setminus E_\varepsilon(\mathbf{x}_0+\xi\mathbf{v})} r(\mathbf{x},\xi)\mathrm{d}\mathbf{x} &= \frac{\mathrm{d}}{\mathrm{d}\xi}\int_\Omega \hat{r}(\mathbf{x},\xi)\mathrm{d}\mathbf{x} - \frac{\mathrm{d}}{\mathrm{d}\xi}\int_{E_\varepsilon(\mathbf{x}_0+\xi\mathbf{v})} \hat{r}(\mathbf{x},\xi)\mathrm{d}\mathbf{x} \\
&= \int_\Omega \partial_\xi\hat{r}(\mathbf{x},\xi)\mathrm{d}\mathbf{x} - \int_{E_\varepsilon(\mathbf{x}_0)} \partial_\xi\hat{r}(\mathbf{x}+\xi\mathbf{v},\xi)\mathrm{d}\mathbf{x} - \int_{\partial E_\varepsilon(\mathbf{x}_0)} \hat{r}(\mathbf{x}+\xi\mathbf{v},\xi)\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}s.
\end{aligned}$$

Setting $\xi = 0$ and combining the first two integrals on the right side yields (5.6). □

Remark 5.3. Lemma 5.2 applies to the vector-valued $\mathbf{k}_i$. When applying Lemma 5.2 to integrals of $\mathbf{k}(\mathbf{x};\mathbf{z}_\ell+\xi\mathbf{v})$ over $E_\varepsilon(\mathbf{z}_\ell+\xi\mathbf{v})$ we will get cancellations from

$$D_\xi\mathbf{k}(\mathbf{x};\mathbf{z}_\ell+\xi\mathbf{v}) = \partial_\xi\mathbf{k}(\mathbf{x};\mathbf{z}_\ell+\xi\mathbf{v}) + D\mathbf{k}(\mathbf{x};\mathbf{z}_\ell+\xi\mathbf{v})\mathbf{v} = D_\ell^{\mathbf{v}}\mathbf{k}_\ell(\mathbf{x}) + D\mathbf{k}_\ell\mathbf{v} = 0. \tag{5.7}$$

The last equality follows from (5.2).

Proof of Equation (4.3). The $-\log\varepsilon$ term in the energy is independent of the positions of the dislocations so it vanishes upon taking the derivative of the energy with respect to $\mathbf{z}_\ell$. To compute the derivative of U with respect to $\mathbf{z}_\ell$ will split $\nabla_{\mathbf{z}_\ell}U$ into $\nabla_{\mathbf{z}_\ell}\widehat{U} + \nabla_{\mathbf{z}_\ell}\overline{U}$. To compute $\nabla_{\mathbf{z}_\ell}\widehat{U}$ we apply (5.6) to get

$$\nabla_{\mathbf{z}_\ell}\widehat{U} = D_\ell^{\mathbf{v}}\left(\int_{\Omega_\varepsilon} W(\mathbf{h}_0)\mathrm{d}\mathbf{x}\right) = \int_{\Omega_\varepsilon} D_\ell^{\mathbf{v}}\mathbf{h}_0\cdot\mathbf{L}\mathbf{h}_0\,\mathrm{d}\mathbf{x} - \int_{\partial E_{\varepsilon,\ell}} W(\mathbf{h}_0)\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}s \tag{5.8}$$

Using (5.3), $\operatorname{div}(\mathbf{L}\mathbf{h}_0) = 0$ in Ω, and $\mathbf{L}\mathbf{h}_0\cdot\mathbf{n} = 0$ on $\partial\Omega$, we have

$$\begin{aligned}
\int_{\Omega_\varepsilon} D_\ell^{\mathbf{v}}\mathbf{h}_0\cdot\mathbf{L}\mathbf{h}_0\,\mathrm{d}\mathbf{x} &= \int_{\Omega_\varepsilon} \nabla(D_\ell^{\mathbf{v}}u_0 - \mathbf{k}_\ell\cdot\mathbf{v})\cdot\mathbf{L}\mathbf{h}_0\,\mathrm{d}\mathbf{x} = \int_{\partial\Omega_\varepsilon} (D_\ell^{\mathbf{v}}u_0 - \mathbf{k}_\ell\cdot\mathbf{v})\mathbf{L}\mathbf{h}_0\cdot\mathbf{n}\,\mathrm{d}s \\
&= -\sum_{j=1}^{N}\int_{\partial E_{\varepsilon,j}} (D_\ell^{\mathbf{v}}u_0 - \mathbf{k}_\ell\cdot\mathbf{v})\mathbf{L}\mathbf{h}_0\cdot\mathbf{n}\,\mathrm{d}s = -\sum_{j=1}^{N}\int_{\partial E_{\varepsilon,j}} w\mathbf{L}\mathbf{h}_0\cdot\mathbf{n}\,\mathrm{d}s
\end{aligned} \tag{5.9}$$

using the notation $w = D_\ell^{\mathbf{v}} u_0 - \mathbf{k}_\ell \cdot \mathbf{v}$ from (5.3). Combining (5.8) and (5.9), and adding and subtracting $\mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)\mathbf{n} \cdot \mathbf{v}$ from the integrand, we have

$$\begin{aligned}
\nabla_{\mathbf{z}_\ell} \widehat{U} &= -\sum_{j=1}^{N} \int_{\partial E_{\varepsilon,j}} (D_\ell^{\mathbf{v}} u_0 - \mathbf{k}_\ell \cdot \mathbf{v}) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n} \,\mathrm{d}s - \int_{\partial E_{\varepsilon,\ell}} W(\mathbf{h}_0) \mathbf{v} \cdot \mathbf{n} \,\mathrm{d}s \\
&= -\int_{\partial E_{\varepsilon,\ell}} \{W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)\} \,\mathbf{n} \cdot \mathbf{v} \,\mathrm{d}s - \sum_{j \neq \ell} \int_{\partial E_{\varepsilon,j}} (D_\ell^{\mathbf{v}} u_0 - \mathbf{k}_\ell \cdot \mathbf{v}) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n} \,\mathrm{d}s \,+ \\
&\qquad - \int_{\partial E_{\varepsilon,\ell}} [(D_\ell^{\mathbf{v}} u_0 - \mathbf{k}_\ell \cdot \mathbf{v}) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n} + \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)\mathbf{n} \cdot \mathbf{v}] \,\mathrm{d}s;
\end{aligned}$$

also, $\mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)\mathbf{n} \cdot \mathbf{v} = (\mathbf{h}_0 \cdot \mathbf{v})(\mathbf{L}\mathbf{h}_0 \cdot \mathbf{n}) = (\nabla u_0 \cdot \mathbf{v} + \sum_{i=1}^{N} \mathbf{k}_i \cdot \mathbf{v})(\mathbf{L}\mathbf{h}_0 \cdot \mathbf{n})$, so

$$\begin{aligned}
(D_\ell^{\mathbf{v}} u_0 - \mathbf{k}_\ell \cdot \mathbf{v}) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n} + \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)\mathbf{n} \cdot \mathbf{v} &= \left(D_\ell^{\mathbf{v}} u_0 - \mathbf{k}_\ell \cdot \mathbf{v} + \nabla u_0 \cdot \mathbf{v} + \sum_{i=1}^{N} \mathbf{k}_i \cdot \mathbf{v} \right) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n} \\
&= \left(D_\xi u_0 + \sum_{i \neq \ell} \mathbf{k}_i \cdot \mathbf{v} \right) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n}
\end{aligned}$$

where $D_\xi u_0 = D_\ell^{\mathbf{v}} u_0 + \nabla u_0 \cdot \mathbf{v}$. Hence,

$$\begin{aligned}
\nabla_{\mathbf{z}_\ell} \widehat{U} &= -\int_{\partial E_{\varepsilon,\ell}} \{W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)\} \,\mathbf{n} \cdot \mathbf{v} \,\mathrm{d}s \\
&\quad - \sum_{j \neq \ell} \int_{\partial E_{\varepsilon,j}} (D_\ell^{\mathbf{v}} u_0 - \mathbf{k}_\ell \cdot \mathbf{v}) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n} \,\mathrm{d}s - \int_{\partial E_{\varepsilon,\ell}} \left(D_\xi u_0 + \sum_{i \neq \ell} \mathbf{k}_i \cdot \mathbf{v} \right) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n} \,\mathrm{d}s
\end{aligned} \tag{5.10}$$

We compute $\nabla_{\mathbf{z}_\ell} \overline{U}$ in several steps. We split the first sum in the right side of (5.1) into the integral over $E_{\varepsilon,\ell}$ and the rest of the terms

$$\sum_{i=1}^{N} \sum_{m \neq i} \int_{E_{\varepsilon,m}} W(\mathbf{k}_i) \mathrm{d}\mathbf{x} = \int_{E_{\varepsilon,\ell}} \sum_{m \neq \ell} W(\mathbf{k}_m) \mathrm{d}\mathbf{x} + \sum_{m \neq \ell} \int_{E_{\varepsilon,m}} \sum_{i \neq m} W(\mathbf{k}_i) \mathrm{d}\mathbf{x}. \tag{5.11}$$

In the first of these, each $\mathbf{k}_m$ does not vary as $\mathbf{z}_\ell \to \mathbf{z}_\ell + \xi \mathbf{v}$ because $m \neq \ell$. Hence we apply (5.4) directly with $D_\xi \mathbf{k}_m = \partial_\xi \mathbf{k}_m + D_\ell^{\mathbf{v}} \mathbf{k}_m = \nabla(\mathbf{k}_m \cdot \mathbf{v})$ because $\partial_\xi \mathbf{k}_m = 0$. We have

$$\begin{aligned}
D_\ell^{\mathbf{v}} \left(\sum_{m \neq \ell} \int_{E_{\varepsilon,\ell}} W(\mathbf{k}_m) \,\mathrm{d}\mathbf{x} \right) &= \sum_{m \neq \ell} \int_{E_{\varepsilon,\ell}} D_\xi \mathbf{k}_m \cdot \mathbf{L}\mathbf{k}_m \,\mathrm{d}\mathbf{x} = \sum_{m \neq \ell} \int_{E_{\varepsilon,\ell}} \nabla(\mathbf{k}_m \cdot \mathbf{v}) \cdot \mathbf{L}\mathbf{k}_m \,\mathrm{d}\mathbf{x} \\
&= \int_{\partial E_{\varepsilon,\ell}} \sum_{m \neq \ell} (\mathbf{k}_m \cdot \mathbf{v}) \mathbf{L}\mathbf{k}_m \cdot \mathbf{n} \,\mathrm{d}s,
\end{aligned} \tag{5.12}$$

where we used $\operatorname{div}(\mathbf{L}\mathbf{k}_m) = 0$.

The second term from (5.11) involves integrals over $E_{\varepsilon,m}$ for $m \neq \ell$, so these domains do not move as $\mathbf{z}_\ell \to \mathbf{z}_\ell + \xi \mathbf{v}$. Also, the terms $W(\mathbf{k}_i)$ for $i \neq \ell$ vanish when we apply $D_\ell^{\mathbf{v}}$, so

$$\begin{aligned}
D_\ell^{\mathbf{v}} \left(\sum_{m \neq \ell} \int_{E_{\varepsilon,m}} \sum_{i \neq m} W(\mathbf{k}_i) \,\mathrm{d}\mathbf{x} \right) &= \sum_{m \neq \ell} \int_{E_{\varepsilon,m}} D_\ell^{\mathbf{v}} \mathbf{k}_\ell \cdot \mathbf{L}\mathbf{k}_\ell \,\mathrm{d}\mathbf{x} = \sum_{m \neq \ell} \int_{E_{\varepsilon,m}} -\nabla(\mathbf{k}_\ell \cdot \mathbf{v}) \cdot \mathbf{L}\mathbf{k}_\ell \,\mathrm{d}\mathbf{x} \\
&= -\sum_{m \neq \ell} \int_{\partial E_{\varepsilon,m}} (\mathbf{k}_\ell \cdot \mathbf{v}) \mathbf{L}\mathbf{k}_\ell \cdot \mathbf{n} \,\mathrm{d}s,
\end{aligned} \tag{5.13}$$

where we used (5.2) and $\operatorname{div}(\mathbf{L}\mathbf{k}_\ell) = 0$.

The second sum from (5.1) is split into the integral over $E_{\varepsilon,\ell}$ and the rest of the terms

$$\sum_{m=1}^{N}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\int_{E_{\varepsilon,m}}\mathbf{k}_j\cdot\mathbf{L}\mathbf{k}_i\,\mathrm{d}\mathbf{x}=\int_{E_{\varepsilon,\ell}}\sum_{i<j}\mathbf{k}_j\cdot\mathbf{L}\mathbf{k}_i\,\mathrm{d}\mathbf{x}+\sum_{m\neq\ell}\int_{E_{\varepsilon,m}}\sum_{i<j}\mathbf{k}_j\cdot\mathbf{L}\mathbf{k}_i\,\mathrm{d}\mathbf{x}. \tag{5.14}$$

Applying (5.4) to the first term on the right side yields

$$\begin{aligned}D_\ell^{\mathbf{v}}\left(\int_{E_{\varepsilon,\ell}}\sum_{i<j}\mathbf{k}_j\cdot\mathbf{L}\mathbf{k}_i\,\mathrm{d}\mathbf{x}\right)&=\int_{E_{\varepsilon,\ell}}\sum_{i<j}D_\xi\mathbf{k}_j\cdot\mathbf{L}\mathbf{k}_i+D_\xi\mathbf{k}_i\cdot\mathbf{L}\mathbf{k}_j\,\mathrm{d}\mathbf{x}\\&=\int_{E_{\varepsilon,\ell}}\sum_{i,j\neq\ell,i<j}\nabla(\mathbf{k}_j\cdot\mathbf{v})\cdot\mathbf{L}\mathbf{k}_i+\nabla(\mathbf{k}_i\cdot\mathbf{v})\cdot\mathbf{L}\mathbf{k}_j\,\mathrm{d}\mathbf{x}\\&=\sum_{i\neq\ell}\sum_{j\neq i}\int_{E_{\varepsilon,\ell}}\nabla(\mathbf{k}_j\cdot\mathbf{v})\cdot\mathbf{L}\mathbf{k}_i\,\mathrm{d}\mathbf{x}=\sum_{i\neq\ell}\sum_{j\neq i}\int_{\partial E_{\varepsilon,\ell}}(\mathbf{k}_j\cdot\mathbf{v})\cdot\mathbf{L}\mathbf{k}_i\cdot\mathbf{n}\,\mathrm{d}s\end{aligned} \tag{5.15}$$

Between the first and second lines we used $D_\xi\mathbf{k}_i=\nabla(\mathbf{k}_i\cdot\mathbf{v})$ for $i\neq\ell$ and $D_\xi\mathbf{k}_\ell=0$ by (5.7), and in the third line we used $\operatorname{div}(\mathbf{L}\mathbf{k}_i)=0$.

For the second sum of (5.14), using (5.2) from Lemma 5.1, we have

$$\begin{aligned}D_\ell^{\mathbf{v}}\left(\sum_{m\neq\ell}\int_{E_{\varepsilon,m}}\sum_{i<j}\mathbf{k}_j\cdot\mathbf{L}\mathbf{k}_i\,\mathrm{d}\mathbf{x}\right)&=\sum_{m\neq\ell}\sum_{i\neq\ell}\int_{E_{\varepsilon,m}}D_\ell^{\mathbf{v}}\mathbf{k}_\ell\cdot\mathbf{L}\mathbf{k}_i\,\mathrm{d}\mathbf{x}=-\sum_{m\neq\ell}\sum_{i\neq\ell}\int_{E_{\varepsilon,m}}\nabla(\mathbf{k}_\ell\cdot\mathbf{v})\cdot\mathbf{L}\mathbf{k}_i\,\mathrm{d}\mathbf{x}\\&=-\sum_{m\neq\ell}\sum_{i\neq\ell}\int_{\partial E_{\varepsilon,m}}(\mathbf{k}_\ell\cdot\mathbf{v})\mathbf{L}\mathbf{k}_i\cdot\mathbf{n}\,\mathrm{d}s\end{aligned} \tag{5.16}$$

The third term comprising $\overline{U}$ in (5.1) is split as

$$\sum_{m=1}^{N}\int_{E_{\varepsilon,m}}W(\nabla u_0)\,\mathrm{d}\mathbf{x}=\int_{E_{\varepsilon,\ell}}W(\nabla u_0)\,\mathrm{d}\mathbf{x}+\sum_{m\neq\ell}\int_{E_{\varepsilon,m}}W(\nabla u_0)\,\mathrm{d}\mathbf{x}. \tag{5.17}$$

To compute the derivative of the first term on the right side of (5.17), we use (5.4), but integrate the D_ξ term by parts directly. Using $D_\xi u_0=D_\ell^{\mathbf{v}}u_0+\nabla u_0\cdot\mathbf{v}$ and $\operatorname{div}(\mathbf{L}\nabla u_0)=0$ we have

$$\begin{aligned}D_\ell^{\mathbf{v}}\left(\int_{E_{\varepsilon,\ell}}W(\nabla u_0)\,\mathrm{d}\mathbf{x}\right)&=\int_{E_{\varepsilon,\ell}}\nabla(D_\xi u_0)\mathbf{L}\nabla u_0\,\mathrm{d}\mathbf{x}=\int_{\partial E_{\varepsilon,\ell}}(D_\xi u_0)\mathbf{L}\nabla u_0\cdot\mathbf{n}\,\mathrm{d}s\\&=\int_{\partial E_{\varepsilon,\ell}}(D_\ell^{\mathbf{v}}u_0+\nabla u_0\cdot\mathbf{v})\mathbf{L}\nabla u_0\cdot\mathbf{n}\,\mathrm{d}s.\end{aligned} \tag{5.18}$$

Computing the derivative of the second term on the right side of (5.17) is almost the same as in (5.18) except the domains $E_{\varepsilon,m}$ do not depend on $\mathbf{z}_\ell$ because $m\neq\ell$. Hence

$$D_\ell^{\mathbf{v}}\left(\sum_{m\neq\ell}\int_{E_{\varepsilon,m}}W(\nabla u_0)\,\mathrm{d}\mathbf{x}\right)=\sum_{m\neq\ell}\int_{E_{\varepsilon,m}}\nabla(D_\ell^{\mathbf{v}}u_0)\cdot\mathbf{L}\nabla u_0\,\mathrm{d}\mathbf{x}=\sum_{m\neq\ell}\int_{\partial E_{\varepsilon,m}}D_\ell^{\mathbf{v}}u_0\cdot\mathbf{L}\nabla u_0\cdot\mathbf{n}\,\mathrm{d}s. \tag{5.19}$$

Turning to the the final term in (5.1), which we split as

$$\sum_{m=1}^{N}\sum_{i=1}^{N}\int_{\partial E_{\varepsilon,m}}u_0\mathbf{L}\mathbf{k}_i\cdot\mathbf{n}\,\mathrm{d}s=\sum_{i=1}^{N}\int_{\partial E_{\varepsilon,\ell}}u_0\mathbf{L}\mathbf{k}_i\cdot\mathbf{n}\,\mathrm{d}s+\sum_{m\neq\ell}\int_{\partial E_{\varepsilon,m}}\sum_{i=1}^{N}u_0\mathbf{L}\mathbf{k}_i\cdot\mathbf{n}\,\mathrm{d}s, \tag{5.20}$$

we compute the derivative of the first term using (5.5) to get

$$D_\ell^{\mathbf{v}}\left(\sum_{i=1}^{N}\int_{\partial E_{\varepsilon,\ell}}u_0\mathbf{L}\mathbf{k}_i\cdot\mathbf{n}\,\mathrm{d}s\right)=\sum_{i=1}^{N}\int_{\partial E_{\varepsilon,\ell}}(D_\xi u_0)\mathbf{L}\mathbf{k}_i\cdot\mathbf{n}\,\mathrm{d}s+\sum_{i=1}^{N}\int_{\partial E_{\varepsilon,\ell}}u_0\mathbf{L}(D_\xi\mathbf{k}_i)\cdot\mathbf{n}\,\mathrm{d}s. \tag{5.21}$$

From (5.7) we have $D_\xi \mathbf{k}_\ell = 0$ and from (5.2) we have $D_\xi \mathbf{k}_i = \nabla(\mathbf{k}_i \cdot \mathbf{v})$ for $i \neq \ell$. Hence, for $i \neq \ell$ we have

$$\begin{aligned}\int_{\partial E_{\varepsilon,\ell}} u_0 \mathbf{L}(D_\xi \mathbf{k}_i) \cdot \mathbf{n}\,\mathrm{d}s &= \int_{\partial E_{\varepsilon,\ell}} u_0 \mathbf{L}\nabla(\mathbf{k}_i \cdot \mathbf{v}) \cdot \mathbf{n}\,\mathrm{d}s = \int_{E_{\varepsilon,\ell}} \operatorname{div}\left(u_0 \mathbf{L}\nabla(\mathbf{k}_i \cdot \mathbf{v})\right)\,\mathrm{d}\mathbf{x} \\ &= \int_{E_{\varepsilon,\ell}} \nabla u_0 \cdot \mathbf{L}\nabla(\mathbf{k}_i \cdot \mathbf{v})\,\mathrm{d}\mathbf{x} + \int_{E_{\varepsilon,\ell}} u_0 \operatorname{div}\left(\mathbf{L}\nabla(\mathbf{k}_i \cdot \mathbf{v})\right)\,\mathrm{d}\mathbf{x} \\ &= \int_{E_{\varepsilon,\ell}} \nabla(\mathbf{k}_i \cdot \mathbf{v}) \cdot \mathbf{L}\nabla u_0\,\mathrm{d}\mathbf{x} = \int_{E_{\varepsilon,\ell}} (\mathbf{k}_i \cdot \mathbf{v}) \cdot \mathbf{L}\nabla u_0 \cdot \mathbf{n}\,\mathrm{d}s.\end{aligned} \tag{5.22}$$

We used $\operatorname{div}\left(\mathbf{L}\nabla(\mathbf{k}_i \cdot \mathbf{v})\right) = (\mathbf{v} \cdot \nabla)(\operatorname{div}(\mathbf{L}\mathbf{k}_i)) = 0$, which follows from $\operatorname{curl} \mathbf{k}_i = 0$ and $\operatorname{div}(\mathbf{L}\mathbf{k}_i) = 0$. Combining (5.21) and (5.22) we get

$$D_\ell^{\mathbf{v}} \left(\sum_{i=1}^{N} \int_{\partial E_{\varepsilon,\ell}} u_0 \mathbf{L}\mathbf{k}_i \cdot \mathbf{n}\,\mathrm{d}s \right) = \sum_{i=1}^{N} \int_{\partial E_{\varepsilon,\ell}} (D_\xi u_0)\mathbf{L}\mathbf{k}_i \cdot \mathbf{n}\,\mathrm{d}s + \sum_{i \neq \ell} \int_{\partial E_{\varepsilon,\ell}} (\mathbf{k}_i \cdot \mathbf{v})\mathbf{L}\nabla u_0 \cdot \mathbf{n}\,\mathrm{d}s \tag{5.23}$$

Finally, the derivative of the second term in (5.20) is computed similarly to the first, but is simpler because the domains of integration are independent of $\mathbf{z}_\ell$. Hence,

$$D_\ell^{\mathbf{v}} \left(\sum_{m \neq \ell} \int_{\partial E_{\varepsilon,m}} \sum_{i=1}^{N} u_0 \mathbf{L}\mathbf{k}_i \cdot \mathbf{n}\,\mathrm{d}s \right) = \sum_{m \neq \ell} \int_{\partial E_{\varepsilon,m}} u_0 \mathbf{L}(D_\ell^{\mathbf{v}} \mathbf{k}_\ell) \cdot \mathbf{n}\,\mathrm{d}s + \sum_{m \neq \ell} \sum_{i=1}^{N} \int_{\partial E_{\varepsilon,m}} (D_\ell^{\mathbf{v}} u_0)\mathbf{L}\mathbf{k}_i \cdot \mathbf{n}\,\mathrm{d}s \tag{5.24}$$

because $D_\ell^{\mathbf{v}} \mathbf{k}_i = 0$ when $i \neq \ell$. Using $\operatorname{div}\left(\mathbf{L}\nabla(\mathbf{k}_i \cdot \mathbf{v})\right) = 0$, as we did to get (5.22), we have

$$\begin{aligned}\int_{\partial E_{\varepsilon,m}} u_0 \mathbf{L}(D_\ell^{\mathbf{v}} \mathbf{k}_\ell) \cdot \mathbf{n}\,\mathrm{d}s &= -\int_{\partial E_{\varepsilon,m}} u_0 \mathbf{L}\nabla(\mathbf{k}_\ell \cdot \mathbf{v}) \cdot \mathbf{n}\,\mathrm{d}s = -\int_{E_{\varepsilon,m}} \operatorname{div}(u_0 \mathbf{L}\nabla(\mathbf{k}_\ell \cdot \mathbf{v}))\,\mathrm{d}\mathbf{x} \\ &= -\int_{E_{\varepsilon,m}} \nabla u_0 \mathbf{L}\nabla(\mathbf{k}_\ell \cdot \mathbf{v})\,\mathrm{d}\mathbf{x} = -\int_{\partial E_{\varepsilon,m}} (\mathbf{k}_\ell \cdot \mathbf{v})\mathbf{L}\nabla u_0 \cdot \mathbf{n}\,\mathrm{d}s\end{aligned} \tag{5.25}$$

Then (5.24) and (5.25) give

$$D_\ell^{\mathbf{v}} \left(\sum_{m=1}^{N} \sum_{i=1}^{N} \int_{\partial E_{\varepsilon,m}} u_0 \mathbf{L}\mathbf{k}_i \cdot \mathbf{n}\,\mathrm{d}s \right) = \sum_{m \neq \ell} \int_{\partial E_{\varepsilon,m}} \left(\sum_{i=1}^{N} D_\ell^{\mathbf{v}} u_0 \cdot \mathbf{L}\mathbf{k}_i \cdot \mathbf{n} - (\mathbf{k}_\ell \cdot \mathbf{v})\mathbf{L}\nabla u_0 \cdot \mathbf{n} \right) \mathrm{d}s \tag{5.26}$$

Combining (5.12), (5.15), (5.18), and (5.23) we have

$$\begin{aligned}&\int_{\partial E_{\varepsilon,\ell}} \left\{ \sum_{i \neq \ell} (\mathbf{k}_i \cdot \mathbf{v})\mathbf{L}\mathbf{k}_i \cdot \mathbf{n} + \sum_{i \neq \ell} \sum_{j \neq i} (\mathbf{k}_j \cdot \mathbf{v}) \cdot \mathbf{L}\mathbf{k}_i \cdot \mathbf{n} + \right. \\ &\qquad \left. + \, (D_\xi u_0)\mathbf{L}\nabla u_0 \cdot \mathbf{n} + \sum_{i=1}^{N} (D_\xi u_0)\mathbf{L}\mathbf{k}_i \cdot \mathbf{n} + \sum_{i \neq \ell} (\mathbf{k}_i \cdot \mathbf{v})\mathbf{L}\nabla u_0 \cdot \mathbf{n} \right\} \mathrm{d}s \\ &\qquad = \int_{\partial E_{\varepsilon,\ell}} \left\{ \sum_{i \neq \ell} (\mathbf{k}_i \cdot \mathbf{v}) \left(\mathbf{L}\nabla u_0 + \sum_{j=1}^{N} \mathbf{L}\mathbf{k}_j \right) + D_\xi u_0 \left(\mathbf{L}\nabla u_0 + \sum_{j=1}^{N} \mathbf{L}\mathbf{k}_j \right) \right\} \cdot \mathbf{n}\,\mathrm{d}s \\ &\qquad = \int_{\partial E_{\varepsilon,\ell}} \left(D_\xi u_0 + \sum_{i \neq \ell} \mathbf{k}_i \cdot \mathbf{v} \right) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n}\,\mathrm{d}s\end{aligned} \tag{5.27}$$

Combining (5.13), (5.16), (5.19), and (5.26) we have

$$\begin{aligned}&\sum_{m \neq \ell} \int_{\partial E_{\varepsilon,m}} \left\{ -(\mathbf{k}_\ell \cdot \mathbf{v})\mathbf{L}\mathbf{k}_\ell - \sum_{i \neq \ell} (\mathbf{k}_\ell \cdot \mathbf{v})\mathbf{L}\mathbf{k}_i + D_\ell^{\mathbf{v}} u_0 \cdot \mathbf{L}\nabla u_0 + \sum_{i=1}^{N} D_\ell^{\mathbf{v}} u_0 \cdot \mathbf{L}\mathbf{k}_i - (\mathbf{k}_\ell \cdot \mathbf{v})\mathbf{L}\nabla u_0 \right\} \cdot \mathbf{n}\,\mathrm{d}s \\ &\qquad = \sum_{m \neq \ell} \int_{\partial E_{\varepsilon,m}} \left(D_\ell^{\mathbf{v}} u_0 - \mathbf{k}_\ell \cdot \mathbf{v} \right) \mathbf{L}\mathbf{h}_0 \cdot \mathbf{n}\,\mathrm{d}s.\end{aligned} \tag{5.28}$$

Thus, (5.10), (5.27), and (5.28) together give

$$D_{\mathbf{z}_\ell} U(\mathbf{v}) = \nabla_{\mathbf{z}_\ell} U \cdot \mathbf{v} = \left(\nabla_{\mathbf{z}_\ell} \widehat{U} + \nabla_{\mathbf{z}_\ell} \overline{U}\right) \cdot \mathbf{v} = -\int_{\partial E_{\varepsilon,\ell}} \{W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0 \otimes (\mathbf{L}\mathbf{h}_0)\}\,\mathbf{n}\,\mathrm{d}s \cdot \mathbf{v},$$

which establishes (4.3). □

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