

## STABILITY OF DISLOCATION NETWORKS OF LOW ANGLE GRAIN BOUNDARIES USING A CONTINUUM ENERGY FORMULATION

**ABSTRACT.** Low angle grain boundaries can be modeled as arrays of line defects (dislocations) in crystalline materials. The classical continuum models for energetics and dynamics of curved grain boundaries are mainly based on those with equilibrium dislocation structures without the long-range elastic interaction, leading to a capillary force proportional to the local curvature of the grain boundary. The new continuum model recently derived by Zhu and Xiang (J. Mech. Phys. Solids, 69, 175-194, 2014) incorporates both the long-range dislocation interaction energy and the local dislocation line energy, and enables the study of low angle grain boundaries with non-equilibrium dislocation structures that involves the long-range elastic interaction. Using this new energy formulation, we show that the orthogonal network of two arrays of screw dislocations on a planar twist low angle grain boundary is always stable subject to both perturbations of the constituent dislocations within the grain boundary and the perturbations of the grain boundary itself.

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**1. Introduction.** A grain boundary is the interface between two grains that have the same crystal structure but different orientations in a polycrystalline solid [16, 8]. The structures and properties of grain boundaries play important roles in plastic deformation, fracture, corrosion and phase transformations of the crystalline materials. If the misorientation angle between the two grains are small, the grain boundary in between is called a low angle grain boundary, and in this case, the grain boundary can be modeled as arrays of dislocations – line defects in crystals [16, 8].

Dislocations are characterized by their Burgers vectors. The elastic displacement vector increases by a constant vector along any small loop enclosing a dislocation, and this vector increment is the Burgers vector of this dislocation. For an edge dislocation (or at an edge point on a dislocation), the Burgers vector is perpendicular to the dislocation (or the line direction of the dislocation); while for a screw dislocation (or at a screw point), the Burgers vector is parallel to the dislocation

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(or the line direction of the dislocation). In a general case, the dislocation line may have an arbitrary angle to its Burgers vector, and the dislocation is of mixed type of edge and screw [8, 18].

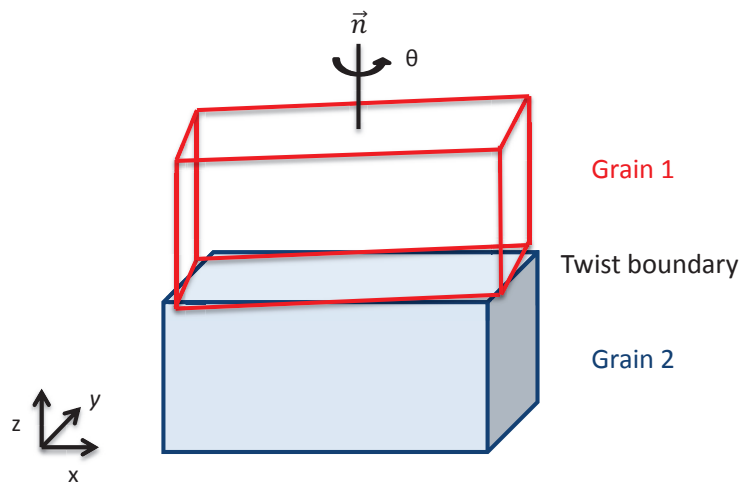
Grain boundary properties are strongly coupled with their structures. The classical continuum frameworks for energetics and dynamics of curved grain boundaries are mainly based on the classical Read-Shockley energy formula derived from equilibrium planar grain boundaries consisting of regular arrays of straight dislocations [16, 8, 15], and the capillary force proportional to the local curvature of the grain boundary [7]. Discrete dislocation dynamics models [9, 5, 19, 1] have been employed to study the energetics and dynamics of low angle grain boundaries with nonequilibrium dislocation structures [10, 13, 11], to which the classical continuum models of grain boundaries do not apply. An attempt was made in Ref. [12] to construct a phenomenological piecewise quadratic energy density function on a plane whose minimizer is in the form of structural units [17] and is able to approximate the orthogonal dislocation network structure on a planar twist boundary.

Recently Zhu and Xiang [21] derived a continuum model for dislocation structure on low angle grain boundaries that are allowed to be nonplanar or nonequilibrium. They introduced a scalar dislocation density potential function on a grain boundary surface to describe the the orientation dependent continuous distribution of dislocations with same Burgers vector. This continuum formulation incorporates both the long-range dislocation interaction and the local dislocation line energy, and are derived from the discrete dislocation model. When a grain boundary has an equilibrium dislocation structure, the long-range elastic energy cancels out, and the new continuum formulation reduces to the classical Read-Shockley energy formula.

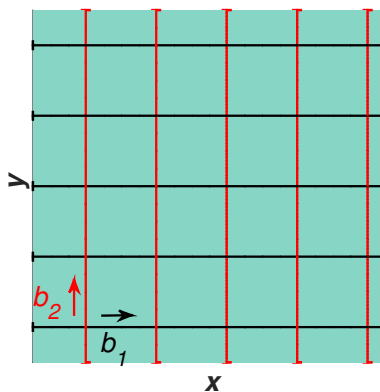
In this paper, we study the local stability of dislocation network structures of low angle grain boundaries using the new continuum energy formulation of Zhu and Xiang [21]. In the literature, continuum models for the motion of grain boundaries were developed under the assumption that the underlying dislocation structures are always in equilibrium (i.e., the long-range elastic energy always cancels out) [4, 3, 15], and as a result, a planar grain boundary is stabilized by the capillary force proportional to the local curvature of the grain boundary [7]. The classical Read-Shockley energy density formula [15] takes the form of  $\theta \log(1/\theta)$ , where  $\theta$  is the rotation angle of the grain boundary (See Eq. (12) in the next section for an example). This formula does not give the stability of the dislocation structure of a grain boundary with rotation angle  $\theta$ . (See the discussion after Eq. (12) in the next section.) Previously in [20], Zhu and Xiang studied the stability of a perturbed symmetric low angle tilt boundary consisting of single array of edge dislocations under the glide Peach-Koehler force (in which the perturbations are limited to the slip planes), using both the discrete dislocation dynamics model and the continuum force formulation they derived that includes the long-range effect. In this paper, we study the full stabilities of low angle grain boundaries in terms of the energy that include the stability subject to perturbations of the constituent dislocations within the grain boundaries as well as that subject to perturbations of the grain boundaries in their normal directions. We use the continuum energy formulation of Zhu and Xiang [21], which is able to examine the long-range elastic energy associated with these perturbations.

We focus on the stabilities of a planar low angle twist boundary that consists of two orthogonally intersecting screw dislocation arrays, see Fig. 1. We show that in the physically relevant regime, the second variation of the total elastic energy with

respect to the change of the grain boundary and the change of dislocation structure on the grain boundary are positive definite, thus the grain boundary is always stable. This study also provides a basis for further investigations of energetics and dynamics of the low angle grain boundaries using the new continuum energy formulation of Zhu and Xiang [21].



(a)



(b)

FIGURE 1. (a) Schematic illustration of a twist boundary. (b) Dislocation network consisting of two orthogonally intersecting screw dislocation arrays on a low angle twist boundary.

The rest of this paper is organized as follows. In section 2, the continuum model of Zhu and Xiang is reviewed, and the orthogonal dislocation network on a low angle twist boundary is described. We then present our main result on stability

in section 3. Proof of the main theorem is presented in section 4. Some lemmas needed in the proof of the main theorem are summarized in section 5.

**2. Review of the continuum model and dislocation network on a twist boundary.** We first review the continuum model introduced by Zhu and Xiang [21]. Consider the dislocation structure on a grain boundary surface  $S$ . A dislocation density potential function  $\eta$  defined on  $S$  is introduced to describe the distribution of the constituent dislocations on  $S$  with the same Burgers vector. It is a scalar function such that these constituent dislocations are given by its level sets  $\{\eta = j, \text{ where } j \text{ is an integer}\}$ . Under this definition, the local dislocation line direction is represented by

$$\mathbf{t} = \frac{\nabla_S \eta \times \mathbf{n}}{\|\nabla_S \eta\|},$$

and the inter-dislocation distance on  $S$  is

$$D = \frac{1}{\|\nabla_S \eta\|}.$$

Here  $\mathbf{n}$  is the unit normal vector of  $S$  and  $\nabla_S \eta = \nabla \eta - (\mathbf{n} \cdot \nabla \eta) \mathbf{n}$  is the surface gradient of  $\eta$  on  $S$ .

We consider  $J$  dislocation arrays on a low angle grain boundary  $S$  with Burgers vector  $\mathbf{b}^{(j)}$ ,  $j = 1, \dots, J$ . These arrays of dislocations are represented by dislocation density potential functions  $\eta_j$ ,  $j = 1, \dots, J$ . The continuum formulation of elastic energy of these dislocation arrays on  $S$  is given by

$$E_S = E_{\text{long}} + E_{\text{local}}, \quad (1)$$

where

$$\begin{aligned} E_{\text{long}} &= \frac{1}{2} \sum_{i=1}^J \sum_{j=1}^J \int_S dS_x \int_S dS_y \left[ -\frac{\mu}{2\pi} \frac{(\nabla_S \eta_i(x) \times \mathbf{n}(x)) \times (\nabla_S \eta_j(y) \times \mathbf{n}(y)) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)})}{\|x-y\|} \right. \\ &\quad + \frac{\mu}{4\pi} \frac{(\nabla_S \eta_i(x) \times \mathbf{n}(x) \cdot \mathbf{b}^{(i)}) (\nabla_S \eta_j(y) \times \mathbf{n}(y) \cdot \mathbf{b}^{(j)})}{\|x-y\|} \\ &\quad + \frac{\mu}{4\pi(1-\nu)} \left( \nabla_S \eta_i(x) \times \mathbf{n}(x) \times \mathbf{b}^{(i)} \right) \\ &\quad \left. \cdot \nabla_x \otimes \nabla_x \|x-y\| \cdot \left( \nabla_S \eta_j(y) \times \mathbf{n}(y) \times \mathbf{b}^{(j)} \right) \right], \quad (2) \end{aligned}$$

and

$$E_{\text{local}} = \sum_{i=1}^J \int_S \frac{\mu(b^{(i)})^2}{4\pi(1-\nu)} \left[ 1 - \nu \frac{(\nabla_S \eta_i \times \mathbf{n} \cdot \mathbf{b}^{(i)})^2}{(b^{(i)})^2 \|\nabla_S \eta_i\|^2} \right] \|\nabla_S \eta_i\| \log \frac{1}{r_g \|\nabla_S \eta_i\|} dS. \quad (3)$$

Here  $\mu$  is the shear modulus,  $\nu$  is the Poisson ratio,  $b^{(i)} = \|\mathbf{b}^{(i)}\|$ , and  $r_g$  is a constant parameter of the order of the dislocation core radius. The energy  $E_{\text{long}}$  represents the energy due to the long range interaction of dislocations, and the energy  $E_{\text{local}}$  is the local dislocation line energy.

When equilibrium state of the grain boundary is reached, the following equations hold:

$$\begin{cases} \frac{\delta E}{\delta r} = -\mathbf{f}_S^{\text{total}} \cdot \mathbf{n} = 0 & \text{when } \delta \mathbf{r} = \mathbf{n} \delta r \\ \frac{\delta E}{\delta \eta_j} = \mathbf{f}_S^{(j)} \cdot \frac{\nabla_S \eta_j}{\|\nabla_S \eta_j\|} = 0, & j = 1, 2, \dots, J. \end{cases} \quad (4)$$

The first equation describes the equilibrium with respect to the evolution of grain boundary  $S$ , and the second one gives the equilibrium state with respect to the motion of the constituent dislocations on the surface  $S$  when it is fixed. Here  $\mathbf{f}_S^{\text{total}}$  is the total force on the grain boundary  $S$  and  $\mathbf{f}_S^{(j)}$  is the force on the  $j$ -th dislocation array which can be written as

$$\mathbf{f}_S^{\text{total}} = \sum_{j=1}^J \|\nabla_S \eta_j\| \mathbf{f}_S^{(j)}, \quad (5)$$

$$\mathbf{f}_S^{(j)} = \mathbf{f}_0^{(j)} + \mathbf{f}_{\text{lt}}^{(j)} + \mathbf{f}_{\text{p}}^{(j)}. \quad (6)$$

The force  $\mathbf{f}_0^{(j)}$  consists of three parts. The long-range Peach-Koehler force  $\mathbf{f}_0^{(j)}$  comes from variations of the long-range energy  $E_{\text{long}}$  and is calculated by

$$\mathbf{f}_0^{(j)} = \left( \boldsymbol{\sigma}^{\text{tot}} \cdot \mathbf{b}^{(j)} \right) \times \left( \frac{\nabla_S \eta_j}{\|\nabla_S \eta_j\|} \times \mathbf{n} \right). \quad (7)$$

Here  $\boldsymbol{\sigma}^{\text{tot}} = \boldsymbol{\sigma} + \boldsymbol{\sigma}^{\text{other}}$  is the total stress field, where  $\boldsymbol{\sigma}$  is the long-range stress field generated by the dislocation arrays on  $S$  and  $\boldsymbol{\sigma}^{\text{other}}$  is the stress tensor due to other effect such as the lattice misfit across the interface or the applied stress. The continuum expression of  $\boldsymbol{\sigma}$  is

$$\begin{aligned} \boldsymbol{\sigma}(X) = & \sum_j \frac{\mu}{4\pi} \int_S \left[ \left( \nabla \frac{1}{\|X-x\|} \times \mathbf{b}^{(j)} \right) \otimes (\nabla_S \eta_j(x) \times \mathbf{n}(x)) \right. \\ & + (\nabla_S \eta_j(x) \times \mathbf{n}(x)) \otimes \left( \nabla \frac{1}{\|X-x\|} \times \mathbf{b}^{(j)} \right) \\ & \left. + \frac{1}{1-\nu} \left( \mathbf{b}^{(j)} \times (\nabla_S \eta_j \times \mathbf{n}) \cdot \nabla \right) (\nabla \otimes \nabla - I\Delta) \|X-x\| \right] dS, \quad (8) \end{aligned}$$

where  $\nabla$  and  $\Delta$  are taken with respect to  $X$ .

The variations of the local dislocation line energy  $E_{\text{local}}$  give two local forces  $\mathbf{f}_{\text{lt}}^{(j)}$  and  $\mathbf{f}_{\text{p}}^{(j)}$ . The force  $\mathbf{f}_{\text{lt}}^{(j)}$  is the local dislocation line tension force, which is calculated by

$$\mathbf{f}_{\text{lt}}^{(j)} = f_N^{(j)} \mathbf{n}_d + \mathbf{f}_B^{(j)} \mathbf{t} \times \mathbf{n}_d, \quad (9)$$

where the force component in the normal direction  $\mathbf{n}_d$  of the constituent dislocation is

$$f_N^{(j)} = \frac{\mu}{4\pi(1-\nu)} \kappa \left[ (1+\nu) \left( b_t^{(j)} \right)^2 + (1-2\nu) \left( b_N^{(j)} \right)^2 + \left( b_B^{(j)} \right)^2 \right] \log \frac{1}{r_g \|\nabla_S \eta_j\|}, \quad (10)$$

and the force component in the binormal direction  $\mathbf{t} \times \mathbf{n}_d$  of the constituent dislocation is

$$f_B^{(j)} = \frac{\mu\nu}{2\pi(1-\nu)} \kappa b_N b_B \log \frac{1}{r_g \|\nabla_S \eta_j\|}.$$

Here  $\kappa$  is the curvature of the local constituent dislocation,  $\kappa$  and  $\mathbf{n}_d$  can be calculated by

$$\kappa \mathbf{n}_d = (\nabla_S \mathbf{t}) \cdot \mathbf{t},$$

and  $b_t^{(j)} = \mathbf{b}^{(j)} \cdot \mathbf{t}$ ,  $b_N^{(j)} = \mathbf{b}^{(j)} \cdot \mathbf{n}_d$ ,  $b_B^{(j)} = \mathbf{b}^{(j)} \cdot \mathbf{t} \times \mathbf{n}_d$ .

The force  $\mathbf{f}_p^{(j)}$  is

$$\mathbf{f}_p^{(j)} = \frac{\mu}{4\pi(1-\nu)} \left( b^{(j)2} - \nu b_t^{(j)2} \right) \left( \kappa_p^{(j)} \mathbf{n}_p^{(j)} + \frac{\Delta_S \eta_j}{\|\nabla_S \eta_j\|^2} \nabla_S \eta_j \right), \quad (11)$$

where  $\kappa_p^{(j)}$  and  $\mathbf{n}_p^{(j)}$  are respectively the curvature and normal direction of the curve on  $S$  that is normal to the constituent dislocations in the  $j$ -th array, and they are determined by

$$\kappa_p \mathbf{n}_p = \nabla_S \left( \frac{\nabla_S \eta}{\|\nabla_S \eta\|} \right) \cdot \frac{\nabla_S \eta}{\|\nabla_S \eta\|}.$$

Consider an orthogonal network of two equidistant arrays of straight screw dislocations on a plane, see Fig. 1(b). The interdislocation distance in both arrays is  $D$  in this network. Under this continuum model, this dislocation network is represented by  $J = 2$ ,  $\eta_1(x, y) = \frac{y}{D}$ , and  $\eta_2(x, y) = -\frac{x}{D}$ , where  $\eta_1(x, y)$  and  $\eta_2(x, y)$  describe the distribution of the two dislocation arrays parallel to the  $x$  and  $y$  axes and with Burgers vector  $\mathbf{b}^{(1)} = (b, 0)$  and  $\mathbf{b}^{(2)} = (0, b)$ , respectively. It is easy to verify that this dislocation network satisfies the equilibrium conditions in Eq. (4). It represents the equilibrium dislocation structure on a low angle twist boundary with rotation angle  $\theta = \frac{b}{D}$  [16, 8], see Fig. 1(a). Note that this dislocation structure can also be obtained by Frank's formula [4, 3, 15, 21] that is equivalent to the cancellation of the long-range elastic energy.

In this equilibrium state, the long-range energy  $E_{\text{long}}$  vanishes, and the local dislocation line energy can be written as  $E_{\text{local}} = \int_S \gamma dS$ , where the energy density

$$\gamma = \frac{\mu b}{2\pi} \theta \log \frac{b}{r_g \theta}. \quad (12)$$

This recovers the classical Read-Shockley energy formula for a planar low angle twist boundary [16, 8, 15].

In the literature, continuum models for the motion of grain boundaries were developed under the assumption that the underlying dislocation structures are always in equilibrium in which the long-range elastic energy always cancels out [16, 8, 15], and the motions of grain boundaries including their stabilities are then governed by the capillary force proportional to the local curvature of the grain boundary [7] which comes from a surface energy corresponding to the local energy  $E_{\text{local}}$  in Eq. (3). The classical Read-Shockley energy formula in Eq. (12) is not able to give the stability of the dislocation structure of the low angle twist boundary with rotation angle  $\theta$ . In fact, the energy formula in Eq. (12) is a concave function of  $\theta$ , making any state with nonzero  $\theta$  unstable. Whereas in reality, the dislocation structure of a twist boundary with rotation angle  $\theta$  is stabilized subject to small perturbations of the constituent dislocations by the dislocation interaction energy, except for the perturbation of the rotation angle  $\theta$  which means a uniform change of all the constituent dislocations. The reason that Eq. (12) fails to give this stability is that it does not include the long-range elastic energy of dislocations.

In this paper, we shall use the total elastic energy formula in Eqs. (1)-(3) from [21] that includes both the long-range dislocation interaction energy  $E_{\text{long}}$  and the local dislocation line energy  $E_{\text{local}}$ , to study the stabilities of this planar low angle twist boundary subject to both perturbations of the constituent dislocations within the grain boundary and the perturbations of the grain boundary itself. In our study, the over-simplified assumption, yet commonly used in the existing continuum models, that the long-range elastic energy always cancels out, is removed, thus our

study will provide a complete understanding of the stabilities of the low angle grain boundaries.

**3. The main stability result.** In the rest of the paper, we shall take the grain boundary  $S$  to be a periodic surface in  $\mathbb{R}^3$  parametrized by  $(u, v)$  with period  $l_1$  in  $u$  and period  $l_2$  in  $v$ .

Suppose that there are  $J$  dislocation arrays described by the dislocation density potential functions  $\eta_i$  for  $i \in J$ , and each  $\eta_i$  has the same period as  $S$ . In this case, we consider the total energy over one period  $V$  of  $S$ , that is

$$\begin{aligned} E_{\text{long}} &= \frac{1}{2} \sum_{i=1}^J \sum_{j=1}^J \int_V dS_x \int_S dS_y \left[ -\frac{\mu}{2\pi} \frac{(\nabla_S \eta_i(x) \times \mathbf{n}(x)) \times (\nabla_S \eta_j(y) \times \mathbf{n}(y)) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)})}{\|x-y\|} \right. \\ &\quad + \frac{\mu}{4\pi} \frac{(\nabla_S \eta_i(x) \times \mathbf{n}(x) \cdot \mathbf{b}^{(i)}) (\nabla_S \eta_j(y) \times \mathbf{n}(y) \cdot \mathbf{b}^{(j)})}{\|x-y\|} \\ &\quad + \frac{\mu}{4\pi(1-\nu)} \left( \nabla_S \eta_i(x) \times \mathbf{n}(x) \times \mathbf{b}^{(i)} \right) \\ &\quad \left. \cdot \nabla_x \otimes \nabla_x \|x-y\| \cdot \left( \nabla_S \eta_j(y) \times \mathbf{n}(y) \times \mathbf{b}^{(j)} \right) \right], \end{aligned} \quad (13)$$

and

$$E_{\text{local}} = \sum_{i=1}^J \int_V \frac{\mu(b^{(i)})^2}{4\pi(1-\nu)} \left[ 1 - \nu \frac{(\nabla_S \eta_i \times \mathbf{n} \cdot \mathbf{b}^{(i)})^2}{(b^{(i)})^2 \|\nabla_S \eta_i\|^2} \right] \|\nabla_S \eta_i\| \log \frac{1}{r_g \|\nabla_S \eta_i\|} dS.$$

The total energy

$$E(\eta, S) = E_{\text{long}} + E_{\text{local}}.$$

Given dislocation density function  $\eta$  and grain boundary  $S$  such that  $E(\eta, S) < \infty$ . Consider perturbations of these dislocations and the grain boundary  $S$  given by

$$\eta_i^\varepsilon(u, v) = \eta_i(u, v) + \varepsilon_i \varphi_i(u, v), \quad (14)$$

$$\mathbf{r}^\delta(u, v) = \mathbf{r}(u, v) + \delta \psi(u, v) \mathbf{n}(u, v), \quad (15)$$

where functions  $\varphi_i(u, v)$  and  $\psi(u, v)$  have the same period as  $S$ . Let  $\eta = (\eta_1, \dots, \eta_J)$  and  $\varphi = (\varphi_1, \dots, \varphi_J)$ . Denote the perturbed grain boundary by  $S^\delta$  and the perturbed dislocation density function  $\eta^\varepsilon = \eta + \varepsilon \varphi$ . We shall consider periodic perturbations  $\varphi_i(u, v)$  and  $\psi(u, v) \in W^{1,2}(V)$ .

Let

$$J_\alpha(\phi, \mathbf{l}) = \int_S \frac{\nabla_S \phi(y) \times \mathbf{n}(y) \cdot \mathbf{l}}{\|x-y\|^{2-\alpha}} dS_y.$$

We claim  $J_\alpha(\phi, \mathbf{l}) \in L^2(V)$  for any vector  $\mathbf{l} \in \mathbb{R}^3$  and any periodic function  $\phi \in W^{1,2}(V)$ . In fact, we can rewrite  $J_\alpha(\phi)$  as follows

$$\begin{aligned} J_\alpha(\phi, \mathbf{l}) &= \int_S \frac{\mathbf{l} \times \nabla \phi(y) \cdot \mathbf{n}(y)}{\|x-y\|^{2-\alpha}} dS_y \\ &= \int_S \frac{\nabla \times (\phi(y) \mathbf{l}) \cdot d\mathbf{S}_y}{\|x-y\|^{2-\alpha}} \end{aligned}$$

By Stokes theorem and the assumption that  $\phi$  is periodic, we have

$$\int_V \nabla \times (\phi(y) \mathbf{l}) \cdot d\mathbf{S}_y = \int_V \phi(y) \mathbf{l} \cdot d\mathbf{r} = 0. \quad (16)$$

For

$$I_s f = 2^{-s} \pi^{-\frac{d}{2}} \frac{\Gamma\left(\frac{d-s}{2}\right)}{\Gamma\left(\frac{s}{2}\right)} \int_{\mathbb{R}^d} \frac{f(y)}{|x-y|^{d-s}} dy$$

We quote the following Hardy-Littlewood-Sobolev inequality on periodic regions.

**Lemma 3.1.** ([2] Prop 2.1 and Cor 2.2, see also [6, 14]) *Let  $u$  be a function on  $\mathbb{T}^d$  with mean zero. Suppose  $s > 0$  and  $1 < p < q < \infty$  satisfy  $\frac{s}{d} \geq \frac{1}{p} - \frac{1}{q}$ . Then we have*

$$\|I_s f\|_{L^q(\mathbb{T}^d)} \lesssim \|f\|_{L^p(\mathbb{T}^d)}.$$

Given  $S$  a periodic surface in  $\mathbb{R}^3$ , we have  $\|x - y\| \simeq |\tilde{x} - \tilde{y}|$  for any  $x, y \in S$ . Here  $\tilde{x}$  is the corresponding point of  $x$  in the parametrization space  $\mathbb{R}^2$ . Taking into account of (16), we can apply Lemma 3.1 for  $d = 2$ ,  $p = q = 2$  and  $s > 0$  to conclude  $J_\alpha(\phi, \mathbf{l}) \in L^2(V)$  for any vector  $\mathbf{l} \in \mathbb{R}^3$ . From this, we can check via direct calculation that  $E(\eta^\varepsilon, S^\delta)$ , the first variations  $\frac{d}{d\varepsilon_i} E(\eta^\varepsilon, S^\delta)$ ,  $\frac{d}{d\delta} E(\eta^\varepsilon, S^\delta)$  and the second variations  $\frac{d^2}{d\varepsilon_i d\varepsilon_j} E(\eta^\varepsilon, S^\delta)$ ,  $\frac{d^2}{d\varepsilon_i d\delta} E(\eta^\varepsilon, S^\delta)$ ,  $\frac{d^2}{d\delta^2} E(\eta^\varepsilon, S^\delta)$  are well defined for  $\varphi_i, \psi \in W^{1,2}(V)$ , for  $i = 1, \dots, J$ .

Our main result is the following theorem that describes the local stability of the orthogonal network dislocation structure on a low angle twist boundary (as shown in Fig. 1) subject to periodic perturbations of the constituent dislocations and the grain boundary.

**Theorem 3.2.** *Given a planar grain boundary  $S$  represented by  $\mathbf{r} = (x, y, 0)$ . There are  $J = 2$  arrays of dislocations with Burgers vectors  $\mathbf{b}^{(1)} = (b, 0, 0)$  and  $\mathbf{b}^{(2)} = (0, b, 0)$ , described by dislocation density potential functions  $\eta_1(x, y) = \frac{y}{D}$  and  $\eta_2(x, y) = -\frac{x}{D}$ , respectively. For perturbations of this grain boundary and its dislocation structure given in Eqs. (14) and (15), with periodic  $\varphi_1, \varphi_2, \psi \in W^{1,2}(V)$ , we have*

(i) *The first variations vanish:*

$$\left. \frac{d}{d\varepsilon_1} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = \left. \frac{d}{d\varepsilon_2} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = \left. \frac{d}{d\delta} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = 0.$$

(ii) *The second variation matrix*

$$\left( \begin{array}{ccc} \frac{d^2}{d\varepsilon_1^2} E(\eta^\varepsilon, S^\delta) & \frac{d^2}{d\varepsilon_1 d\varepsilon_2} E(\eta^\varepsilon, S^\delta) & \frac{d^2}{d\varepsilon_1 d\delta} E(\eta^\varepsilon, S^\delta) \\ \frac{d^2}{d\varepsilon_2 d\varepsilon_1} E(\eta^\varepsilon, S^\delta) & \frac{d^2}{d\varepsilon_2^2} E(\eta^\varepsilon, S^\delta) & \frac{d^2}{d\varepsilon_2 d\delta} E(\eta^\varepsilon, S^\delta) \\ \frac{d^2}{d\delta d\varepsilon_1} E(\eta^\varepsilon, S^\delta) & \frac{d^2}{d\delta d\varepsilon_2} E(\eta^\varepsilon, S^\delta) & \frac{d^2}{d\delta^2} E(\eta^\varepsilon, S^\delta) \end{array} \right) \Bigg|_{\varepsilon_1=\varepsilon_2=\delta=0} \geq 0, \quad (17)$$

if the perturbation wavelengths of  $\varphi$  satisfies

$$\frac{1}{\lambda_1^2} + \frac{1}{\lambda_2^2} \leq \frac{1}{D^2}, \quad (18)$$

where  $\lambda_1$  and  $\lambda_2$  are perturbation wavelengths of  $\varphi_1$  and  $\varphi_2$ , respectively. Here “ $\geq$ ” in Eq. (17) means the  $3 \times 3$  matrix is semipositive definite. Moreover, this dislocation network is strictly stable to any nonzero perturbation if the condition in Eq. (18) is satisfied.

**Remark 1.** The assumption that the perturbation wavelengths of  $\varphi$  satisfies Eq. (18) is physically good enough for the stability of the dislocation structure. This assumption basically means that the perturbation wavelength is not very small so that there is at least one dislocation in each perturbation period of the dislocation structure. Any perturbation with wavelength less than this value is not physically relevant.



In fact, the destabilizing effect comes from the local energy  $E_{\text{local}}$ , due to perturbations in the direction normal to the constituent dislocations. This instability is always stabilized by the long-range energy  $E_{\text{long}}$  in the physically relevant regime.

Mathematically, the continuum energy formulation presented in the previous section may indeed lead to physically irrelevant instability for perturbations with very small wavelengths. An attempt has been made in Ref. [21] to simply remove some small terms that may result in such a instability. Systematic treatment for the improvement of the continuum model will be explored in the future work.

**Remark 2.** This stability theorem ensures the stability of any numerical scheme for the continuum model whose numerical grid constant  $\Delta \gg D$ . This condition is easy to satisfy because the inter-dislocation distance  $D$  is a microscopic length which is much smaller than the length scale of the continuum model.

**Remark 3.** Theorem 3.2 tells us that the grain boundary and its dislocation structure is stable subject to periodic perturbations. Now we briefly discuss the stability when there are uniform perturbations of inter-dislocation distance, i.e. the inter-dislocation distance in the first array becomes  $D + \varepsilon_1$  and the inter-dislocation distance in the second array becomes  $D + \varepsilon_2$ . Accordingly, the dislocation density potential functions change to  $\eta_1^\varepsilon(x, y) = y/(D + \varepsilon_1)$  and  $\eta_2^\varepsilon(x, y) = -x/(D + \varepsilon_2)$ .

When  $\varepsilon_1 \neq \varepsilon_2$ , there is a constant long-range stress field in the infinity three dimensional space, and the long-range elastic energy  $E_{\text{long}}$  becomes  $+\infty$ . Thus in this case, the grain boundary is still stable.

When  $\varepsilon_1 = \varepsilon_2$ , the long-range elastic energy  $E_{\text{long}}$  still vanishes, and

$$\left. \frac{dE_{\text{local}}}{d\varepsilon_i} \right|_{\varepsilon_1=\varepsilon_2=0} = \frac{\mu b^2}{4\pi D^2} \int_S \left( 1 - \log \frac{D}{r_g} \right) dS < 0.$$

Thus in this case, the grain boundary is unstable. This instability is included in the classical Read-Shockley energy formula in Eq. (12).

**4. Proof of Theorem 3.2.** To prove our theorem, we divide our calculations on second variation of  $E$  with respect to  $\varepsilon$  and  $\delta$  into several lemmas.

Let  $V = [0, l_1] \times [0, l_2]$  be the periodic domain for the parameters  $(u, v)$  for the grain boundary  $S$  and the perturbed boundary  $S^\delta$ . We write the energies in Eqs. (13) and (??) in terms of  $(u, v)$  as follows.

$$E_{\text{long}}(\eta^\varepsilon, S^\delta) = \frac{1}{2} \sum_{i=1}^J \sum_{j=1}^J \int_V \int_{S^\delta} \left( -\frac{\mu}{2\pi} A_{ij} + \frac{\mu}{4\pi} B_{ij} + \frac{\mu}{4\pi(1-\nu)} C_{ij} \right) dudvd\tilde{u}d\tilde{v}, \quad (19)$$

and

$$E_{\text{local}} = \sum_{i=1}^J \int_V \frac{\mu (b^{(i)})^2}{4\pi(1-\nu)} A_i \theta_i^{\varepsilon, \delta} \log \frac{1}{r_g \theta_i^{\varepsilon, \delta}} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| dudv, \quad (20)$$

where

$$\begin{aligned} A_{ij} &= \frac{(\nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v)) \times (\nabla_{S^\delta} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v})) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)})}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \\ &\quad \cdot \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_{\tilde{u}}^\delta \times \mathbf{r}_{\tilde{v}}^\delta\| \\ &= a_{ij} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_{\tilde{u}}^\delta \times \mathbf{r}_{\tilde{v}}^\delta\| \\ &= \frac{L_{ij}}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_{\tilde{u}}^\delta \times \mathbf{r}_{\tilde{v}}^\delta\|, \end{aligned}$$

hence  $A_{ij} = A_{ji}$  and  $A_{ii} = 0$ ,

$$\begin{aligned}
B_{ij} &= \frac{(\nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \cdot \mathbf{b}^{(i)}) (\nabla_{S^\delta} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \cdot \mathbf{b}^{(j)})}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \\
&\quad \cdot \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \\
&= b_{ij} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \\
&= \frac{M_{ij}}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\|, \\
C_{ij} &= \left[ (\nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)}) \cdot \nabla_{\mathbf{r}(u, v)} \otimes \nabla_{\mathbf{r}(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \right. \\
&\quad \left. \cdot (\nabla_{S^\delta} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)}) \right] \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \\
&= c_{ij} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\|, \\
A_i &= \left( 1 - \nu \frac{(\nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \cdot \mathbf{b}^{(i)})^2}{(b^{(i)})^2 \|\nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v))\|^2} \right), \\
\theta_i^{\varepsilon, \delta} &= \|\nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v))\|.
\end{aligned}$$

Derivatives of these expressions with respect to  $\varepsilon = (\varepsilon_1, \dots, \varepsilon_J)$ , and  $\delta$  for a general periodic grain boundary  $S$  (could be nonplanar) with  $J$  arrays of dislocations on it are given in the next section. Using these results, we have the following lemmas for the the perturbed twist boundary  $S^\delta$  in the theorem, where parameters  $(u, v) = (x, y)$ .

**Lemma 4.1.** *For the perturbed twist boundary  $S^\delta$  in Theorem 3.2, the followings hold at  $\varepsilon_1 = \varepsilon_2 = \delta = 0$ . Here  $i, k, l = 1$  or  $2$ , and  $\delta_{kl} = 1$  when  $k = l$  and  $0$  when  $k \neq l$ .*

$$\begin{aligned}
\left. \frac{d\mathbf{n}^\delta}{d\delta} \right|_{\delta=0} &= -\psi_u \mathbf{r}_u - \psi_v \mathbf{r}_v; & \left. \frac{d^2 \mathbf{n}^\delta}{d\delta^2} \right|_{\delta=0} &= -(\psi_u^2 + \psi_v^2) \mathbf{n}; \\
\left. \frac{d\|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\|}{d\delta} \right|_{\delta=0} &= 0; & \left. \frac{d^2 \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\|}{d\delta^2} \right|_{\delta=0} &= \psi_u^2 + \psi_v^2; \\
\left. \frac{d\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|}{d\delta} \right|_{\delta=0} &= 0; & \left. \frac{d^2 \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|}{d\delta^2} \right|_{\delta=0} &= \frac{|\psi(u, v) - \psi(\tilde{u}, \tilde{v})|^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|}; \\
\left. \frac{d\|\nabla_{S^\delta} \eta_i^\varepsilon\|}{d\delta} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= 0; & \left. \frac{d\|\nabla_{S^\delta} \eta_i^\varepsilon\|}{d\varepsilon_k} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= \frac{\nabla_S \eta_i \cdot \nabla_S \varphi_i}{\|\nabla_S \eta_i\|} \delta_{ik}; \\
\left. \frac{d^2 \|\nabla_{S^\delta} \eta_i^\varepsilon\|}{d\varepsilon_k d\delta} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= 0; & \left. \frac{d^2 \|\nabla_{S^\delta} \eta_i^\varepsilon\|}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= \frac{\|\nabla_S \eta_i \times \nabla_S \varphi_i\|^2}{(\theta_i)^3} \delta_{ik} \delta_{il}; \\
\left. \frac{d^2 \|\nabla_{S^\delta} \eta_1^\varepsilon\|}{d\delta^2} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= -\frac{1}{D} \psi_u^2; & \left. \frac{d^2 \|\nabla_{S^\delta} \eta_2^\varepsilon\|}{d\delta^2} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= -\frac{1}{D} \psi_v^2; \\
\left. \frac{d\nabla_{S^\delta} \eta_1^\varepsilon}{d\delta} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= \frac{\psi_u}{D} \mathbf{n}; & \left. \frac{d\nabla_{S^\delta} \eta_2^\varepsilon}{d\delta} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= -\frac{\psi_v}{D} \mathbf{n}; \\
\left. \frac{d^2 \nabla_{S^\delta} \eta_1^\varepsilon}{d\delta^2} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= -\frac{2\psi_u \psi_u}{D} \mathbf{r}_u - \frac{2\psi_u^2}{D} \mathbf{r}_v; & \left. \frac{d^2 \nabla_{S^\delta} \eta_2^\varepsilon}{d\delta^2} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= \frac{2\psi_v \psi_u}{D} \mathbf{r}_v + \frac{2\psi_v^2}{D} \mathbf{r}_u; \\
\left. \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_i^\varepsilon \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= \delta_{ik} \nabla_S \varphi_i; & \left. \frac{d^2}{d\varepsilon_k d\varepsilon_l} \nabla_{S^\delta} \eta_i^\varepsilon \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= 0; \\
\left. \frac{d^2}{d\varepsilon_k d\delta} \nabla_{S^\delta} \eta_i^\varepsilon \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} &= \delta_{ik} (\psi_u \varphi_{iu} + \psi_v \varphi_{iv}) \mathbf{n}.
\end{aligned}$$

A direct result of Lemma 4.1 is the following corollary on some of the terms that frequently appear in the derivatives of  $E$ .

**Lemma 4.2.** *The followings hold.*

$$\begin{aligned}
\left. \frac{d}{d\delta} (\nabla_{S^s} \eta_1^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v)) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{\psi_u}{D} \mathbf{n}; \\
\left. \frac{d}{d\delta} (\nabla_{S^s} \eta_2^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v)) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{\psi_v}{D} \mathbf{n}; \\
\left. \frac{d^2}{d\delta d\varepsilon_k} \nabla_{S^s} \eta_i^\varepsilon \cdot \nabla_{S^s} \eta_i^\varepsilon \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 0; \\
\left. \frac{d}{d\delta} \left( \frac{d}{d\varepsilon_k} \nabla_{S^s} \eta_1^\varepsilon \times \mathbf{n}^\delta \right) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= (\psi_u \varphi_{1v} - \varphi_{1u} \psi_v) \mathbf{n}; \\
\left. \frac{d}{d\delta} \left( \frac{d}{d\varepsilon_k} \nabla_{S^s} \eta_2^\varepsilon \times \mathbf{n}^\delta \right) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= (\psi_u \varphi_{2v} - \varphi_{2u} \psi_v) \mathbf{n}; \\
\left. \frac{d}{d\delta} (\nabla_{S^s} \eta_i^\varepsilon \times \mathbf{n}^\delta \cdot \mathbf{b}^{(i)}) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 0; \\
\left. \frac{d}{d\delta} \left( \frac{d}{d\varepsilon_k} \nabla_{S^s} \eta_i^\varepsilon \times \mathbf{n}^\delta \cdot \mathbf{b}^{(i)} \right) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 0;
\end{aligned}$$

$$\begin{aligned}
\left. \frac{d^2}{d\delta^2} \nabla_{S^s} \eta_1^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{2\psi_v \psi_u}{D} \mathbf{r}_v - \frac{2\psi_v^2}{D} \mathbf{r}_u; \\
\left. \frac{d^2}{d\delta^2} \nabla_{S^s} \eta_2^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{2\psi_v \psi_u}{D} \mathbf{r}_u - \frac{2\psi_u^2}{D} \mathbf{r}_v; \\
\left. \frac{d}{d\delta} \nabla_{S^s} \eta_1^\varepsilon (\mathbf{r}^\delta(u, v)) \times \frac{d}{d\delta} \mathbf{n}^\delta(u, v) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{\psi_v^2}{D} \mathbf{r}_u - \frac{\psi_v \psi_u}{D} \mathbf{r}_v; \\
\left. \frac{d}{d\delta} \nabla_{S^s} \eta_2^\varepsilon (\mathbf{r}^\delta(u, v)) \times \frac{d}{d\delta} \mathbf{n}^\delta(u, v) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{\psi_v \psi_u}{D} \mathbf{r}_u + \frac{\psi_u^2}{D} \mathbf{r}_v; \\
\left. \frac{d^2}{d\delta^2} (\nabla_{S^s} \eta_1^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v)) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{\psi_u^2 + \psi_v^2}{D} \mathbf{r}_u; \\
\left. \frac{d^2}{d\delta^2} (\nabla_{S^s} \eta_2^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v)) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{\psi_u^2 + \psi_v^2}{D} \mathbf{r}_v.
\end{aligned}$$

The following Lemmas hold for terms that appear in  $E_{\text{long}}$  and  $E_{\text{local}}$ .

**Lemma 4.3.**  $A_{11} = A_{22} = 0$  and the followings hold at  $\varepsilon_1 = \varepsilon_2 = \delta = 0$ .

$$\begin{aligned}
\left. \frac{dA_{12}}{d\varepsilon_1} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2 \varphi_{1v}(u, v)}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|}; \\
\left. \frac{dA_{12}}{d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2 \varphi_{2\tilde{u}}(\tilde{u}, \tilde{v})}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|}; \\
\left. \frac{dA_{21}}{d\varepsilon_1} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2 \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v})}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|}; \\
\left. \frac{dA_{21}}{d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2 \varphi_{2u}(u, v)}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|}; \\
\left. \frac{dA_{ij}}{d\delta} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \left. \frac{d^2 A_{ij}}{d\delta d\varepsilon_k} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = 0; \\
\left. \frac{d^2 A_{12}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2 (\varphi_{1u}(u, v) \varphi_{2\tilde{v}}(\tilde{u}, \tilde{v}) - \varphi_{1v}(u, v) \varphi_{2\tilde{u}}(\tilde{u}, \tilde{v}))}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} (\delta_{1k} \delta_{2l} + \delta_{1l} \delta_{2k}); \\
\left. \frac{d^2 A_{21}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2 (-\varphi_{2u}(u, v) \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}) + \varphi_{2v}(u, v) \varphi_{1\tilde{u}}(\tilde{u}, \tilde{v}))}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} (\delta_{2k} \delta_{1l} + \delta_{2l} \delta_{1k}); \\
\left. \frac{d^2 A_{12}}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2 |\psi(u, v) - \psi(\tilde{u}, \tilde{v})|^2}{D^2 \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|^3}; \\
\left. \frac{d^2 A_{21}}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2 |\psi(u, v) - \psi(\tilde{u}, \tilde{v})|^2}{D^2 \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|^3}.
\end{aligned}$$

**Lemma 4.4.** The followings hold for  $B_{ij}$  at  $\varepsilon_1 = \varepsilon_2 = \delta = 0$ .

$$\begin{aligned}
\left. \frac{dB_{ij}}{d\delta} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \left. \frac{d^2 B_{ij}}{d\delta d\varepsilon_k} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = 0; \\
\left. \frac{dB_{11}}{d\varepsilon_1} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} (\varphi_{1v}(u, v) + \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v})); \\
\left. \frac{dB_{11}}{d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \left. \frac{dB_{22}}{d\varepsilon_1} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = 0; \\
\left. \frac{dB_{12}}{d\varepsilon_1} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{1v}(u, v); \\
\left. \frac{dB_{12}}{d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{2\tilde{u}}(\tilde{u}, \tilde{v}); \\
\left. \frac{dB_{21}}{d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{2u}(u, v); \\
\left. \frac{dB_{21}}{d\varepsilon_1} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}); \\
\left. \frac{dB_{22}}{d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2}{D \|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} (\varphi_{2u}(u, v) + \varphi_{2\tilde{u}}(\tilde{u}, \tilde{v}));
\end{aligned}$$

$$\begin{aligned}
\left. \frac{d^2 B_{11}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{1v}(u, v) \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}) (\delta_{1k}\delta_{1l} + \delta_{1l}\delta_{1k}); \\
\left. \frac{d^2 B_{12}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{1v}(u, v) \varphi_{2\tilde{u}}(\tilde{u}, \tilde{v}) (\delta_{1k}\delta_{2l} + \delta_{1l}\delta_{2k}); \\
\left. \frac{d^2 B_{21}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{2u}(u, v) \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}) (\delta_{2k}\delta_{1l} + \delta_{2l}\delta_{1k}); \\
\left. \frac{d^2 B_{22}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{2u}(u, v) \varphi_{2\tilde{u}}(\tilde{u}, \tilde{v}) (\delta_{2k}\delta_{2l} + \delta_{2l}\delta_{2k}); \\
\left. \frac{d^2 B_{ij}}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{b^2}{D^2} \frac{|\psi(u, v) - \psi(\tilde{u}, \tilde{v})|^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|^3}.
\end{aligned}$$

**Lemma 4.5.** For  $C_{ij}$ , we have

$$\begin{aligned}
\left. \frac{d}{d\varepsilon_k} C_{ij} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \left. \frac{d}{d\delta} C_{ij} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = \left. \frac{d^2}{d\delta d\varepsilon_k} C_{ij} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = 0; \\
\left. \frac{d^2 C_{11}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{1u}(u, v) \varphi_{1\tilde{u}}(\tilde{u}, \tilde{v}) (\delta_{1k}\delta_{1l} + \delta_{1l}\delta_{1k}); \\
\left. \frac{d^2 C_{12}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{1u}(u, v) \varphi_{2\tilde{v}}(\tilde{u}, \tilde{v}) (\delta_{1k}\delta_{2l} + \delta_{2k}\delta_{1l}); \\
\left. \frac{d^2 C_{21}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{2v}(u, v) \varphi_{1\tilde{u}}(\tilde{u}, \tilde{v}) (\delta_{1k}\delta_{2l} + \delta_{2k}\delta_{1l}); \\
\left. \frac{d^2 C_{22}}{d\varepsilon_k d\varepsilon_l} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{b^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|} \varphi_{2v}(u, v) \varphi_{2\tilde{v}}(\tilde{u}, \tilde{v}) (\delta_{2k}\delta_{2l} + \delta_{2l}\delta_{2k}); \\
\left. \frac{d^2}{d\delta^2} C_{11} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{2b^2}{D} \psi_u(u, v) \psi_{\tilde{u}}(\tilde{u}, \tilde{v}) \frac{(v - \tilde{v})^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|^3}; \\
\left. \frac{d^2}{d\delta^2} C_{12} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{2b^2}{D} \psi_u(u, v) \psi_{\tilde{v}}(\tilde{u}, \tilde{v}) \left( \frac{(u - \tilde{u})(v - \tilde{v})}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|^3} \right); \\
\left. \frac{d^2}{d\delta^2} C_{21} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{2b^2}{D} \psi_v(u, v) \psi_{\tilde{u}}(\tilde{u}, \tilde{v}) \left( \frac{(u - \tilde{u})(v - \tilde{v})}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|^3} \right); \\
\left. \frac{d^2}{d\delta^2} C_{22} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{2b^2}{D} \psi_v(u, v) \psi_{\tilde{v}}(\tilde{u}, \tilde{v}) \frac{(u - \tilde{u})^2}{\|\mathbf{r}(u, v) - \mathbf{r}(\tilde{u}, \tilde{v})\|^3}.
\end{aligned}$$

**Lemma 4.6.** The followings hold for  $A_i$  when  $\varepsilon_1 = \varepsilon_2 = \delta = 0$ .

$$\begin{aligned}
\left. \frac{d}{d\varepsilon_k} A_i \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 0; & \left. \frac{d}{d\delta} A_i \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 0; \\
\left. \frac{d^2}{d\delta d\varepsilon_k} A_i \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 0; & \left. \frac{d^2}{d\varepsilon_k d\varepsilon_l} A_1 \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 2\nu D^2 (\varphi_{1u})^2 \delta_{1k}\delta_{1l}; \\
\left. \frac{d^2}{d\varepsilon_k d\varepsilon_l} A_2 \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 2\nu D^2 (\varphi_{2v})^2 \delta_{2k}\delta_{2l}; & \left. \frac{d^2}{d\delta^2} A_1 \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 2\nu \psi_v^2; \\
\left. \frac{d^2}{d\delta^2} A_2 \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 2\nu \psi_u^2.
\end{aligned}$$

We are now ready to give expressions of the second variations of  $E$  with respect to  $\varepsilon$  and  $\delta$ , which are summarized in the following proposition.

**Proposition 1.** *For the perturbed twist boundary  $S^\delta$  and the perturbed dislocation density potential functions  $\eta^\varepsilon = (\eta_1^\varepsilon, \eta_2^\varepsilon)$  in Theorem 3.2, we have*

$$\begin{aligned} \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{\mu b^2 l_1 l_2}{2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\kappa_n^2 |\widehat{\varphi}_1|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} \\ &\quad + \frac{\mu b^2 l_1 l_2}{2(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 |\widehat{\varphi}_1|^2}{\sqrt{\xi_n^2 + \kappa_n^2}}, \\ \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_2^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{\mu b^2 l_1 l_2}{2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 |\widehat{\varphi}_2|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} \\ &\quad + \frac{\mu b^2 l_1 l_2}{2(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\kappa_n^2 |\widehat{\varphi}_2|^2}{\sqrt{\xi_n^2 + \kappa_n^2}}, \\ \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1 d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{\mu \nu b^2 l_1 l_2}{4(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n \kappa_n}{\sqrt{\xi_n^2 + \kappa_n^2}} \left( \widehat{\varphi}_1 \overline{\widehat{\varphi}_2} + \widehat{\varphi}_2 \overline{\widehat{\varphi}_1} \right), \\ \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{2\mu b^2 l_1 l_2}{(1-\nu) D^2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 \kappa_n^2}{(\xi_n^2 + \kappa_n^2)^{\frac{3}{2}}} |\widehat{\psi}|^2, \\ \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_k d\delta} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 0, \\ \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{\mu b^2 D}{4\pi} \int_V (\varphi_{1v})^2 dudv \\ &\quad + \frac{\mu b^2 D}{4\pi(1-\nu)} \int_V (\varphi_{1u})^2 \left[ (1+\nu) \log \frac{D}{r_g} - (1-\nu) \right] dudv, \\ \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_2^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= -\frac{\mu b^2 D}{4\pi} \int_V (\varphi_{2u})^2 dudv \\ &\quad + \frac{\mu b^2 D}{4\pi(1-\nu)} \int_V (\varphi_{2v})^2 \left[ (1+\nu) \log \frac{D}{r_g} - (1-\nu) \right] dudv, \\ \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1 d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 0, \\ \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{\mu b^2}{4\pi(1-\nu) D} \int_V (\psi_u^2 + \psi_v^2) \left[ (1+\nu) \log \frac{D}{r_g} + (1-\nu) \right] dudv, \\ \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_k d\delta} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= 0. \end{aligned}$$

Here  $\mathbf{Z}$  is the set of all integers, and  $\widehat{\varphi}$  is the Fourier transform of  $\varphi$  which is defined by  $\widehat{\varphi}(\xi_n, \kappa_n) = \frac{1}{l_1 l_2} \int_V \varphi(u, v) e^{-i(\xi_n u + \kappa_n v)} dudv$ .

**Proof:** We first evaluate the derivatives of  $E_{\text{long}}$ . Recall that for the unperturbed twist boundary,  $\mathbf{r}(u, v) = (u, v)$ .

$$\begin{aligned}
& \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= \frac{1}{2} \int_V \int_S \left( \frac{\mu}{4\pi} \frac{d^2}{d\varepsilon_1^2} B_{11} + \frac{\mu}{4\pi(1-\nu)} \frac{d^2}{d\varepsilon_1^2} C_{11} \right) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudvd\tilde{u}d\tilde{v} \\
&= \frac{\mu b^2}{4\pi} \int_V \int_S \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{1v}(u, v) \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}) dudvd\tilde{u}d\tilde{v} \\
&\quad + \frac{\mu b^2}{4\pi(1-\nu)} \int_V \int_S \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{1u}(u, v) \varphi_{1\tilde{u}}(\tilde{u}, \tilde{v}) dudvd\tilde{u}d\tilde{v} \\
&= \frac{\mu b^2 l_1 l_2}{2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\kappa_n^2 |\widehat{\varphi}_1|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} + \frac{\mu b^2 l_1 l_2}{2(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 |\widehat{\varphi}_1|^2}{\sqrt{\xi_n^2 + \kappa_n^2}}.
\end{aligned}$$

Note that here the grain boundary  $S = \mathbf{R}^2$ .

Here in order to get the result in the Fourier space, we have used the following calculation, using the first term as an example.

$$\begin{aligned}
& \int_V \int_{\mathbf{R}^2} \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{1v}(u, v) \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}) dudvd\tilde{u}d\tilde{v} \\
&= \int_V \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}) d\tilde{u}d\tilde{v} \int_{\mathbf{R}^2} \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{1v}(u, v) dudv \\
&= \int_V \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}) f(\tilde{u}, \tilde{v}) d\tilde{u}d\tilde{v}, \tag{21}
\end{aligned}$$

where  $f(\tilde{u}, \tilde{v}) = \int_{\mathbf{R}^2} \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{1v}(u, v) dudv$  is also a periodic function over  $V$ . It is easy to calculate the Fourier transform of the function  $f(\tilde{u}, \tilde{v})$  by

$$\begin{aligned}
\widehat{f}(\xi_n, \kappa_n) &= \frac{1}{l_1 l_2} \int_V f(\tilde{u}, \tilde{v}) e^{-i(\xi_n \tilde{u} + \kappa_n \tilde{v})} d\tilde{u}d\tilde{v} \\
&= \frac{1}{l_1 l_2} \int_V e^{-i(\xi_n \tilde{u} + \kappa_n \tilde{v})} d\tilde{u}d\tilde{v} \int_{\mathbf{R}^2} \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{1v}(u, v) dudv \\
&= \frac{1}{l_1 l_2} \int_V e^{-i(\xi_n \tilde{u} + \kappa_n \tilde{v})} d\tilde{u}d\tilde{v} \int_{\mathbf{R}^2} \frac{1}{\|(u, v)\|} \varphi_{1\tilde{v}}(\tilde{u} - u, \tilde{v} - v) dudv \\
&= \int_{\mathbf{R}^2} \frac{1}{\|(u, v)\|} e^{-i(\xi_n u + \kappa_n v)} dudv \\
&\quad \cdot \frac{1}{l_1 l_2} \int_V e^{-i[\xi_n(\tilde{u}-u) + \kappa_n(\tilde{v}-v)]} \varphi_{1\tilde{v}}(\tilde{u} - u, \tilde{v} - v) d(\tilde{u} - u) d(\tilde{v} - v) \\
&= \frac{2\pi}{\sqrt{\xi_n^2 + \kappa_n^2}} \widehat{\varphi_{1v}}(\xi_n, \kappa_n).
\end{aligned}$$

The result follows using Parseval identity and  $\widehat{\varphi_{1v}} = i\kappa_n \widehat{\varphi}$ .

Similarly, we have

$$\begin{aligned}
& \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_2^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= \frac{1}{2} \int_V \int_S \left( \frac{\mu}{4\pi} \frac{d^2}{d\varepsilon_2^2} B_{22} + \frac{\mu}{4\pi(1-\nu)} \frac{d^2}{d\varepsilon_2^2} C_{22} \right) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudvd\tilde{u}\tilde{v} \\
&= \frac{\mu b^2}{4\pi} \int_V \int_S \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{2u}(u, v) \varphi_{2\tilde{u}}(\tilde{u}, \tilde{v}) dudvd\tilde{u}\tilde{v} \\
&\quad + \frac{\mu b^2}{4\pi(1-\nu)} \int_V \int_S \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{2v}(u, v) \varphi_{2\tilde{v}}(\tilde{u}, \tilde{v}) dudvd\tilde{u}\tilde{v} \\
&= \frac{\mu b^2 l_1 l_2}{2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 |\widehat{\varphi}_2|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} + \frac{\mu b^2 l_1 l_2}{2(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\kappa_n^2 |\widehat{\varphi}_2|^2}{\sqrt{\xi_n^2 + \kappa_n^2}},
\end{aligned}$$

$$\begin{aligned}
& \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1 d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= -\frac{\mu}{4\pi} \int_V \int_S \left( \frac{d^2}{d\varepsilon_1 d\varepsilon_2} A_{12} + \frac{d^2}{d\varepsilon_1 d\varepsilon_2} A_{21} \right) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudvd\tilde{u}\tilde{v} \\
&\quad + \frac{\mu}{8\pi} \int_V \int_S \left( \frac{d^2}{d\varepsilon_1 d\varepsilon_2} B_{12} + \frac{d^2}{d\varepsilon_1 d\varepsilon_2} B_{21} \right) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudvd\tilde{u}\tilde{v} \\
&\quad + \frac{\mu}{8\pi(1-\nu)} \int_V \int_S \left( \frac{d^2}{d\varepsilon_1 d\varepsilon_2} C_{12} + \frac{d^2}{d\varepsilon_1 d\varepsilon_2} C_{21} \right) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudvd\tilde{u}\tilde{v} \\
&= -\frac{\mu b^2}{4\pi} \int_V \int_S \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} [\varphi_{1u}(u, v) \varphi_{2\tilde{v}}(\tilde{u}, \tilde{v}) - \varphi_{1v}(u, v) \varphi_{2\tilde{u}}(\tilde{u}, \tilde{v})] dudvd\tilde{u}\tilde{v} \\
&\quad - \frac{\mu b^2}{4\pi} \int_V \int_S \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} [-\varphi_{2u}(u, v) \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}) + \varphi_{2v}(u, v) \varphi_{1\tilde{u}}(\tilde{u}, \tilde{v})] dudvd\tilde{u}\tilde{v} \\
&\quad - \frac{\mu b^2}{8\pi} \int_V \int_S \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} [\varphi_{2u}(u, v) \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v}) + \varphi_{1v}(u, v) \varphi_{2\tilde{u}}(\tilde{u}, \tilde{v})] dudvd\tilde{u}\tilde{v} \\
&\quad + \frac{\mu b^2}{8\pi(1-\nu)} \int_V \int_S \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{1u}(u, v) \varphi_{2\tilde{v}}(\tilde{u}, \tilde{v}) dudvd\tilde{u}\tilde{v} \\
&\quad + \frac{\mu b^2}{8\pi(1-\nu)} \int_V \int_S \frac{1}{\|(u, v) - (\tilde{u}, \tilde{v})\|} \varphi_{2v}(u, v) \varphi_{1\tilde{u}}(\tilde{u}, \tilde{v}) dudvd\tilde{u}\tilde{v} \\
&= \frac{\mu \nu b^2 l_1 l_2}{4(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n \kappa_n}{\sqrt{\xi_n^2 + \kappa_n^2}} \left( \widehat{\varphi}_1 \overline{\widehat{\varphi}_2} + \widehat{\varphi}_2 \overline{\widehat{\varphi}_1} \right).
\end{aligned}$$

We also have

$$\begin{aligned}
& \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_k d\delta} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= \frac{1}{2} \sum_{i=1}^2 \sum_{j=1}^2 \int_V \int_S \left( -\frac{\mu}{2\pi} \frac{d^2}{d\varepsilon_k d\delta} A_{ij} + \frac{\mu}{4\pi} \frac{d^2}{d\varepsilon_k d\delta} B_{ij} + \frac{\mu}{4\pi(1-\nu)} \frac{d^2}{d\varepsilon_k d\delta} C_{ij} \right) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudvd\tilde{u}\tilde{v} \\
&= 0,
\end{aligned}$$



$$\begin{aligned}
& \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= \frac{1}{2} \sum_{i=1}^2 \sum_{j=1}^2 \int_V \int_S \left( -\frac{\mu}{2\pi} \frac{d^2}{d\delta^2} A_{ij} + \frac{\mu}{4\pi} \frac{d^2}{d\delta^2} B_{ij} + \frac{\mu}{4\pi(1-\nu)} \frac{d^2}{d\delta^2} C_{ij} \right) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudvd\tilde{u}\tilde{v} \\
&= \frac{\mu}{4\pi} \int_V \int_S \frac{2b^2}{D^2} \frac{|\psi(u, v) - \psi(\tilde{u}, \tilde{v})|^2}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} dudvd\tilde{u}\tilde{v} \\
&\quad + \frac{\mu}{8\pi} \int_V \int_S \frac{(-4b^2)}{D^2} \frac{|\psi(u, v) - \psi(\tilde{u}, \tilde{v})|^2}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} dudvd\tilde{u}\tilde{v} \\
&\quad + \frac{\mu b^2}{4\pi(1-\nu)D^2} \int_V \int_S \left[ \psi_u(u, v) \psi_{\tilde{u}}(\tilde{u}, \tilde{v}) \frac{(v - \tilde{v})^2}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} \right. \\
&\quad \left. + \psi_u(u, v) \psi_{\tilde{v}}(\tilde{u}, \tilde{v}) \frac{(u - \tilde{u})(v - \tilde{v})}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} + \psi_v(u, v) \psi_{\tilde{u}}(\tilde{u}, \tilde{v}) \frac{(u - \tilde{u})(v - \tilde{v})}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} \right. \\
&\quad \left. + \psi_v(u, v) \psi_{\tilde{v}}(\tilde{u}, \tilde{v}) \frac{(u - \tilde{u})^2}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} \right] dudvd\tilde{u}\tilde{v} \\
&= \frac{\mu b^2}{4\pi(1-\nu)D^2} \int_V \int_S \left[ \psi_u(u, v) \psi_{\tilde{u}}(\tilde{u}, \tilde{v}) \frac{(v - \tilde{v})^2}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} \right. \\
&\quad \left. + \psi_u(u, v) \psi_{\tilde{v}}(\tilde{u}, \tilde{v}) \frac{(u - \tilde{u})(v - \tilde{v})}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} + \psi_v(u, v) \psi_{\tilde{u}}(\tilde{u}, \tilde{v}) \frac{(u - \tilde{u})(v - \tilde{v})}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} \right. \\
&\quad \left. + \psi_v(u, v) \psi_{\tilde{v}}(\tilde{u}, \tilde{v}) \frac{(u - \tilde{u})^2}{\|(u, v) - (\tilde{u}, \tilde{v})\|^3} \right] dudvd\tilde{u}\tilde{v} \\
&= \frac{2\mu b^2 l_1 l_2}{(1-\nu)D^2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 \kappa_n^2}{(\xi_n^2 + \kappa_n^2)^{\frac{3}{2}}} |\hat{\psi}|^2. \tag{22}
\end{aligned}$$

Here we have used

$$\begin{aligned}
\left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} &= \frac{\mu b^2}{4\pi(1-\nu)D^2} \int_V [\psi_{\tilde{u}}(\tilde{u}, \tilde{v}) f_{11}(\tilde{u}, \tilde{v}) + \psi_{\tilde{v}}(\tilde{u}, \tilde{v}) f_{21}(\tilde{u}, \tilde{v}) \\
&\quad + \psi_{\tilde{u}}(\tilde{u}, \tilde{v}) f_{12}(\tilde{u}, \tilde{v}) + \psi_{\tilde{v}}(\tilde{u}, \tilde{v}) f_{22}(\tilde{u}, \tilde{v})] d\tilde{u}\tilde{v},
\end{aligned}$$

where

$$f_{11}(\tilde{u}, \tilde{v}) = \int_{\mathbf{R}^2} \psi_u(u, v) \frac{\partial^2}{\partial v^2} \|(u, v) - (\tilde{u}, \tilde{v})\| dudv,$$

$$f_{21}(\tilde{u}, \tilde{v}) = \int_{\mathbf{R}^2} \psi_u(u, v) \frac{\partial^2}{\partial u \partial v} \|(u, v) - (\tilde{u}, \tilde{v})\| dudv,$$

$$f_{12}(\tilde{u}, \tilde{v}) = \int_{\mathbf{R}^2} \psi_v(u, v) \frac{\partial^2}{\partial u \partial v} \|(u, v) - (\tilde{u}, \tilde{v})\| dudv,$$

$$f_{22}(\tilde{u}, \tilde{v}) = \int_{\mathbf{R}^2} \psi_v(u, v) \frac{\partial^2}{\partial u^2} \|(u, v) - (\tilde{u}, \tilde{v})\| dudv.$$

The Fourier transforms of these functions are

$$\begin{aligned}
\widehat{f_{11}}(\xi_n, \kappa_n) &= \frac{1}{l_1 l_2} \int_V f_{11}(\tilde{u}, \tilde{v}) e^{-i(\xi_n \tilde{u} + \kappa_n \tilde{v})} d\tilde{u} d\tilde{v} \\
&= \frac{1}{l_1 l_2} \int_V e^{-i(\xi_n \tilde{u} + \kappa_n \tilde{v})} d\tilde{u} d\tilde{v} \int_{\mathbf{R}^2} \psi_u(u, v) \frac{\partial^2}{\partial^2 v^2} \|(u, v) - (\tilde{u}, \tilde{v})\| dudv \\
&= \frac{1}{l_1 l_2} \int_V e^{-i(\xi_n \tilde{u} + \kappa_n \tilde{v})} d\tilde{u} d\tilde{v} \int_{\mathbf{R}^2} \psi_{\tilde{u}}(\tilde{u} - u, \tilde{v} - v) \frac{\partial^2}{\partial^2 v^2} \|(u, v)\| dudv \\
&= \int_{\mathbf{R}^2} e^{-i(\xi_n u + \kappa_n v)} \frac{\partial^2}{\partial^2 v^2} \|(u, v)\| dudv \\
&\quad \cdot \frac{1}{l_1 l_2} \int_V e^{-i[\xi_n(\tilde{u}-u) + \kappa_n(\tilde{v}-v)]} \psi_{\tilde{u}}(\tilde{u} - u, \tilde{v} - v) d(\tilde{u} - u) d(\tilde{v} - v) \\
&= \frac{2\pi \kappa_n^2}{(\xi_n^2 + \kappa_n^2)^{\frac{3}{2}}} \widehat{\psi}_u(\xi_n, \kappa_n).
\end{aligned}$$

Similarly,

$$\begin{aligned}
\widehat{f_{21}}(\xi_n, \kappa_n) &= \frac{2\pi \xi_n \kappa_n}{(\xi_n^2 + \kappa_n^2)^{\frac{3}{2}}} \widehat{\psi}_u(\xi_n, \kappa_n), \\
\widehat{f_{12}}(\xi_n, \kappa_n) &= \frac{2\pi \xi_n \kappa_n}{(\xi_n^2 + \kappa_n^2)^{\frac{3}{2}}} \widehat{\psi}_v(\xi_n, \kappa_n), \\
\widehat{f_{22}}(\xi_n, \kappa_n) &= \frac{2\pi \xi_n^2}{(\xi_n^2 + \kappa_n^2)^{\frac{3}{2}}} \widehat{\psi}_v(\xi_n, \kappa_n).
\end{aligned}$$

Eq. (22) then follows using Parseval identity.

We now find the second derivatives of  $E_{\text{local}}$ .

$$\begin{aligned}
&\frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_k d\varepsilon_l} \\
&= \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} \frac{d^2}{d\varepsilon_k d\varepsilon_l} A_i \cdot \theta_i^{\varepsilon, \delta} \log \frac{1}{r_g \theta_i^{\varepsilon, \delta}} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| dudv \\
&\quad + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} \frac{d}{d\varepsilon_k} A_i \cdot \frac{d}{d\varepsilon_l} \theta_i^{\varepsilon, \delta} \cdot \left( \log \frac{1}{r_g \theta_i^{\varepsilon, \delta}} - 1 \right) \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| dudv \\
&\quad + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} \frac{d}{d\varepsilon_l} A_i \cdot \frac{d}{d\varepsilon_k} \theta_i^{\varepsilon, \delta} \cdot \left( \log \frac{1}{r_g \theta_i^{\varepsilon, \delta}} - 1 \right) \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| dudv \\
&\quad + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} A_i \cdot \frac{d^2}{d\varepsilon_k d\varepsilon_l} \theta_i^{\varepsilon, \delta} \cdot \left( \log \frac{1}{r_g \theta_i^{\varepsilon, \delta}} - 1 \right) \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| dudv \\
&\quad - \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} A_i \cdot \frac{1}{\theta_i^{\varepsilon, \delta}} \frac{d}{d\varepsilon_k} \theta_i^{\varepsilon, \delta} \frac{d}{d\varepsilon_l} \theta_i^{\varepsilon, \delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| dudv.
\end{aligned}$$

It then follows

$$\left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1 d\varepsilon_2} \right|_{\varepsilon_1 = \varepsilon_2 = \delta = 0} = 0,$$

$$\begin{aligned}
& \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= \frac{\mu b^2 D}{4\pi(1-\nu)} \int_V \left[ 2\nu \log \frac{D}{r_g} (\varphi_{1u})^2 + (1-\nu) (\varphi_{1u})^2 \left( \log \frac{D}{r_g} - 1 \right) - (1-\nu) (\varphi_{1v})^2 \right] dudv \\
&= -\frac{\mu b^2 D}{4\pi} \int_V (\varphi_{1v})^2 dudv + \frac{\mu b^2 D}{4\pi(1-\nu)} \int_V (\varphi_{1u})^2 \left[ (1+\nu) \log \frac{D}{r_g} - (1-\nu) \right] dudv,
\end{aligned}$$

$$\begin{aligned}
& \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_2^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= \frac{\mu b^2 D}{4\pi(1-\nu)} \int_V \left[ 2\nu \log \frac{D}{r_g} (\varphi_{2v})^2 + (1-\nu) (\varphi_{2v})^2 \left( \log \frac{D}{r_g} - 1 \right) - (1-\nu) (\varphi_{2u})^2 \right] dudv \\
&= -\frac{\mu b^2 D}{4\pi} \int_V (\varphi_{2u})^2 dudv + \frac{\mu b^2 D}{4\pi(1-\nu)} \int_V (\varphi_{2v})^2 \left[ (1+\nu) \log \frac{D}{r_g} - (1-\nu) \right] dudv,
\end{aligned}$$

$$\begin{aligned}
& \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_k d\delta} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} \frac{d^2}{d\varepsilon_k d\delta} A_i \cdot \theta_i^{\varepsilon,\delta} \log \frac{1}{r_g \theta_i^{\varepsilon,\delta}} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
&\quad + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} \frac{d}{d\varepsilon_k} A_i \cdot \theta_i^{\varepsilon,\delta} \log \frac{1}{r_g \theta_i^{\varepsilon,\delta}} \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
&\quad + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} \frac{d}{d\varepsilon_k} A_i \cdot \frac{d}{d\delta} \theta_i^{\varepsilon,\delta} \cdot \left( \log \frac{1}{r_g \theta_i^{\varepsilon,\delta}} - 1 \right) \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
&\quad + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} A_i \cdot \frac{d}{d\varepsilon_k} \theta_i^{\varepsilon,\delta} \cdot \left( \log \frac{1}{r_g \theta_i^{\varepsilon,\delta}} - 1 \right) \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
&\quad + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} A_i \cdot \frac{d^2}{d\varepsilon_k d\delta} \theta_i^{\varepsilon,\delta} \cdot \left( \log \frac{1}{r_g \theta_i^{\varepsilon,\delta}} - 1 \right) \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
&\quad - \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} A_i \cdot \frac{1}{\theta_i^{\varepsilon,\delta}} \frac{d}{d\delta} \theta_i^{\varepsilon,\delta} \cdot \frac{d}{d\varepsilon_k} \theta_i^{\varepsilon,\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
&\quad + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} \frac{d}{d\delta} A_i \cdot \frac{d}{d\varepsilon_k} \theta_i^{\varepsilon,\delta} \cdot \left( \log \frac{1}{r_g \theta_i^{\varepsilon,\delta}} - 1 \right) \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
&= 0,
\end{aligned}$$

$$\begin{aligned}
& \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
= & \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} \frac{d^2}{d\delta^2} A_i \cdot \theta_i^{\varepsilon, \delta} \log \frac{1}{r_g \theta_i^{\varepsilon, \delta}} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
& + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} A_i \cdot \frac{d^2}{d\delta^2} \theta_i^{\varepsilon, \delta} \cdot \left( \log \frac{1}{r_g \theta_i^{\varepsilon, \delta}} - 1 \right) \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
& + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} A_i \cdot \theta_i^{\varepsilon, \delta} \log \frac{1}{r_g \theta_i^{\varepsilon, \delta}} \frac{d^2}{d\delta^2} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
= & \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} \frac{d^2}{d\delta^2} A_i \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} \cdot \frac{1}{D} \log \frac{D}{r_g} dudv \\
& + \int_V \frac{\mu b^2}{4\pi(1-\nu)} (1-\nu) \cdot \left( -\frac{1}{D} \psi_v^2 \right) \cdot \left( \log \frac{D}{r_g} - 1 \right) dudv \\
& + \int_V \frac{\mu b^2}{4\pi(1-\nu)} (1-\nu) \cdot \left( -\frac{1}{D} \psi_u^2 \right) \cdot \left( \log \frac{D}{r_g} - 1 \right) dudv \\
& + \sum_{i=1}^2 \int_V \frac{\mu b^2}{4\pi(1-\nu)} (1-\nu) \cdot \frac{1}{D} \log \frac{D}{r_g} (\psi_u^2 + \psi_v^2) dudv \\
= & \frac{\mu b^2}{4\pi(1-\nu)D} \int_V (\psi_u^2 + \psi_v^2) \left[ (1+\nu) \log \frac{D}{r_g} + (1-\nu) \right] dudv.
\end{aligned}$$

**Proof of Theorem 3.2:**

(i) Consider the first variations. From the lemmas above, it is easy to see that

$$\left. \frac{d}{d\delta} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = 0.$$

For the derivative with respect to  $\varepsilon_1$ , we have

$$\begin{aligned}
& \left. \frac{d}{d\varepsilon_1} E_{\text{long}}(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
= & \frac{1}{2} \sum_{i=1}^2 \sum_{j=1}^2 \int_V \int_{\mathbf{R}^2} \left[ -\frac{\mu}{2\pi} \frac{dA_{ij}}{d\varepsilon_1} + \frac{\mu}{4\pi} \frac{dB_{ij}}{d\varepsilon_1} + \frac{\mu}{4\pi(1-\nu)} \frac{dC_{ij}}{d\varepsilon_1} \right] \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv d\tilde{u} d\tilde{v} \\
= & \frac{1}{2} \int_V \int_{\mathbf{R}^2} \left[ -\frac{\mu b^2}{2\pi D} \frac{\varphi_{1v}(u, v) + \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v})}{\|(u, v) - (\tilde{u}, \tilde{v})\|} + \frac{\mu b^2}{2\pi D} \frac{\varphi_{1v}(u, v) + \varphi_{1\tilde{v}}(\tilde{u}, \tilde{v})}{\|(u, v) - (\tilde{u}, \tilde{v})\|} + 0 \right] dudv d\tilde{u} d\tilde{v} \\
= & 0.
\end{aligned}$$

$$\begin{aligned}
& \left. \frac{d}{d\varepsilon_1} E_{\text{local}}(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
= & \frac{\mu b^2}{4\pi(1-\nu)} \int_V \log \frac{D}{er_g} \frac{d\|\nabla_{S^\delta} \eta_1^\varepsilon\|}{d\varepsilon_1} \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} dudv \\
= & \frac{\mu b^2}{4\pi(1-\nu)} \log \frac{D}{er_g} \int_V \varphi_v(u, v) dudv \\
= & 0.
\end{aligned}$$

The last equation is due to the periodicity of  $\varphi$ .

Thus

$$\frac{d}{d\varepsilon_1} E(\eta^\varepsilon, S^\delta) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} = \frac{d}{d\varepsilon_1} E_{\text{long}}(\eta^\varepsilon, S^\delta) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} + \frac{d}{d\varepsilon_1} E_{\text{local}}(\eta^\varepsilon, S^\delta) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} = 0.$$

Similarly, we have

$$\frac{d}{d\varepsilon_2} E(\eta^\varepsilon, S^\delta) \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} = 0.$$

(ii) Consider the second variations. Using **Proposition 1**, we have

$$\begin{aligned} & \frac{d^2 E(\eta^\varepsilon, S^\delta)}{d\varepsilon_1^2} \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} \\ = & \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1^2} \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} + \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1^2} \Big|_{\varepsilon_1=\varepsilon_2=\delta=0} \\ = & \frac{\mu b^2 l_1 l_2}{2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\kappa_n^2 |\widehat{\varphi}_1|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} + \frac{\mu b^2 l_1 l_2}{2(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 |\widehat{\varphi}_1|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} \\ & - \frac{\mu b^2 D}{4\pi} \int_V (\varphi_{1v})^2 dudv + \frac{\mu b^2 D}{4\pi(1-\nu)} \int_V (\varphi_{1u})^2 \left[ (1+\nu) \log \frac{D}{r_g} - (1-\nu) \right] dudv \\ = & \frac{\mu b^2 l_1 l_2}{2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\kappa_n^2 |\widehat{\varphi}_1|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} + \frac{\mu b^2 l_1 l_2}{2(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 |\widehat{\varphi}_1|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} \\ & - \frac{\mu b^2 D l_1 l_2}{4\pi} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \kappa_n^2 |\widehat{\varphi}_1|^2 \\ & + \frac{\mu b^2 D l_1 l_2}{4\pi(1-\nu)} \left[ (1+\nu) \log \frac{D}{r_g} - (1-\nu) \right] \sum_{(\xi_n, \kappa_n^2) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \xi_n^2 |\widehat{\varphi}_1|^2, \end{aligned}$$

$$\begin{aligned}
& \left. \frac{d^2 E(\eta^\varepsilon, S^\delta)}{d\varepsilon_2^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
= & \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_2^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} + \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_2^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
= & \frac{\mu b^2 l_1 l_2}{2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 |\widehat{\varphi}_2|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} + \frac{\mu b^2 l_1 l_2}{2(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\kappa_n^2 |\widehat{\varphi}_2|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} \\
& - \frac{\mu b^2 D}{4\pi} \int_V (\varphi_{2u})^2 dudv \\
& + \frac{\mu b^2 D}{4\pi(1-\nu)} \int_V (\varphi_{2v})^2 \left[ (1+\nu) \log \frac{D}{r_g} - (1-\nu) \right] dudv \\
= & \frac{\mu b^2 l_1 l_2}{2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 |\widehat{\varphi}_2|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} + \frac{\mu b^2 l_1 l_2}{2(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\kappa_n^2 |\widehat{\varphi}_2|^2}{\sqrt{\xi_n^2 + \kappa_n^2}} \\
& - \frac{\mu b^2 D l_1 l_2}{4\pi} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \xi_n^2 |\widehat{\varphi}_2|^2 \\
& + \frac{\mu b^2 D l_1 l_2}{4\pi(1-\nu)} \left[ (1+\nu) \log \frac{D}{r_g} - (1-\nu) \right] \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \kappa_n^2 |\widehat{\varphi}_2|^2,
\end{aligned}$$

$$\begin{aligned}
& \left. \frac{d^2 E(\eta^\varepsilon, S^\delta)}{d\varepsilon_1 d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = \left. \frac{d^2 E(\eta^\varepsilon, S^\delta)}{d\varepsilon_2 d\varepsilon_1} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
= & \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1 d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} + \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_1 d\varepsilon_2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
= & \frac{\mu \nu b^2 l_1 l_2}{4(1-\nu)} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n \kappa_n}{\sqrt{\xi_n^2 + \kappa_n^2}} \left( \widehat{\varphi}_1 \widehat{\varphi}_2 + \widehat{\varphi}_2 \widehat{\varphi}_1 \right),
\end{aligned}$$

$$\begin{aligned}
& \left. \frac{d^2 E(\eta^\varepsilon, S^\delta)}{d\varepsilon_k d\delta} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
= & \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_k d\delta} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} + \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\varepsilon_k d\delta} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} = 0.
\end{aligned}$$

$$\begin{aligned}
& \left. \frac{d^2}{d\delta^2} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= \left. \frac{d^2 E_{\text{long}}(\eta^\varepsilon, S^\delta)}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} + \left. \frac{d^2 E_{\text{local}}(\eta^\varepsilon, S^\delta)}{d\delta^2} \right|_{\varepsilon_1=\varepsilon_2=\delta=0} \\
&= \frac{2\mu b^2 l_1 l_2}{(1-\nu) D^2} \sum_{(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}} \frac{\xi_n^2 \kappa_n^2}{(\xi_n^2 + \kappa_n^2)^{\frac{3}{2}}} |\widehat{\psi}|^2 \\
&\quad + \frac{\mu b^2}{4\pi(1-\nu) D} \int_V (\psi_u^2 + \psi_v^2) \left[ (1+\nu) \log \frac{D}{r_g} + (1-\nu) \right] dudv.
\end{aligned}$$

Therefore, the second variation matrix at  $\varepsilon_1 = \varepsilon_2 = \delta = 0$  takes the form

$$\left( \begin{array}{ccc}
\left. \frac{d^2}{d\varepsilon_1^2} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} & \left. \frac{d^2}{d\varepsilon_1 d\varepsilon_2} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} & 0 \\
\left. \frac{d^2}{d\varepsilon_2 d\varepsilon_1} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} & \left. \frac{d^2}{d\varepsilon_2^2} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0} & 0 \\
0 & 0 & \left. \frac{d^2}{d\delta^2} E(\eta^\varepsilon, S^\delta) \right|_{\varepsilon_1=\varepsilon_2=\delta=0}
\end{array} \right).$$

It is easy to see that this matrix is semipositive definite when

$$\frac{1}{\sqrt{\xi_n^2 + \kappa_n^2}} - \frac{D}{2\pi} \geq 0, \quad (23)$$

for all  $(\xi_n, \kappa_n) \in \frac{2\pi}{l_1} \mathbf{Z} \times \frac{2\pi}{l_2} \mathbf{Z}$ . If we use the perturbation wavelengths  $\lambda_1 = 2\pi/\xi_n$  and  $\lambda_2 = 2\pi/\kappa_n$  in the  $x$  and  $y$  directions, respectively, this condition is the one in Eq. (18) in the theorem. Note that the  $-\frac{D}{2\pi}$  term in Eq. (23) is destabilizing and comes from the local energy  $E_{\text{local}}$ , which is due to perturbations in the direction normal to the constituent dislocations. This instability is stabilized by the long-range energy  $E_{\text{long}}$  when the perturbation wavelengths are not very small so that the condition in Eq. (18) is satisfied.

We can also conclude from these expressions of the second variations that the dislocation structure in the theorem is strictly stable to nonzero perturbations.

**5. Derivatives with respect to  $\varepsilon$  and  $\delta$ .** In this last section, we present the derivatives with respect to  $\varepsilon = (\varepsilon_1, \dots, \varepsilon_J)$ , and  $\delta$  of those terms in the expressions of  $E_{\text{long}}$  and  $E_{\text{local}}$  in Eqs. (19) and (20). Note that these results hold for general periodic grain boundary  $S$  (could be nonplanar) with  $J$  arrays of dislocations on it.

**Lemma 5.1.** *The followings hold for  $A_{ij}$ .*

$$\begin{aligned}
\frac{d}{d\delta} A_{ij} &= \frac{d}{d\delta} a_{ij} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \\
&\quad + a_{ij} \left( \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| + \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \right); \\
\frac{d^2}{d\delta^2} A_{ij} &= a_{ij} \cdot \left( \frac{d^2}{d\delta^2} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| + \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d^2}{d\delta^2} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| + 2 \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \right) \\
&\quad + 2 \frac{d}{d\delta} a_{ij} \left( \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| + \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \right) \\
&\quad + \frac{d^2}{d\delta^2} a_{ij} \cdot \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\|;
\end{aligned}$$

$$\begin{aligned}\frac{d}{d\varepsilon_k}A_{ij} &= \frac{\|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\|}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \frac{d}{d\varepsilon_k}L_{ij}; \\ \frac{d^2}{d\varepsilon_k d\varepsilon_l}A_{ij} &= \frac{\|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\|}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \frac{d^2}{d\varepsilon_k d\varepsilon_l}L_{ij};\end{aligned}$$

$$\begin{aligned}\frac{d^2}{d\delta d\varepsilon_k}A_{ij} &= \frac{d^2}{d\delta d\varepsilon_k}a_{ij} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \\ &\quad + \frac{1}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \left( \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| + \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \right) \frac{d}{d\varepsilon_k}L_{ij};\end{aligned}$$

$$\frac{d}{d\delta}a_{ij} = \frac{1}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \frac{d}{d\delta}L_{ij} - \frac{L_{ij}}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|^2} \frac{d}{d\delta} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|;$$

$$\begin{aligned}\frac{d}{d\delta}L_{ij} &= \left( \frac{d}{d\delta} \nabla_{S^s} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right) \times \left( \nabla_{S^s} \eta_j(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \right) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)}) \\ &\quad + \left( \nabla_{S^s} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \frac{d}{d\delta} \mathbf{n}^\delta(u, v) \right) \times \left( \nabla_{S^s} \eta_j(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \right) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)}) \\ &\quad + \left( \nabla_{S^s} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right) \times \left( \frac{d}{d\delta} \nabla_{S^s} \eta_j(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \right) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)}) \\ &\quad + \left( \nabla_{S^s} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right) \times \left( \nabla_{S^s} \eta_j(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \frac{d}{d\delta} \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \right) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)}); \end{aligned}$$

$$\begin{aligned}\frac{d}{d\varepsilon_k}L_{ij} &= \left( \frac{d}{d\varepsilon_k} \nabla_{S^s} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right) \times \left( \nabla_{S^s} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \right) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)}) \\ &\quad + \left( \nabla_{S^s} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right) \times \left( \frac{d}{d\varepsilon_k} \nabla_{S^s} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \right) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)}); \end{aligned}$$

$$\begin{aligned}\frac{d^2}{d\delta^2}L_{ij} &= \frac{d^2}{d\delta^2} \left( \nabla_{S^s} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right) \times \left( \nabla_{S^s} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \right) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)}) \\ &\quad + \left( \nabla_{S^s} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right) \times \frac{d^2}{d\delta^2} \left( \nabla_{S^s} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \right) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)}) \\ &\quad + 2 \frac{d}{d\delta} \left( \nabla_{S^s} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \right) \times \frac{d}{d\delta} \left( \nabla_{S^s} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \right) \cdot (\mathbf{b}^{(i)} \times \mathbf{b}^{(j)}); \end{aligned}$$

$$\begin{aligned}\frac{d^2}{d\delta^2}a_{ij} &= \frac{1}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \frac{d^2}{d\delta^2}L_{ij} + 2 \frac{d}{d\delta}L_{ij} \cdot \frac{d}{d\delta} \frac{1}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \\ &\quad + L_{ij} \frac{d^2}{d\delta^2} \frac{1}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|}; \end{aligned}$$

$$\begin{aligned}\frac{d^2}{d\delta d\varepsilon_k}a_{ij} &= \frac{1}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|} \frac{d^2}{d\delta d\varepsilon_k}L_{ij} \\ &\quad - \frac{1}{\|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|^2} \frac{d}{d\varepsilon_k}L_{ij} \cdot \frac{d}{d\delta} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\|; \end{aligned}$$







**Lemma 5.3.** *The followings hold for  $C_{ij}$ .*

$$\begin{aligned} \frac{d}{d\delta} C_{ij} &= \frac{d}{d\delta} c_{ij} \cdot \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \\ &\quad + c_{ij} \left( \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| + \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \right); \end{aligned}$$

$$\begin{aligned} \frac{d^2}{d\delta^2} C_{ij} &= \frac{d^2}{d\delta^2} c_{ij} \cdot \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \\ &\quad + 2 \frac{d}{d\delta} c_{ij} \cdot \left( \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| + \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \right) \\ &\quad + c_{ij} \cdot \left( \frac{d^2}{d\delta^2} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| + \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d^2}{d\delta^2} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \right. \\ &\quad \left. + 2 \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \right); \end{aligned}$$

$$\begin{aligned} \frac{d}{d\varepsilon_k} C_{ij} &= \frac{d}{d\varepsilon_k} c_{ij} \cdot \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\|; \\ \frac{d^2}{d\varepsilon_k d\varepsilon_l} C_{ij} &= \frac{d^2}{d\varepsilon_k d\varepsilon_l} c_{ij} \cdot \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\|; \end{aligned}$$

$$\begin{aligned} \frac{d^2}{d\delta d\varepsilon_k} C_{ij} &= \frac{d^2}{d\delta d\varepsilon_k} c_{ij} \cdot \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \\ &\quad + \frac{d}{d\varepsilon_k} c_{ij} \left( \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| + \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \frac{d}{d\delta} \|\mathbf{r}_u^\delta \times \mathbf{r}_v^\delta\| \right); \end{aligned}$$

$$\begin{aligned} \frac{d}{d\delta} c_{ij} &= \frac{d}{d\delta} \left( \nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\ &\quad \cdot \left( \nabla_{S^\delta} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\ &\quad + \left( \nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\ &\quad \cdot \frac{d}{d\delta} \left( \nabla_{S^\delta} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\ &\quad + \left( \nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \frac{d}{d\delta} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\ &\quad \cdot \left( \nabla_{S^\delta} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right); \end{aligned}$$

$$\begin{aligned} \frac{d}{d\varepsilon_k} c_{ij} &= \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\ &\quad \cdot \left( \nabla_{S^\delta} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\ &\quad + \left( \nabla_{S^\delta} \eta_i^\varepsilon(\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\ &\quad \cdot \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_j^\varepsilon(\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right); \end{aligned}$$

$$\begin{aligned}
\frac{d^2}{d\varepsilon_k d\varepsilon_l} c_{ij} &= \left( \frac{d^2}{d\varepsilon_k d\varepsilon_l} \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&\quad + \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \frac{d}{d\varepsilon_l} \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&\quad + \left( \frac{d}{d\varepsilon_l} \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&\quad + \left( \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \frac{d^2}{d\varepsilon_k d\varepsilon_l} \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&= \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \frac{d}{d\varepsilon_l} \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&\quad + \left( \frac{d}{d\varepsilon_l} \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right);
\end{aligned}$$

$$\begin{aligned}
\frac{d^2}{d\varepsilon_k d\delta} c_{ij} &= \frac{d}{d\delta} \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&\quad + \frac{d}{d\delta} \left( \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&\quad + \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \frac{d}{d\delta} \left( \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&\quad + \left( \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \frac{d}{d\delta} \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&\quad + \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \frac{d}{d\delta} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right) \\
&\quad + \left( \nabla_{S^\delta} \eta_i^\varepsilon (\mathbf{r}^\delta(u, v)) \times \mathbf{n}^\delta(u, v) \times \mathbf{b}^{(i)} \right) \cdot \nabla_{\mathbf{r}^\delta(u, v)} \otimes \nabla_{\mathbf{r}^\delta(u, v)} \frac{d}{d\delta} \|\mathbf{r}^\delta(u, v) - \mathbf{r}^\delta(\tilde{u}, \tilde{v})\| \\
&\quad \cdot \left( \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_j^\varepsilon (\mathbf{r}^\delta(\tilde{u}, \tilde{v})) \times \mathbf{n}^\delta(\tilde{u}, \tilde{v}) \times \mathbf{b}^{(j)} \right);
\end{aligned}$$





**Lemma 5.5.** *The followings hold for  $\theta_i^{\varepsilon, \delta}$ .*

$$\begin{aligned} \frac{d\theta_i^{\varepsilon, \delta}}{d\varepsilon_k} &= \delta_{ik} \frac{\varepsilon_i \|\nabla_{S^\delta} \varphi_i\|^2 + \nabla_{S^\delta} \eta_i \cdot \nabla_{S^\delta} \varphi_i}{\theta_i^{\varepsilon, \delta}}; \\ \frac{d\theta_i^{\varepsilon, \delta}}{d\delta} &= \frac{\frac{d}{d\delta} \nabla_{S^\delta} \eta_i^\varepsilon \cdot \nabla_{S^\delta} \eta_i^\varepsilon}{\theta_i^{\varepsilon, \delta}}; \\ \frac{d^2 \theta_i^{\varepsilon, \delta}}{d\varepsilon_k d\varepsilon_l} &= \frac{\|\nabla_{S^\delta} \eta_i \times \nabla_{S^\delta} \varphi_i\|^2}{\left(\theta_i^{\varepsilon, \delta}\right)^3} \delta_{il} \delta_{ik}; \\ \frac{d^2 \theta_i^{\varepsilon, \delta}}{d\varepsilon_k d\delta} &= \frac{\frac{d}{d\delta} \nabla_{S^\delta} \eta_i^\varepsilon \cdot \frac{d}{d\varepsilon_k} \nabla_{S^\delta} \eta_i^\varepsilon + \frac{d^2}{d\delta d\varepsilon_k} \nabla_{S^\delta} \eta_i^\varepsilon \cdot \nabla_{S^\delta} \eta_i^\varepsilon}{\theta_i^{\varepsilon, \delta}} \\ &\quad - \frac{\frac{d}{d\delta} \nabla_{S^\delta} \eta_i^\varepsilon \cdot \nabla_{S^\delta} \eta_i^\varepsilon}{\left(\theta_i^{\varepsilon, \delta}\right)} \cdot \frac{\varepsilon_i \|\nabla_{S^\delta} \varphi_i\|^2 + \nabla_{S^\delta} \eta_i \cdot \nabla_{S^\delta} \varphi_i}{\theta_i^{\varepsilon, \delta}} \delta_{ik}; \\ \frac{d^2 \theta_i^{\varepsilon, \delta}}{d\delta^2} &= \frac{\frac{d^2}{d\delta^2} \nabla_{S^\delta} \eta_i^\varepsilon \cdot \nabla_{S^\delta} \eta_i^\varepsilon + \frac{d}{d\delta} \nabla_{S^\delta} \eta_i^\varepsilon \cdot \frac{d}{d\delta} \nabla_{S^\delta} \eta_i^\varepsilon}{\theta_i^{\varepsilon, \delta}} - \frac{\left(\frac{d}{d\delta} \nabla_{S^\delta} \eta_i^\varepsilon \cdot \nabla_{S^\delta} \eta_i^\varepsilon\right)^2}{\left(\theta_i^{\varepsilon, \delta}\right)^3}. \end{aligned}$$

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