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OF SINGLE DISLOCATIONS

by

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NON-LINEAR EFFECTS IN THE ELASTIC FIELD OF SINGLE DISLOCATIONS

I. ITERATION SCHEME FOR SOLVING NON-LINEAR DISLOCATION PROBLEMS

by C. TEODOSIU * and E. SOÓS **

The present paper deals with the extension of Willis' iteration scheme for the determination of the non-linear elastic field produced by single dislocation loops in anisotropic bodies. The first part of the paper gives the Eulerian formulation of the boundary-value problem for both finite and infinite media, under consideration of the core boundary conditions. The uniqueness of the solutions to the successive linear boundary-value problems occurring in the iteration scheme, and the complementary conditions at infinity are discussed in some detail. The second part of the paper will be devoted to the determination of the second-order elastic effects produced by an edge dislocation in an infinite anisotropic medium.

INTRODUCTION

The first systematic iterative method for the solution of non-linear elastic boundary-value problems has been elaborated by Signorini [1], who further developed his ideas in [2, 3]. Willis [4] has adapted Signorini's scheme to the case of continuous distributions of dislocations by using Eulerian co-ordinates

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and Green's function techniques. He has also treated the case of a screw dislocation in an infinite anisotropic elastic medium by ignoring, however, the core conditions.

Alternative iteration schemes using Lagrangian co-ordinates have been also developed and applied for determining the non-linear elastic field of screw and edge dislocations in anisotropic media by Seeger and Mann [5] , Teodosiu [6] , vol. 2, Sect. 15, Seeger, Teodosiu, and Petrasch [7] . However, as shown by Petrasch [8] and by the present authors [9] , the Eulerian formulation should be generally preferred, since it avoids the rather complicated discussion implied by the correct formulation of the boundary-value problem in terms of Lagrangian co-ordinates.

In the first part of this paper, Willis' scheme in Eulerian co-ordinates will be extended to include the influence of the core conditions on the non-linear elastic field produced by single dislocation loops in anisotropic finite bodies or infinite media. A special attention is given to the conditions assuring the uniqueness of the solutions to the successive linear boundary-value problems, as well as to the complementary conditions to be fulfilled for unbounded media.

In the second part of the paper, the iteration scheme will be applied to determine the second-order effects produced by an edge dislocation lying along a two-fold symmetry axis in an infinite anisotropic elastic medium. In particular, the results obtained by Seeger, Teodosiu, and Petrasch [7] are completed and partly corrected; by removing some residual discontinuities occurring across the cut surface in the second step of the iteration, which are shown to correspond to a generalized Somigliana dislocation [10] . Similar results have been obtained by Petrasch

[8] in the particular case of the orthotropic medium, by using a different reasoning based on symmetry and continuity conditions.

1. EULERIAN FORMULATION OF THE BOUNDARY-VALUE PROBLEM

Consider an elastic body \mathcal{B} free of body forces and surface tractions, occupying a simply-connected region \mathcal{V} bounded by a surface \mathcal{A} , and containing a single dislocation loop of line L . Denote by (k) this configuration of \mathcal{B} and by \underline{x} the position vector of a current particle X of \mathcal{B} in (k) .

We apply the (non-linear) elasticity theory outside a thin tube \mathcal{V}_0 of boundary \mathcal{O}_0 having the dislocation line as axis and with circular cross section of radius r_0 , and denote $\mathcal{V}_0 = \mathcal{V} \setminus \mathcal{V}_0$. It has been shown in [9] that the boundary-value problem associated with the determination of the elastic state produced by the dislocation loop may be given the following Eulerian formulation.

Find an invertible second-order tensor field $\underline{\underline{A}} = \underline{\underline{A}}(\underline{x})$ of class C^1 in \mathcal{V}_0 that satisfies the equilibrium equations

$$\operatorname{div} \underline{\underline{T}} = \underline{\underline{0}}, \quad T_{kl,l} = 0, \quad (1.1)$$

the constitutive equations

$$\underline{\underline{T}} = j \underline{\underline{A}} \frac{\partial W(\underline{\underline{D}})}{\partial \underline{\underline{D}}} \underline{\underline{A}}^T, \quad T_{kl} = j A_{km} \frac{\partial W(\underline{\underline{D}})}{\partial D_{mn}} A_{ln}, \quad (1.2)$$

the jump condition

$$\int_c \underline{\underline{A}}^{-1}(\underline{x}) d\underline{x} = \underline{\underline{b}}, \quad \int_c \underline{\underline{A}}_{kl}^{-1}(\underline{x}) dx_l = b_k, \quad (1.3)$$

and the boundary conditions

$$\underline{T} \underline{n} = \begin{cases} \underline{0} & \text{on } \Delta \\ \underline{\hat{t}} & \text{on } \sigma_0, \end{cases} \quad T_{kl} n_l = \begin{cases} 0 & \text{on } \Delta \\ \hat{t}_k & \text{on } \sigma_0, \end{cases} \quad (1.4)$$

where \underline{A} is the elastic distortion, \underline{T} is the Cauchy stress tensor, W is the strain-energy density per unit underformed volume,

$$\underline{D} = \frac{1}{2} (\underline{A}^T \underline{A} - \underline{1}), \quad D_{kl} = \frac{1}{2} (A_{pk} A_{pl} - \delta_{kl}) \quad (1.5)$$

is the finite strain tensor,

$$j = \det \underline{A}^{-1} > 0, \quad (1.6)$$

\underline{c} denotes any smooth curve which encircles once τ_0 in the right-handed sense with respect to the positive sense chosen on L , \underline{b} is the true Burgers vector of the dislocation, \underline{n} is the outward unit normal to $\Delta \cup \sigma_0$, and $\underline{\hat{t}}$ is the traction acting on σ_0 from the dislocation core τ_0 . Here and in the following we write the main relationships both in direct notation and in the rectangular Cartesian component form.

The value of $\underline{\hat{t}}$ may be determined only by combining the elastic model with the atomistic model of the dislocation core, by using a semidiscrete method. For stationary dislocations, since the dislocated body is in equilibrium, we must require that the resultant force \underline{P} and couple \underline{M} of the tractions acting on σ_0 vanish, i.e.

$$\underline{P} \equiv \int_{\sigma_0} \underline{\hat{t}} \, ds = \underline{0}, \quad (1.7)$$

$$\underline{M} \equiv \int_{\sigma_0} \underline{x} \times \underline{\hat{t}} \, ds = \underline{0}. \quad (1.8)$$

From (1.3) it follows [9] that

$$\underline{A}^{-1} = \text{grad } \chi^*, \quad A_{kl}^{-1} = \chi_{k,l}^*, \quad (1.9)$$

where $\underline{\chi}^*$ is a class C^2 vector field in V_0 defined by

$$\underline{\chi}^*(\underline{x}) = \underline{\chi}_0^* + \int_{\underline{x}_0}^{\underline{x}} \underline{A}^{-1}(\underline{x}) d\underline{x}. \quad (1.10)$$

The line integral in (1.10) is to be calculated on any smooth curve in V_0 connecting an arbitrary fixed point $\underline{x}_0 \in V_0$ with the current point \underline{x} , while $\underline{\chi}_0^*$ is an arbitrary constant vector. By (1.3), $\underline{\chi}^*$ is generally a multiple-valued function having b as cyclic period.

Alternatively, we may obtain a single-valued function $\underline{\chi}^*$ satisfying (1.9) by introducing a two-sided barrier s bounded by L and rendering V_0 simply-connected. Let s_0 be the part of s outside \mathcal{C}_0 , and \underline{n} the unit normal to s_0 directed in the right-handed sense with respect to the positive sense on L . Denote by s_0^+ the face of s_0 into which points \underline{n} and by s_0^- the opposite face of s_0 . Then, from (1.3) and (1.9) it follows that $\underline{\chi}^*$ is of class C^2 in $V_0 \setminus s_0$ and satisfies the jump relation

$$\underline{\chi}^*(\underline{x}^+) - \underline{\chi}^*(\underline{x}^-) = -b \quad \text{for } \underline{x} \in s_0. \quad (1.11)$$

Here and in the following the superscripts $+$ and $-$ are used to distinguish between the limiting values on s_0^+ and s_0^- , respectively.

By introducing the displacement field \underline{u}^* , defined by

$$\underline{u}^*(\underline{x}) = \underline{x} - \underline{\chi}^*(\underline{x}) \quad (1.12)$$

relations (1.11) and (1.9) become

$$\underline{u}^*(\underline{x}^+) - \underline{u}^*(\underline{x}^-) = b \quad \text{for } \underline{x} \in s_0, \quad (1.13)$$

$$\underline{A}^{-1} = \underline{1} - \underline{H}^*, \quad \underline{A}_{km}^{-1} = \delta_{km} - H_{km}^*, \quad (1.14)$$

where \underline{H}^* is the displacement gradient given by

$$\underline{H}^* = \text{grad } \underline{u}^*, \quad H_{km}^* = u_{k,m}^*. \quad (1.15)$$

We may now formulate the boundary-value problem in terms of \underline{u}^* as follows. Find a (single-valued) vector field $\underline{u}^* = \underline{u}^*(\underline{x})$ of class C^2 in $V_0 \setminus s_0$ that satisfies the jump condition (1.13) on s_0 and whose gradient \underline{H}^* satisfies the field equations (1.1), (1.2), and (1.14), and the boundary conditions (1.4).

On physical grounds we should require the continuity of the stress vector $\underline{t} = \underline{T} \underline{n}$ through the barrier s_0 . In our case, however, this condition is merely a consequence of the assumed continuity of \underline{A} through s_0 and of the constitutive equation (1.2).

2. ITERATION SCHEME

We will solve the non-linear boundary-value problem formulated in the preceding section by an iteration scheme, based on the following hypotheses :

(i) The prescribed traction on σ_0 and the true Burgers vector are proportional to a small parameter ε , i.e.

$$\hat{\underline{t}} = \varepsilon \hat{\underline{t}}^{(1)}, \quad \underline{b} = \varepsilon \underline{b}^{(1)}. \quad (2.1)$$

This hypothesis is justified by the fact that $\hat{\underline{t}}$ vanishes together with \underline{b} . The numerical choice of ε is immaterial, since it appears in the final result only through the combinations $\varepsilon \hat{\underline{t}}^{(1)}$ and $\varepsilon \underline{b}^{(1)}$.

(ii) There exists a solution $\underline{u}^*(\underline{x})$ of the boundary-value problem that depends analytically on ε and vanishes for $\varepsilon = 0$, i.e.

$$\underline{u}^* = \varepsilon \underline{u}^{*(1)} + \varepsilon^2 \underline{u}^{*(2)} + \dots \quad (2.2)$$

Let us put

$$\underline{A} = \underline{1} + \underline{H}, \quad A_{kl} = \delta_{kl} + H_{kl}. \quad (2.3)$$

Introducing (1.14) and (2.3) into the relation $\underline{A} \underline{A}^{-1} = \underline{1}$, we obtain

$$\underline{H} = \underline{H}^* + \underline{H} \underline{H}^*, \quad H_{kl} = H_{kl}^* + H_{kp} H_{pl}^*. \quad (2.4)$$

On the other hand, we have from (1.15) and (2.2)

$$H_{kl}^* = \varepsilon u_{k,l}^{*(1)} + \varepsilon^2 u_{k,l}^{*(2)} + \dots \quad (2.5)$$

and hence, by (2.4)₂,

$$H_{kl} = \varepsilon u_{k,l}^{*(1)} + \varepsilon^2 (u_{k,l}^{*(2)} + u_{k,p}^{*(1)} u_{p,l}^{*(1)}) + \dots \quad (2.6)$$

Next, substituting (2.6) into (1.5) yields

$$\begin{aligned} D_{kl} = \frac{\varepsilon}{2} (u_{k,l}^{*(1)} + u_{l,k}^{*(1)}) + \frac{\varepsilon^2}{2} (u_{k,l}^{*(2)} + u_{l,k}^{*(2)} + u_{k,p}^{*(1)} u_{p,l}^{*(1)} + \\ + u_{p,k}^{*(1)} u_{p,l}^{*(1)} + u_{p,l}^{*(1)} u_{l,p}^{*(1)}) + \dots \end{aligned} \quad (2.7)$$

In order to obtain the expansion of the stress tensor we first rewrite Eqs. (1.2) and (1.6) in the form

$$T_{kl} = j (\delta_{km} + H_{km}) \frac{\partial W(D)}{\partial D_{mn}} (\delta_{ln} + H_{ln}), \quad (2.8)$$

$$j = \det [\delta_{pq} - H_{pq}^*]. \quad (2.9)$$

Assuming that W may be developed in a power series of \underline{D} , we have

$$\frac{\partial W(D)}{\partial D_{mn}} = c_{mnpq} D_{pq} + \frac{1}{2} C_{mnpqrs} D_{pq} D_{rs} + \dots \quad (2.10)$$

where c and C are the tensors of the second- and third-order elastic constants, respectively.

Introducing now (2.7) into (2.10), (2.5) into (2.9), and putting the results obtained into (2.8), we deduce that

$$T_{kl} = \varepsilon T_{kl}^{(1)} + \varepsilon^2 T_{kl}^{(2)} + \dots \quad (2.11)$$

where

$$T_{kl}^{(1)} = c_{klmn} u_{m,n}^{*(1)}, \quad T_{kl}^{(2)} = c_{klmn} u_{m,n}^{*(2)} + \tau_{kl}, \quad (2.12)$$

$$\begin{aligned} \tau_{kl} = & -u_{m,m}^{*(1)} T_{kl}^{(1)} + u_{k,m}^{*(1)} T_{ml}^{(1)} + u_{l,m}^{*(1)} T_{km}^{(1)} + \\ & + c_{klmn} (u_{m,p}^{*(1)} u_{p,n}^{*(1)} + \frac{1}{2} u_{p,m}^{*(1)} u_{p,n}^{*(1)}) + \frac{1}{2} c_{klmnpq} u_{m,n}^{*(1)} u_{p,q}^{*(1)}. \end{aligned} \quad (2.13)$$

Substituting (2.1), (2.2), and (2.11) into (1.13), (1.1), and (1.4), and equating like powers of ϵ , we obtain a sequence of linear traction boundary-value problems, namely, at the first step

$$\left. \begin{aligned} u_k^{*(1)}(\tilde{x}^+) - u_k^{*(1)}(\tilde{x}^-) &= b_k^{(1)} \text{ for } \tilde{x} \in s_0, \\ T_{kl,l}^{(1)} &= 0, \quad T_{kl}^{(1)} = c_{klmn} u_{m,n}^{*(1)} \text{ in } v_0 \setminus s_0, \\ T_{kl}^{(1)} n_l &= \begin{cases} 0 & \text{on } s \\ \hat{t}_k^{(1)} & \text{on } \sigma_0, \end{cases} \end{aligned} \right\} \quad (2.14)$$

at the second step

$$\left. \begin{aligned} u_k^{*(2)}(\tilde{x}^+) - u_k^{*(2)}(\tilde{x}^-) &= 0 \text{ for } \tilde{x} \in s_0, \\ T_{kl,l}^{(2)} &= 0, \quad T_{kl}^{(2)} = c_{klmn} u_{m,n}^{*(2)} + \tau_{kl} \text{ in } v_0 \setminus s_0, \\ T_{kl}^{(2)} n_l &= 0 \text{ on } s \cup \sigma_0, \end{aligned} \right\} \quad (2.15)$$

and so on. In the following we will consider only the first two steps of the iteration, for the subsequent steps involve elastic constants of fourth and higher orders, which, in general, are not available.

The traction boundary-value problem (2.14) and (2.15) can be formulated in terms of the displacement fields $\underline{u}^{*(1)}$ and $\underline{u}^{*(2)}$, respectively, as

$$\left. \begin{aligned} \underline{u}_R^{*(1)}(\underline{x}^+) - \underline{u}_R^{*(1)}(\underline{x}^-) &= \underline{b}_R^{(1)} \text{ for } \underline{x} \in S_0, \\ c_{klmn} u_{m,nl}^{*(1)} &= 0 \text{ in } V_0 \setminus S_0, \\ c_{klmn} u_{m,n}^{*(1)} n_l &= \begin{cases} 0 & \text{on } S \\ \hat{t}_R^{(1)} & \text{on } \sigma_0, \end{cases} \end{aligned} \right\} \quad (2.16)$$

and

$$\left. \begin{aligned} \underline{u}_R^{*(2)}(\underline{x}^+) - \underline{u}_R^{*(2)}(\underline{x}^-) &= 0 \text{ for } \underline{x} \in S_0, \\ c_{klmn} u_{m,nl}^{*(2)} + \underline{p}_R^{(2)} &= 0 \text{ in } V_0 \setminus S_0, \\ c_{klmn} u_{m,n}^{*(2)} n_l &= \hat{t}_R^{(2)} \text{ on } S \cup \sigma_0, \end{aligned} \right\} \quad (2.17)$$

where

$$\underline{p}_R^{(2)} = \tau_{kl,l}, \quad \hat{t}_R^{(2)} = -\tau_{kl} n_l \quad (2.18)$$

play the role of a body force and a surface traction, respectively. It may be shown, by using Gauss' theorem, that the resultant force and couple of the forces (2.18) are zero.

Clearly, the boundary-value problem to be solved at the first step corresponds to a Volterra dislocation of translational type with prescribed tractions on the boundary of the dislocation core, while the second step involves a classical traction boundary-

value problem of linear elasticity. Assuming that the tensor of second-order elastic constants c is positive definite, it follows that any two solutions of the traction boundary-value problems differ by an infinitesimal rigid displacement.

In the original form of Signorini's scheme the arbitrary infinitesimal rotation corresponding to each step of the iteration is determined such that the body forces and surface tractions corresponding to the following step be equilibrated. On the other side, in the case of a single dislocation, the only external forces acting on the part of the body occupying the region v_0 are those applied on the core boundary σ_0 . Moreover, these forces must be self-equilibrated in the deformed configuration of the body, since the dislocation core itself is in equilibrium. Consequently, when using a semidiscrete method, the infinitesimal rigid rotations occurring at each step must be used as adjustable parameters, together with the tractions on σ_0 and the positions of the atoms inside for minimizing the potential energy of the whole body.

Alternatively, the successive linear boundary-value problems could be formulated in terms of stress functions. However, this approach leads generally to great mathematical difficulties which have been overcome so far only in two particular situations: the isotropic case and the anisotropic boundary-value problems independent of one Cartesian co-ordinate. The first case has been extensively treated by Kröner and Seeger [11] and by Pfleiderer, Seeger, and Kröner [12]. The second case has been considered by Seeger, Teodosiu, and Petrasch [7] and by Petrasch [8]; it will be also illustrated in the second part of the present paper.

3. THE CASE OF THE INFINITE MEDIUM

When studying the elastic field of a single dislocation loop lying in an infinite elastic medium, we shall require, on physical grounds, that the stress tensor \underline{T} vanish and the finite rotation \underline{R} approach the unit tensor at infinity, i.e.

$$\lim_{\|\underline{x}\| \rightarrow \infty} \underline{T}(\underline{x}) = \underline{0}, \quad \lim_{\|\underline{x}\| \rightarrow \infty} \underline{R}(\underline{x}) = \underline{1}, \quad (3.1)$$

since the lattice distortion gradually disappears at large distances from the dislocation line.

When using the iteration scheme explained in the preceding section, the first condition (3.1) is equivalent to

$$\lim_{\|\underline{x}\| \rightarrow \infty} \underline{T}^{(n)}(\underline{x}) = \underline{0}, \quad n=1, 2. \quad (3.2)$$

Analogously, we write

$$\underline{R} = \underline{1} + \epsilon \underline{R}^{(1)} + \epsilon^2 \underline{R}^{(2)} + \dots, \quad (3.3)$$

and require that

$$\lim_{\|\underline{x}\| \rightarrow \infty} \underline{R}^{(n)}(\underline{x}) = \underline{0}, \quad n=1, 2. \quad (3.4)$$

The last condition may be given a more explicit form by expressing $\underline{R}^{(n)}$ in terms of $\text{grad } \underline{u}^{*(n)}$, $n=1, 2$. To this end we start from the polar decomposition

$$\underline{A} = \underline{R} \underline{U} \quad (3.5)$$

where \underline{R} is an orthogonal tensor and \underline{U} is a symmetric tensor.

Since $\underline{R}^T \underline{R} = \underline{1}$ and $\underline{U}^T = \underline{U}$, we have by (3.5) and (2.3)

$$\underline{U}^2 = \underline{A}^T \underline{A} = \underline{1} + \underline{H} + \underline{H}^T + \underline{H}^T \underline{H}. \quad (3.6)$$

By taking

$$\underline{U} = \underline{1} + \varepsilon \underline{U}^{(1)} + \varepsilon^2 \underline{U}^{(2)} + \dots, \quad (3.7)$$

introducing (3.7) and (2.6) into (3.6) and equating the coefficients of ε and ε^2 , we obtain

$$U_{kl}^{(1)} = \frac{1}{2} (u_{k,l}^{*(1)} + u_{l,k}^{*(1)}), \quad (3.8)$$

$$U_{kl}^{(2)} = \frac{1}{2} \left[u_{k,l}^{*(2)} + u_{l,k}^{*(2)} + \frac{3}{4} (u_{k,p}^{*(1)} u_{p,l}^{*(1)} + u_{l,p}^{*(1)} u_{p,k}^{*(1)} + u_{p,k}^{*(1)} u_{p,l}^{*(1)}) - \frac{1}{4} u_{k,p}^{*(1)} u_{l,p}^{*(1)} \right]. \quad (3.9)$$

Next, introducing (2.6), (3.3) and (3.7) into the relation $\underline{1} + \underline{H} = \underline{R} \underline{U}$, equating like powers of ε , and considering (3.9) we obtain after some algebraic calculation

$$R_{kl}^{(1)} = \Omega_{kl}^{(1)}, \quad (3.10)$$

$$R_{kl}^{(2)} = \Omega_{kl}^{(2)} + \frac{1}{8} (3 u_{k,p}^{*(1)} u_{p,l}^{*(1)} - u_{p,k}^{*(1)} u_{l,p}^{*(1)} - u_{p,l}^{*(1)} u_{p,k}^{*(1)} - u_{k,p}^{*(1)} u_{l,p}^{*(1)}), \quad (3.11)$$

where

$$\Omega_{kl}^{(1)} = \frac{1}{2} (u_{k,l}^{*(1)} - u_{l,k}^{*(1)}), \quad \Omega_{kl}^{*(2)} = \frac{1}{2} (u_{k,l}^{*(2)} - u_{l,k}^{*(2)}) \quad (3.12)$$

are the (antisymmetric) infinitesimal rotation tensors corresponding to the first two steps of the iteration.

By (2.12)₁ and (3.2) the symmetric part of $\text{grad } \underline{u}^{*(1)}$ must vanish at infinity. On the other hand, by (3.4), (3.10), and (3.12)₁ the antisymmetric part of $\text{grad } \underline{u}^{*(1)}$ must also vanish at infinity, and hence

$$\lim_{\|x\| \rightarrow \infty} \text{grad } \underline{u}^{*(1)}(x) = \underline{0}. \quad (3.13)$$

Next, (3.13) and (2.13) imply that \underline{t} vanishes at infinity. Since $\underline{T}^{(2)}$ vanishes also at infinity, we deduce from (2.12) that the symmetric part of $\text{grad } \underline{u}^{*(2)}$ vanishes at infinity, too. On the other hand, by (3.4) and (3.13) we see from (3.11) and (3.12)₂ that the antisymmetric part of $\text{grad } \underline{u}^{*(2)}$ has the same property, and hence

$$\lim_{\|x\| \rightarrow \infty} \text{grad } \underline{u}^{*(2)}(x) = \underline{0}. \quad (3.14)$$

Conversely, Eqs. (3.13) and (3.14) assure that conditions (3.2) and (3.4) are fulfilled. Consequently, the boundary conditions on Δ corresponding to the first two boundary-value problems must be replaced in the case of an infinite medium by (3.13) and (3.14). Alternatively, we may retain the conditions (3.2) and replace (3.4) by

$$\lim_{\|x\| \rightarrow \infty} \underline{\omega}^{(n)}(x) = \underline{0}, \quad (3.15)$$

where $\underline{\omega}^{(n)}$ denotes the axial vector corresponding to the antisymmetric second-order tensor $\underline{\Omega}^{(n)}$, i.e.

$$\omega^{(n)} = -\frac{1}{2} \text{curl } \underline{u}^{*(n)}, \quad \omega_R^{(n)} = -\frac{1}{2} \epsilon_{mrs} u_{r,s}^{*(n)}, \quad n=1,2, \quad (3.16)$$

while ϵ_{mrs} denotes the permutation tensor.

By virtue of Bézier's uniqueness theorem [13], we conclude that the solutions of the linear traction boundary-value problems corresponding to the first two steps and satisfying the complementary conditions (3.2) and (2.15) at infinity are unique to within an infinitesimal translation.

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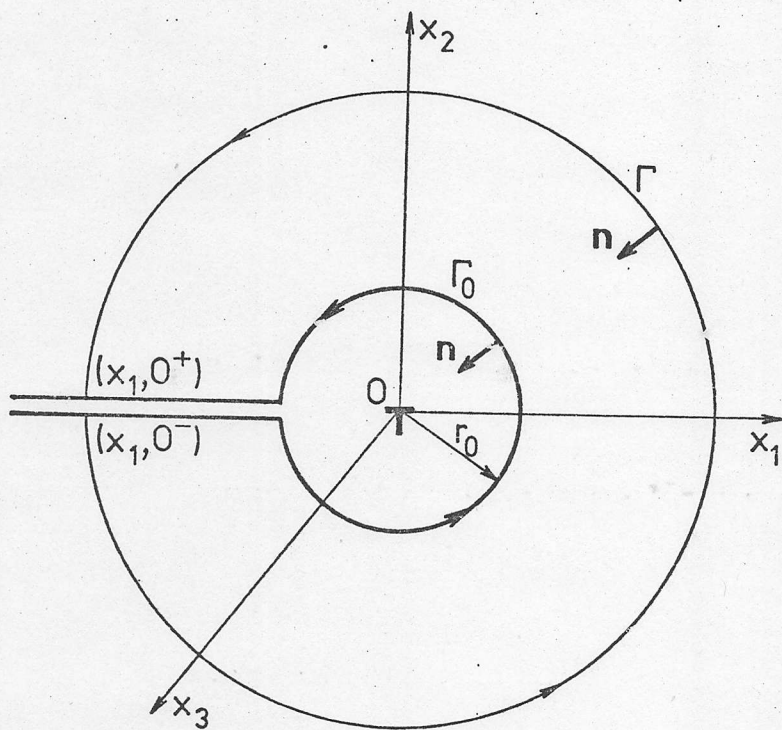


Fig.1

NON-LINEAR EFFECTS IN THE ELASTIC FIELD OF SINGLE DISLOCATIONS

II. SECOND-ORDER ELASTIC EFFECTS OF AN EDGE DISLOCATIONS

by C. TEODOSIU^{*} and E. SOCS^{**}

The first part of this paper is devoted to the extension of Willis' iteration scheme for the determination of the non-linear elastic field produced by single dislocation loops in anisotropic media under consideration of the core boundary conditions. The second part of the paper will be concerned with the determination of the second-order elastic effects produced by an edge dislocation lying along a two-fold symmetry axis in an infinite anisotropic elastic medium.

4. ITERATION SCHEME FOR AN EDGE DISLOCATION LYING ALONG A TWO-FOLD AXIS OF MATERIAL SYMMETRY

Second-order effects in the isotropic elastic field of an edge dislocation have been determined by Pfleiderer, Seeger, and Kröner [12], by disregarding core effects and applying an iteration scheme formulated in Eulerian co-ordinates, which had been previously elaborated by Kröner and Seeger [11].

Seeger, Teodosiu, and Petrasch [7] have determined the second-order effects in the anisotropic elastic field of an edge dislocation, under consideration of the core boundary conditions, and using an iteration scheme formulated in Lagrangian co-ordinates. Their results will be completed and partly corrected in the present paper, by removing some residual discontinuities occurring across

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the cut surface in the second step of the iteration, and using Willis' iteration scheme in Lagrangian co-ordinates.

Consider a straight edge dislocation lying in an infinite anisotropic elastic medium \mathcal{V} and take the axes x_1 and x_3 of a Cartesian system of co-ordinates along the true Burgers vector, respectively. Let us assume that the dislocation line lies along a two-fold axis of material symmetry or, equivalently, that any crystallographic plane parallel to the x_1x_2 -plane in the local stress-free configurations¹ is a plane of material symmetry.

We apply the (non-linear) theory of elasticity to the region \mathcal{V}_0 situated outside the dislocation core, the latter being taken as an infinite tube bounded by a circular cylindrical surface σ_0 of radius r_0 and axis x_3 . Let us denote by Γ_0 the intersection line of σ_0 with the x_1x_2 -plane and by Δ_0 the region outside Γ_0 in this plane (Fig. 1). We assume, on physical grounds, that the tractions acting on Γ_0 from the dislocation core do not depend on x_3 , and hence the elastic medium is subjected to a state of plain strain. Then, by taking the half-plane $x_2 = 0, x_1 \leq -r_0$ as cut surface s_0 rendering \mathcal{V}_0 simply-connected, we may define in the region $\mathcal{V}_0 \setminus s_0$ a single-valued displacement field, whose Cartesian components must have the form²

$$u_\alpha^* = u_\alpha^*(x_1, x_2), \quad u_3^* = 0. \quad (4.1)$$

¹cf. [9], Sect. 1.

²Here and in the following Greek indices range over the values 1, 2; the summation over twice repeated Greek indices will be always implied, while other cases of summation will be explicitly indicated by the symbol \sum_α .

It may be shown that (4.1) and the assumed material symmetry imply that $T_{13} = T_{23} = 0$. In addition, although the stress component T_{33} is not zero, it does not intervene in the successive linear boundary-value problems, and its value can be directly obtained from (2.14)₃ and (2.15)₃ after the calculation of $u^{*(1)}$ and $u^{*(2)}$. Consequently, the only stress components that are significant for our problem are $T_{\alpha\beta}$, $\alpha, \beta = 1, 2$.

Since now $b_1 = b$, $b_2 = b_3 = 0$, where $b = \epsilon b^{(1)}$ is the magnitude of the true Burgers vector, the jump condition (1.13) becomes

$$u_{\alpha}^{*}(x_1, 0^+) - u_{\alpha}^{*}(x_1, 0^-) = -\delta_{\alpha 1} b \quad \text{for } x_1 \in (-\infty, -r_0]. \quad (4.2)$$

By virtue of (4.1) and (4.2), the boundary-value problems (2.14) and (2.15), with the complementary conditions at infinity (3.13) and (3.14) become at the first step:

$$\left. \begin{aligned} u_{\alpha}^{*(1)}(x_1, 0^+) - u_{\alpha}^{*(1)}(x_1, 0^-) &= -\delta_{\alpha 1} b^{(1)} \quad \text{for } x_1 \in (-\infty, -r_0], \\ T_{\alpha\beta}^{(1)} &= 0, \quad T_{\alpha\beta}^{(1)} = c_{\alpha\beta\gamma\delta} u_{\gamma,\delta}^{*(1)} \quad \text{in } \Delta_0 \setminus \bar{\tau}_0, \\ u_{\alpha,\beta}^{*(1)} &\text{ continuous across } \bar{\tau}_0, \\ T_{\alpha\beta}^{(1)} n_{\beta} &= \hat{t}_{\alpha}^{(1)} \quad \text{on } \Gamma_0, \\ \lim_{\rho \rightarrow \infty} u_{\alpha,\beta}^{*(1)}(x_1, x_2) &= 0, \end{aligned} \right\} \quad (4.3)$$

and at the second step:

$$\left. \begin{aligned} u_{\alpha}^{*(2)}(x_1, 0^+) - u_{\alpha}^{*(2)}(x_1, 0^-) &= 0 \text{ for } x_1 \in (-\infty, -r_0], \\ T_{\alpha\beta, \beta}^{(2)} &= 0, \quad T_{\alpha\beta}^{(2)} = c_{\alpha\beta\gamma\delta} u_{\gamma, \delta}^{*(2)} + \tau_{\alpha\beta} \text{ in } \Delta_0 \setminus \gamma_0, \\ u_{\alpha, \beta}^{*(2)} &\text{ continuous across } \gamma_0 \\ T_{\alpha\beta}^{(2)} n_{\beta} &= 0 \text{ on } \Gamma_0, \\ \lim_{\rho \rightarrow \infty} u_{\alpha, \beta}^{*(2)}(x_1, x_2) &= 0, \end{aligned} \right\} \quad (4.4)$$

where $\rho = \sqrt{x_1^2 + x_2^2}$, γ_0 is the line $x_2 = x_3 = 0$, $x_1 \in (-\infty, -r_0]$,

while

$$\begin{aligned} \tau_{\alpha\beta} &= -u_{\delta, \gamma}^{*(1)} T_{\alpha\beta}^{(1)} + u_{\alpha, \delta}^{*(1)} T_{\gamma\beta}^{(1)} + u_{\beta, \delta}^{*(1)} T_{\alpha\gamma}^{(1)} + \\ &+ c_{\alpha\beta\gamma\delta} (u_{\gamma, \pi}^{*(1)} u_{\pi, \delta}^{*(1)} + \frac{1}{2} u_{\pi, \gamma}^{*(1)} u_{\pi, \delta}^{*(1)}) + \frac{1}{2} c_{\alpha\beta\gamma\delta} \pi_{\gamma} u_{\gamma, \delta}^{*(1)} u_{\pi, \delta}^{*(1)}. \end{aligned} \quad (4.5)$$

The conditions (1.7) and (1.8), which express the vanishing of the resultant force and couple of the tractions acting on Γ_0 assume the form

$$\int_{\Gamma_0} \hat{t}_{\alpha} d\ell = 0, \quad \int_{\Gamma_0} (x_1 \hat{t}_2 - x_2 \hat{t}_1) d\ell = 0, \quad (4.6)$$

where ℓ denotes the curvilinear abscissa on Γ_0 . As already mentioned in Sect. 1, the continuity of $u_{\alpha, \beta}^{*(1)}$ and $u_{\alpha, \beta}^{*(2)}$ across γ_0 implies the continuity across γ_0 of the stress vector components t_{α} . Consequently, the first equation (4.6) and the equilibrium of the material inside Γ , Γ_0 , and γ_0 imply that

$$\int_{\Gamma} t_{\alpha} d\ell = 0 \quad (4.7)$$

on any smooth closed curve encircling Γ anticlockwise in the x_1x_2 -plane (Fig. 1). Clearly, the last relation is equivalent to within terms of third order in ε with the conditions

$$\int_{\Gamma} t_{\alpha}^{(1)} dl = 0, \quad \int_{\Gamma} t_{\alpha}^{(2)} dl = 0. \quad (4.8)$$

The last two sections of the paper will be devoted to the solving of the linear boundary-value problems (4.3) and (4.4).

5. SOLUTION OF THE FIRST LINEAR BOUNDARY-VALUE PROBLEM

The first linear boundary-value problem (4.3) has been solved by Teodosiu and Nicolae [14], by using a complex-variable technique. Therefore, we reproduce here only the main intermediate results that are further used in the second step of the iteration.

By introducing the complex variables

$$z = x_1 + ix_2, \quad \bar{z} = x_1 - ix_2,$$

the complex displacement

$$U^{(1)} = u_1^{*(1)} + i u_2^{*(1)}, \quad (5.1)$$

and the complex stresses

$$\Theta^{(1)} = T_{11}^{(1)} + T_{22}^{(1)}, \quad \Phi^{(1)} = T_{11}^{(1)} - T_{22}^{(1)} + 2iT_{12}^{(1)}, \quad (5.2)$$

and taking into account that

$$\begin{aligned} \frac{\partial U^{(1)}}{\partial z} &= \frac{1}{2} \left[\frac{\partial u_1^{*(1)}}{\partial x_1} + \frac{\partial u_2^{*(1)}}{\partial x_2} - i \left(\frac{\partial u_1^{*(1)}}{\partial x_2} - \frac{\partial u_2^{*(1)}}{\partial x_1} \right) \right], \\ \frac{\partial U^{(1)}}{\partial \bar{z}} &= \frac{1}{2} \left[\frac{\partial u_1^{*(1)}}{\partial x_1} - \frac{\partial u_2^{*(1)}}{\partial x_2} + i \left(\frac{\partial u_1^{*(1)}}{\partial x_2} + \frac{\partial u_2^{*(1)}}{\partial x_1} \right) \right], \end{aligned} \quad (5.3)$$

where

$$\frac{\partial}{\partial z} = \frac{1}{2} \left(\frac{\partial}{\partial x_1} - i \frac{\partial}{\partial x_2} \right), \quad \frac{\partial}{\partial \bar{z}} = \frac{1}{2} \left(\frac{\partial}{\partial x_1} + i \frac{\partial}{\partial x_2} \right), \quad (5.4)$$

we obtain from (4.3) the jump condition

$$U^{(n)}(x_1, 0^+) - U^{(n)}(x_1, 0^-) = -\delta^{(n)} \text{ for } x_1 \in (-\infty, -r_0], \quad (5.5)$$

the equilibrium equation

$$\frac{\partial \Theta^{(n)}}{\partial \bar{z}} + \frac{\partial \Phi^{(n)}}{\partial z} = 0, \quad (5.6)$$

the constitutive equations

$$\left. \begin{aligned} 2 \frac{\partial U^{(n)}}{\partial \bar{z}} &= A \Phi^{(n)} + B \bar{\Phi}^{(n)} + 2C \Theta^{(n)}, \\ \frac{\partial U^{(n)}}{\partial z} + \frac{\partial \bar{U}^{(n)}}{\partial \bar{z}} &= \bar{C} \Phi^{(n)} + C \bar{\Phi}^{(n)} + 2D \Theta^{(n)}, \end{aligned} \right\} \quad (5.7)$$

and the boundary conditions

$$\frac{1}{2} (\Theta^{(n)} + \Phi^{(n)} e^{-2i\theta}) = \hat{t}_r^{(n)} + i \hat{t}_\theta^{(n)} \text{ for } z = r_0 e^{i\theta}, \theta \in (-\pi, \pi], \quad (5.8)$$

$$\lim_{\rho \rightarrow \infty} \frac{\partial U^{(n)}}{\partial z} = 0, \quad \lim_{\rho \rightarrow \infty} \frac{\partial \bar{U}^{(n)}}{\partial \bar{z}} = 0, \quad (5.9)$$

where $\hat{t}_r^{(n)}$ and $\hat{t}_\theta^{(n)}$ are the radial and tangential components of $\hat{\underline{t}}^{(n)}$, respectively, θ is the polar angle in the $x_1 x_2$ -plane, and

A, B, C, D are determined by the relations

$$4Ad = c_{66}(c_{11} + c_{22} + 2c_{12}) - (c_{16} + c_{26})^2 + c_{11}c_{22} - c_{12}^2,$$

$$4Bd = c_{66}(c_{11} + c_{22} + 2c_{12}) - (c_{16} + c_{26})^2 - c_{11}c_{22} + c_{12}^2 + \\ + 2i[c_{26}(c_{12} + c_{11}) - c_{16}(c_{12} + c_{22})],$$

$$4Cd = c_{66}(c_{22} - c_{11}) + c_{16}^2 - c_{26}^2 + \\ + i[c_{16}(c_{12} - c_{22}) - c_{26}(c_{12} - c_{11})],$$

$$d = c_{66}(c_{11}c_{22} - c_{12}^2) + 2c_{12}c_{16}c_{26} - c_{11}c_{26}^2 - c_{22}c_{16}^2.$$

In view of (4.3)₄ and (5.3) we shall also require the continuity of $\frac{\partial U^{(1)}}{\partial z}$ and $\frac{\partial U^{(1)}}{\partial \bar{z}}$ across $\bar{\sigma}_0$.

Next, the equilibrium equation (5.6) is identically satisfied by setting

$$\Phi^{(1)} = -4 \frac{\partial^2 F^{(1)}}{\partial \bar{z}^2}, \quad \Theta^{(1)} = 4 \frac{\partial^2 F^{(1)}}{\partial z \partial \bar{z}}, \quad (5.10)$$

where $F^{(1)}$ is Airy's stress function. The function $F^{(1)}$ must satisfy the compatibility condition obtained by eliminating $U^{(1)}$ between equations (5.7). After some intermediate calculation, it results

$$\mathcal{L} F^{(1)} = 0, \quad (5.11)$$

where \mathcal{L} is the real differential operator

$$\mathcal{L} \equiv B \frac{\partial^4}{\partial z^4} - 4C \frac{\partial^4}{\partial z^3 \partial \bar{z}} + 2(A+2D) \frac{\partial^4}{\partial z^2 \partial \bar{z}^2} - 4\bar{C} \frac{\partial^4}{\partial z \partial \bar{z}^3} + \bar{B} \frac{\partial^4}{\partial \bar{z}^4}. \quad (5.12)$$

This operator can be decomposed into the product

$$\mathcal{L} \equiv \bar{B} \left(\frac{\partial}{\partial \bar{z}} - \tau_1 \frac{\partial}{\partial z} \right) \left(\frac{\partial}{\partial \bar{z}} - \tau_2 \frac{\partial}{\partial z} \right) \left(\frac{\partial}{\partial \bar{z}} - \tau_3 \frac{\partial}{\partial z} \right) \left(\frac{\partial}{\partial \bar{z}} - \tau_4 \frac{\partial}{\partial z} \right), \quad (5.13)$$

where $\tau_1, \tau_2, \tau_3, \tau_4$ are the roots of the algebraic reciprocal equation

$$\bar{B} \tau^4 - 4\bar{C} \tau^3 + 2(A+2D) \tau^2 - 4C \tau + B = 0. \quad (5.14)$$

As shown by Green and Zerna [15], when the strain energy function is positive definite, the roots of this equation are complex, and their moduli cannot equal unity, and hence they can be labeled such that $|\tau_1| < 1$, $|\tau_2| < 1$, $\tau_3 = 1/\bar{\tau}_1$, $\tau_4 = 1/\bar{\tau}_2$.

In addition, (5.14) yields

$$\frac{\tau_1 \tau_2}{\bar{\tau}_1 \bar{\tau}_2} = \frac{B}{\bar{B}}, \quad \tau_1 + \tau_2 + \frac{1}{\bar{\tau}_1} + \frac{1}{\bar{\tau}_2} = \frac{4\bar{C}}{\bar{B}}. \quad (5.15)$$

We assume ¹ in the following that $\tau_1 \neq \tau_2$. Since the

¹ The case $\tau_1 = \tau_2$ may be studied by a method similar to that used in the isotropic case.

operators $\mathcal{L}_k \equiv \partial/\partial \bar{z} - \tau_k \partial/\partial z$, $k = 1, 2, 3, 4$,

are linear independent and have constant coefficients, it follows by Boggio's theorem that the general solution of (5.12) equals the sum of the general solutions of the equations $\mathcal{L}_k F^{(1)} = 0$, $k = 1, 2, 3, 4$.

By introducing the new complex variables

$$z_1 = z + \tau_1 \bar{z}, \quad \bar{z}_1 = \bar{z} + \bar{\tau}_1 z, \quad (5.16)$$

we find that

$$\left(\frac{\partial}{\partial \bar{z}} - \tau_1 \frac{\partial}{\partial z} \right) \left(\frac{\partial}{\partial \bar{z}} - \frac{1}{\tau_1} \frac{\partial}{\partial z} \right) \equiv - \frac{(1 - \tau_1 \bar{\tau}_1)^2}{\tau_1} \frac{\partial^2}{\partial z_1 \partial \bar{z}_1},$$

and hence the general real solution of the equation $\mathcal{L}_1 \mathcal{L}_3 F^{(1)} = 0$ is

$$F^{(1)}(x_1, x_2) = \Omega_1(z_1) + \overline{\Omega_1(z_1)},$$

where $\Omega_1(z_1)$ is an arbitrary analytic function of z_1 . Analogously, the general real solution of the equation $\mathcal{L}_2 \mathcal{L}_4 F^{(1)} = 0$ is

$$F^{(1)}(x_1, x_2) = \Omega_2(z_2) + \overline{\Omega_2(z_2)},$$

where $\Omega_2(z_2)$ is an arbitrary analytic function of z_2 , and

$$z_2 = z + \tau_2 \bar{z}, \quad \bar{z}_2 = \bar{z} + \bar{\tau}_2 z. \quad (5.17)$$

Hence, the general solution of equation (5.11) is

$$F^{(1)}(x_1, x_2) = 2 \operatorname{Re} [\Omega_1(z_1) + \Omega_2(z_2)]. \quad (5.18)$$

Introducing (5.18) into (5.10) and making use of (5.16)

and (5.17) yields

$$\Phi^{(1)} = -4 \sum_{\alpha} [\tau_{\alpha}^2 \Omega_{\alpha}''(z_{\alpha}) + \overline{\Omega_{\alpha}''(z_{\alpha})}], \quad \Theta^{(1)} = 8 \operatorname{Re} \sum_{\alpha} \tau_{\alpha} \Omega_{\alpha}''(z_{\alpha}). \quad (5.19)$$

Next, by substituting (5.19) into (5.7) and integrating the system of equations obtained, we find

$$U^{(1)}(x_1, x_2) = \sum_{\alpha} [\delta_{\alpha} \Omega'_{\alpha}(z_{\alpha}) + \rho_{\alpha} \overline{\Omega'_{\alpha}(z_{\alpha})}] + \omega_0^{(1)} iz + u_0^{(1)} + i v_0^{(1)}, \quad (5.20)$$

where $\omega_0^{(1)}, u_0^{(1)}, v_0^{(1)}$ are arbitrary real constants and

$$\delta_{\alpha} = -2(A\tau_{\alpha} - 2C + B/\tau_{\alpha}), \quad \rho_{\alpha} = -2(A - 2C\tau_{\alpha} + \tau_{\alpha}^2), \quad (5.21)$$

The expression $\omega_0^{(1)} iz + u_0^{(1)} + i v_0^{(1)}$ corresponds to an infinitesimal rigid displacement. By considering (5.20), it may be seen that both conditions (5.9) can be satisfied by taking

$$\omega_0^{(1)} = 0 \quad (5.22)$$

and requiring that

$$\lim_{\delta \rightarrow 0} \Omega''_{\alpha}(z_{\alpha}) = 0, \quad \alpha = 1, 2. \quad (5.23)$$

As pointed out above, $\partial U^{(1)}/\partial z$ and $\partial U^{(1)}/\partial \bar{z}$ must be continuous across τ_0 . Clearly, this condition is fulfilled when the functions $\Omega'_{\alpha}(z_{\alpha})$, $\alpha = 1, 2$ are single-valued in the regions Δ_{α} corresponding to Δ_0 in the z_{α} -planes, and hence can be developed in Laurent series in those regions. Moreover, by (5.23) these series may contain only negative powers of z_{α} . Consequently, by integrating them with respect to z_{α} , we find

$$\Omega'_{\alpha}(z_{\alpha}) = \kappa_{\alpha} \ln \frac{z_{\alpha}}{1 + \tau_{\alpha}} + \sum_{k=1}^{\infty} a_{k\alpha}^{(1)} z_{\alpha}^{-k}, \quad \alpha = 1, 2, \quad (5.24)$$

where κ_{α} and $a_{k\alpha}^{(1)}$ are arbitrary complex constants. The denominators $1 + \tau_{\alpha}$, $\alpha = 1, 2$ have been introduced in order to define single-valued branches of the logarithmic functions having τ_0 as cut. Indeed, it is well-known that $\ln(x_1 + ix_2)$ may be defined as a single-valued function, by cutting the $x_1 x_2$ -plane, e.g. along the negative x_1 -axis, and taking

$$\ln(x_1 + ix_2) = \ln \rho + i\theta, \quad (5.25)$$

where $\rho = \sqrt{x_1^2 + x_2^2}$,

$$\theta = \begin{cases} \cotan^{-1}(x_1/x_2) & \text{for } x_2 > 0 \\ 0 & \text{for } x_2 = 0, x_1 > 0 \\ \cotan^{-1}(x_1/x_2) - \pi & \text{for } x_2 < 0. \end{cases} \quad (5.26)$$

According to this definition, the limiting values of θ on the upper and lower faces of the cut are π and $-\pi$, respectively. On the other hand, we have

$$\frac{z_\alpha}{1 + \tau_\alpha} = x_1 + i \frac{1 - \tau_\alpha}{1 + \tau_\alpha} x_2 = x_1 + \frac{2 \operatorname{Im} \tau_\alpha}{|1 + \tau_\alpha|^2} x_2 + i \frac{1 - |\tau_\alpha|^2}{|1 + \tau_\alpha|^2} x_2,$$

and, by taking into account that $|\tau_\alpha| < 1$, we see that the discontinuity lines of the functions $\ln [z_\alpha / (1 + \tau_\alpha)]$, $\alpha = 1, 2$, are ^{again} given by $x_2 = 0$, $x_1 \leq 0$, and hence coincide with the cut used to define a single-valued displacement field. Moreover, these functions take also the limiting values π and $-\pi$ on the upper and lower faces of the cut, respectively.

The coefficients κ_1 and κ_2 will be determined by the jump condition (5.5) and by condition (4.8)₁, which expresses the vanishing of the resultant force exerted ^{on} by the dislocation core and the continuity of the stress vector through τ_0 . Clearly, (4.8)₁ is equivalent with

$$\int_{\Gamma} (t_1^{(1)} + i t_2^{(1)}) d\ell = 0. \quad (5.27)$$

Next, inspection of Fig. 1 shows that

$$\begin{aligned} t_1^{(1)} + i t_2^{(1)} &= T_{11}^{(1)} n_1 + T_{12}^{(1)} n_2 + i (T_{12}^{(1)} n_1 + T_{22}^{(1)} n_2) \\ &= - (T_{11}^{(1)} + i T_{12}^{(1)}) \frac{dx_2}{d\ell} + (T_{12}^{(1)} + i T_{22}^{(1)}) \frac{dx_1}{d\ell} \\ &= \frac{i}{2} \left[(T_{11}^{(1)} + T_{22}^{(1)}) \frac{d\bar{z}}{d\ell} - (T_{11}^{(1)} - T_{22}^{(1)} + 2i T_{12}^{(1)}) \frac{dz}{d\ell} \right]. \end{aligned}$$

Consequently, considering also (5.2) and (5.10), we have

$$t_1^{(1)} + i t_2^{(1)} = \frac{i}{2} \left(\Theta^{(1)} \frac{dz}{d\bar{z}} - \Phi^{(1)} \frac{d\bar{z}}{dz} \right) = 2i \frac{d}{d\bar{z}} \left(\frac{\partial F^{(1)}}{\partial \bar{z}} \right),$$

and, introducing this result into (5.27), we deduce that

$$\frac{\partial F^{(1)}}{\partial \bar{z}} (x_1, 0^+) - \frac{\partial F^{(1)}}{\partial \bar{z}} (x_1, 0^-) = 0 \quad \text{for } x_1 \in (-\infty, -r_0]. \quad (5.28)$$

Next, from (5.16 - 18) it follows that

$$\frac{\partial F^{(1)}}{\partial \bar{z}} (x_1, x_2) = \sum_{\alpha} [\delta_{\alpha} \Omega'_{\alpha}(\bar{z}_{\alpha}) + \overline{\Omega'_{\alpha}(\bar{z}_{\alpha})}]. \quad (5.29)$$

Substituting now (5.24) into (5.29) and the result obtained into (5.28) yields

$$\sum_{\alpha} (\delta_{\alpha} \kappa_{\alpha} - \bar{\kappa}_{\alpha}) = 0. \quad (5.30)$$

On the other hand, introducing (5.20) into the jump condition (5.5) and considering (5.24), we find

$$\sum_{\alpha} (\delta_{\alpha} \kappa_{\alpha} - \bar{\kappa}_{\alpha}) = \frac{i b^{(1)}}{2\pi}. \quad (5.31)$$

Conditions (5.30) and (5.31) provide two complex equations for the determination of the parameters κ_1 and κ_2 . Following [14], we first simplify (5.31) by taking into consideration (5.21) and (5.30), thus obtaining

$$\sum_{\alpha} \left(\bar{\delta}_{\alpha}^2 \kappa_{\alpha} - \frac{\kappa_{\alpha}}{\bar{\delta}_{\alpha}} \right) = \frac{i b^{(1)}}{4\pi B}. \quad (5.32)$$

Eliminating $\bar{\kappa}_1$ and $\bar{\kappa}_2$ between equations (5.30), (5.32) and their complex conjugates, we get

$$\begin{aligned} \bar{\delta}_2 \nu_1 \nu_3 \kappa_1 + \bar{\delta}_1 \nu_2 \bar{\nu}_3 \kappa_2 &= -i b^{(1)} \bar{\delta}_1 \bar{\delta}_2 / (4\pi B), \\ \nu_1 \nu_3 \kappa_1 + \nu_2 \bar{\nu}_3 \kappa_2 &= -i b^{(1)} \bar{\delta}_1 \bar{\delta}_2 / (4\pi B), \end{aligned}$$

where

$$\nu_1 = 1 - \sigma_1 \bar{\sigma}_1, \quad \nu_2 = 1 - \sigma_2 \bar{\sigma}_2, \quad \nu_3 = 1 - \sigma_1 \bar{\sigma}_2. \quad (5.33)$$

Making use of (5.15), this system can be further solved to give

$$\kappa_1 = \frac{i b^{(1)} (1 - \sigma_1) \sigma_1 \sigma_2}{4\pi B \nu_1 \nu_3 \nu_4}, \quad \kappa_2 = - \frac{i b^{(1)} (1 - \sigma_2) \sigma_1 \sigma_2}{4\pi B \nu_2 \nu_3 \nu_4}, \quad (5.34)$$

where $\nu_4 = \sigma_1 - \sigma_2$.

In [14] the coefficients $a_{k\alpha}^{(1)}$ ($k = 1, 2, \dots$) have been completely determined in terms of the complex Fourier coefficients of the function $\hat{t}_\varphi^{(1)} + i \hat{t}_\theta^{(1)}$, by using the boundary condition (5.8). However, since these Fourier coefficients are not known a priori, it proves more advantageous, when applying semi-discrete methods, to consider as unknowns besides the positions of the atoms inside Γ_0 the coefficients $a_{k\alpha}^{(1)}$ themselves, instead of the Fourier coefficients. In this case, the solution of the first linear boundary-value problem (4.3) of the iteration scheme is given by (5.19), (5.20), and (5.24), with κ_α determined by (5.34).

6. SOLUTION OF THE SECOND LINEAR BOUNDARY-VALUE PROBLEM

We proceed now to solve the second linear boundary-value problem (4.4) of the iteration scheme. The only differences from the first problem are the presence of the non-linear term \underline{z} in the expression of $\underline{t}^{(2)}$ and the continuity of $\underline{u}^{(2)}$ across the cut σ_0 .

By introducing the complex displacement

$$U^{(2)} = u_1^{*(2)} + i u_2^{*(2)} \quad (6.1)$$

and the complex stresses

$$\Theta^{(2)} = T_{11}^{(2)} + T_{22}^{(2)}, \quad \Phi^{(2)} = T_{11}^{(2)} - T_{22}^{(2)} + 2i T_{12}^{(2)}, \quad (6.2)$$

we obtain from (4.4) the jump condition

$$U^{(2)}(x_1, 0^+) - U^{(2)}(x_1, 0^-) = 0 \quad \text{for } x_1 \in (-\infty, -r_0], \quad (6.3)$$

the equilibrium equation

$$\frac{\partial \Theta^{(2)}}{\partial \bar{z}} + \frac{\partial \Phi^{(2)}}{\partial z} = 0, \quad (6.4)$$

the constitutive equations

$$\left. \begin{aligned} 2 \frac{\partial U^{(2)}}{\partial \bar{z}} &= A(\Phi^{(2)} - \Phi_0) + B(\bar{\Phi}^{(2)} - \bar{\Phi}_0) + 2C(\Theta^{(2)} - \Theta_0), \\ \frac{\partial U^{(2)}}{\partial z} + \frac{\partial U^{(2)}}{\partial \bar{z}} &= \bar{C}(\Phi^{(2)} - \Phi_0) + C(\bar{\Phi}^{(2)} - \bar{\Phi}_0) + 2D(\Theta^{(2)} - \Theta_0), \end{aligned} \right\} \quad (6.5)$$

and the boundary conditions

$$\Theta^{(2)} + \Phi^{(2)} e^{-2i\theta} = 0 \quad \text{for } z = r_0 e^{i\theta}, \quad \theta \in (-\pi, \pi], \quad (6.6)$$

$$\lim_{\xi \rightarrow \infty} \frac{\partial U^{(2)}}{\partial z} = 0, \quad \lim_{\xi \rightarrow \infty} \frac{\partial U^{(2)}}{\partial \bar{z}} = 0, \quad (6.7)$$

where the functions

$$\Theta_0 = \tau_{11} + \tau_{22}, \quad \Phi_0 = \tau_{11} - \tau_{22} + 2i\tau_{12} \quad (6.8)$$

depend only on $\mu_{\alpha, \beta}^{*(4)}$ and hence are known from the first step of the iteration.

The equilibrium condition (6.4) is identically satisfied by putting as before

$$\Phi^{(2)} = -4 \frac{\partial^2 F^{(2)}}{\partial \bar{z}^2}, \quad \Theta^{(2)} = 4 \frac{\partial^2 F^{(2)}}{\partial z \partial \bar{z}}, \quad (6.9)$$

where $F^{(2)}$ is Airy's stress function corresponding to the second iteration step. By a reasoning similar to that leading to (5.28) we conclude that (4.8)₂ implies

$$\frac{\partial F^{(2)}}{\partial \bar{z}}(x_1, 0^+) - \frac{\partial F^{(2)}}{\partial \bar{z}}(x_1, 0^-) = 0 \quad \text{for } x_1 \in (-\infty, -r_0]. \quad (6.10)$$

Clearly, we could derive the compatibility equation to be satisfied by $F^{(2)}$ as above, by eliminating $U^{(2)}$ between equations (6.5). However, the subsequent integration of the equation obtained and of system (6.5) proves to be much more difficult than it was for the first iteration step. That is why it is better to adopt an apparently longer way [7] which, however, greatly simplifies procedure.

We recall that the operator \mathcal{L} assumes a particularly simple form when choosing z_1 and \bar{z}_1 or, alternatively, z_2 and \bar{z}_2 as independent variables, instead of z and \bar{z} . Let us first take z_2 and \bar{z}_2 as independent variables in (6.5) and (6.9). By using the relations

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial z_2} + \bar{\sigma}_2 \frac{\partial}{\partial \bar{z}_2}, \quad \frac{\partial}{\partial \bar{z}} = \sigma_2 \frac{\partial}{\partial z_2} + \frac{\partial}{\partial \bar{z}_2},$$

we obtain after some algebraic manipulation, the system

$$\begin{aligned} \frac{\partial}{\partial z_2} (\bar{U}^{(2)} - \bar{\sigma}_2 U^{(2)}) &= (\rho_2 - \sigma_2 \bar{\sigma}_2) \frac{\partial^2 F^{(2)}}{\partial z_2^2} + (\bar{\sigma}_2 \rho_2 - \bar{\sigma}_2) \frac{\partial^2 F^{(2)}}{\partial z_2 \partial \bar{z}_2} + \\ &+ (4\mu_2)^{-1} [(\bar{\sigma}_2 + \bar{\sigma}_2 \rho_2) \Theta_0 + \bar{\sigma}_2 \bar{\sigma}_2 \Phi_0 + \rho_2 \bar{\Phi}_0], \end{aligned} \quad (6.11)$$

$$\begin{aligned} \frac{\partial U^{(2)}}{\partial z_2} + \frac{\partial \bar{U}^{(2)}}{\partial \bar{z}_2} &= 2 \operatorname{Re} \left\{ \sigma_2 \frac{\partial^2 F^{(2)}}{\partial z_2^2} + \left(\frac{\sigma_2}{\bar{\sigma}_2} + \frac{B \mu_2^2}{\bar{\sigma}_2^2} \right) \frac{\partial^2 F^{(2)}}{\partial z_2 \partial \bar{z}_2} + \right. \\ &\left. + (2\mu_2)^{-1} [(\bar{\sigma}_2 C + \sigma_2 \bar{C} - 2D) \Theta_0 + (A \bar{\sigma}_2 - 2\bar{C} + \bar{B} \sigma_2) \Phi_0] \right\}. \end{aligned} \quad (6.12)$$

Integrating (6.11) with respect to z_2 yields

$$\begin{aligned} \bar{U}^{(2)} - \bar{\sigma}_2 U^{(2)} &= (\rho_2 - \sigma_2 \bar{\sigma}_2) \frac{\partial F^{(2)}}{\partial z_2} + (\bar{\sigma}_2 \rho_2 - \bar{\sigma}_2) \frac{\partial F^{(2)}}{\partial \bar{z}_2} + \\ &+ (4\mu_2)^{-1} \int [(\bar{\sigma}_2 + \bar{\sigma}_2 \rho_2) \Theta_0 + \bar{\sigma}_2 \bar{\sigma}_2 \Phi_0 + \rho_2 \bar{\Phi}_0] dz_2 + \gamma(z_2), \end{aligned}$$

where $\eta(z_2)$ is an arbitrary analytic function of z_2 . Eliminating $\bar{U}^{(2)}$ between this equation and its complex conjugate yields

$$\begin{aligned} \nu_2 U^{(2)} = & (\tau_2 \rho_2 - \tau_2^2 \bar{\delta}_2 + \tau_2 \bar{\rho}_2 - \delta_2) \frac{\partial F^{(2)}}{\partial z_2} + (\tau_2 \bar{\tau}_2 \rho_2 - \tau_2 \bar{\delta}_2 + \bar{\rho}_2 - \bar{\delta}_2 \delta_2) \frac{\partial F^{(2)}}{\partial \bar{z}_2} + \\ & + (4\nu_2)^{-1} \left\{ \tau_2 \left[(\bar{\delta}_2 + \bar{\tau}_2 \rho_2) \Theta_0 + \bar{\tau}_2 \bar{\delta}_2 \Phi_0 + \rho_2 \bar{\Phi}_0 \right] dz_2 + \right. \\ & \left. + \left[(\delta_2 + \tau_2 \bar{\rho}_2) \Theta_0 + \tau_2 \delta_2 \bar{\Phi}_0 + \bar{\rho}_2 \Phi_0 \right] d\bar{z}_2 + \eta'(z_2) + \tau_2 \overline{\eta'(z_2)} \right\}. \quad (6.13) \end{aligned}$$

Finally, introducing (6.13) into (6.12), we find

$$\begin{aligned} \frac{1}{\nu_1^2} \left[-\bar{\nu}_3 \nu_4 \frac{\partial^2 F^{(2)}}{\partial z_2^2} + (\nu_3 \bar{\nu}_3 + \nu_4 \bar{\nu}_4) \frac{\partial^2 F^{(2)}}{\partial z_2 \partial \bar{z}_2} - \nu_3 \bar{\nu}_4 \frac{\partial^2 F^{(2)}}{\partial \bar{z}_2^2} \right] = \\ = 2 \operatorname{Re} \left[k_4 \Theta_0 + k_5 \Phi_0 + \frac{\partial h(z_2, \bar{z}_2)}{\partial \bar{z}_2} + \frac{\nu_2}{k_0} \eta''(z_2) \right], \quad (6.14) \end{aligned}$$

where

$$h(z_2, \bar{z}_2) = \int (k_1 \Theta_0 + k_2 \Phi_0 + k_3 \bar{\Phi}_0) dz_2, \quad (6.15)$$

$$\begin{aligned} k_0 = \frac{2\nu_1^2 \nu_2^2 B}{\tau_1 \tau_2}, \quad k_1 = \frac{\bar{\delta}_2 + \bar{\tau}_2 \rho_2}{4k_0}, \quad k_2 = \frac{\bar{\tau}_2 \bar{\delta}_2}{4k_0}, \quad k_3 = \frac{\rho_2}{4k_0}, \\ k_4 = \frac{(1 + \tau_2 \bar{\tau}_2) D - C \bar{\tau}_2 - \bar{C} \tau_2}{k_0}, \quad k_5 = -\frac{A \bar{\tau}_2 - (1 + \tau_2 \bar{\tau}_2) \bar{C} + \bar{B} \tau_2}{k_0}. \end{aligned}$$

Change now in (6.14) the independent variables z_2 and \bar{z}_2 by z_1 and \bar{z}_1 . Since

$$z_1 = (\nu_3 z_2 + \nu_4 \bar{z}_2) / \nu_2, \quad \bar{z}_1 = (\bar{\nu}_4 z_2 + \bar{\nu}_3 \bar{z}_2) / \nu_2, \quad (6.16)$$

and hence

$$\frac{\partial}{\partial z_2} = \frac{\nu_3}{\nu_2} \frac{\partial}{\partial z_1} + \frac{\bar{\nu}_4}{\nu_2} \frac{\partial}{\partial \bar{z}_1}, \quad \frac{\partial}{\partial \bar{z}_2} = \frac{\nu_4}{\nu_2} \frac{\partial}{\partial z_1} + \frac{\bar{\nu}_3}{\nu_2} \frac{\partial}{\partial \bar{z}_1}, \quad (6.17)$$

it follows that

$$\frac{\partial^2 F^{(2)}}{\partial z_1 \partial \bar{z}_1} = 2 \operatorname{Re} \left[k_4 \Theta_0 + k_5 \Phi_0 + \frac{\partial h(z_1, \bar{z}_1)}{\partial \bar{z}_1} + \frac{\nu_2}{k_0} \eta''(z_1) \right]. \quad (6.18)$$

The general solution of this equation is

$$F^{(2)}(x_1, x_2) = 2 \operatorname{Re} [\omega_1(z_1) + \omega_2(z_2)] + F_0(z_1, \bar{z}_1), \quad (6.19)$$

where $\omega_1(z_1)$ is an arbitrary analytic function of z_1 ,

$$\omega_2(z_2) \equiv -\frac{\nu_1^2 \nu_2}{k_0 \nu_3 \nu_4} \eta(z_2) = \frac{\eta(z_2)}{2(\delta_2 - \tau_2 \bar{\rho}_2)},$$

and $F_0(z_1, \bar{z}_1)$ is a particular solution of the equation

$$\frac{\partial^2 F_0}{\partial z_1 \partial \bar{z}_1} = 2 k_4 \Theta_0 + k_5 \Phi_0 + \bar{k}_5 \bar{\Phi}_0 + \frac{\partial h(z_2, \bar{z}_2)}{\partial \bar{z}_2} + \frac{\overline{\partial h(z_2, \bar{z}_2)}}{\partial z_2}. \quad (6.20)$$

In order to obtain the expression of $U^{(2)}$, we first note that, by virtue of (6.17),

$$\begin{aligned} (\tau_2 \rho_2 - \tau_2^2 \bar{\delta}_2 + \tau_2 \bar{\rho}_2 - \delta_2) \frac{\partial}{\partial z_2} + (\tau_2 \bar{\tau}_2 \rho_2 - \tau_2 \bar{\delta}_2 + \bar{\rho}_2 - \bar{\tau}_2 \delta_2) \frac{\partial}{\partial \bar{z}_2} = \\ = \nu_2 \left(\delta_1 \frac{\partial}{\partial z_1} + \rho_1 \frac{\partial}{\partial \bar{z}_1} \right). \end{aligned}$$

Hence, considering also (6.15), equation (6.13) may be rewritten as

$$U^{(2)}(x_1, x_2) = \delta_1 \frac{\partial F^{(2)}}{\partial z_1} + \rho_1 \frac{\partial F^{(2)}}{\partial \bar{z}_1} + \frac{k_0}{\nu_2^2} [\tau_2 h(z_2, \bar{z}_2) + \overline{h(z_2, \bar{z}_2)}] + \frac{1}{\nu_2} [\eta'(z_2) + \overline{\eta'(z_2)}].$$

Next, replacing $F^{(2)}$ by (6.19) yields

$$U^{(2)}(x_1, x_2) = \sum_{\alpha} [\delta_{\alpha} \omega'_{\alpha}(z_{\alpha}) + \rho_{\alpha} \overline{\omega'_{\alpha}(z_{\alpha})}] + U_0(x_1, x_2), \quad (6.21)$$

where

$$U_0(x_1, x_2) = \delta_1 \frac{\partial F_0}{\partial z_1} + \rho_1 \frac{\partial F_0}{\partial \bar{z}_1} + \frac{k_0}{\nu_2^2} [\tau_2 h(z_2, \bar{z}_2) + \overline{h(z_2, \bar{z}_2)}]. \quad (6.22)$$

Finally, by substituting (6.19) into (6.9), we deduce the complex stresses

$$\left. \begin{aligned} \Phi^{(2)} &= -4 \sum_{\alpha} [\tau_{\alpha}^2 \omega''_{\alpha}(z_{\alpha}) + \overline{\omega''_{\alpha}(z_{\alpha})}] - 4 \frac{\partial^2 F_0}{\partial z^2}, \\ \Theta^{(2)} &= 8 \operatorname{Re} \sum_{\alpha} \tau_{\alpha} \omega''_{\alpha}(z_{\alpha}) + 4 \frac{\partial^2 F_0}{\partial z \partial \bar{z}}. \end{aligned} \right\} \quad (6.23)$$

The complex potentials $\omega_1'(z_1)$ and $\omega_2'(z_2)$ can be determined by using the boundary conditions (6.6), (6.7), and the continuity conditions (6.3), (6.10), provided we are able to calculate two indefinite integrals that are necessary to obtain $h(z_2, \bar{z}_2)$ and $\partial F_0 / \partial \bar{z}_1$ from (6.15) and (6.20), respectively. Since the functions Θ_0 and Φ_0 occurring in (6.15) and (6.20) are quadratic in the partial derivatives of $U^{(1)}$, it is easily seen that the amount of algebra necessary to calculate $h(z_2, \bar{z}_2)$ and $\partial F_0 / \partial \bar{z}_1$ increases very rapidly with the number of terms taken into account in the expression (5.24) of $\Omega_\alpha'(z_\alpha)$. Therefore, following an idea of Seeger, we content ourselves with determining only those terms which are at most of the order $O(\varrho^{-1})$ in the expression of the displacement and $O(\varrho^{-2})$ in the expression of the stresses, as $\varrho \rightarrow \infty$. In this way, we attempt to find out the most significant correction to the classical solution, which neglects boundary conditions on Γ_0 and second-order effects and retains only the terms of order $O(\varrho^{-1})$ in the expression of stresses. The calculation of the functions $h(z_2, \bar{z}_2)$ and $\partial F_0 / \partial \bar{z}_1$ corresponding to this approximation is presented in the Appendix. The final result reads

$$\frac{\partial F_0}{\partial \bar{z}}(x_1, x_2) = \sum_{\alpha} [\delta_{\alpha} \Lambda_{\alpha}(x_1, x_2) + \overline{\Lambda_{\alpha}(x_1, x_2)}], \quad (6.24)$$

$$U_0(x_1, x_2) = \Lambda_0(x_1, x_2) + \sum_{\alpha} [\delta_{\alpha} \Lambda_{\alpha}(x_1, x_2) + \overline{\delta_{\alpha} \Lambda_{\alpha}(x_1, x_2)}], \quad (6.25)$$

where

$$\left. \begin{aligned} \Lambda_0(x_1, x_2) &= \frac{t_1}{z_1} + \frac{t_2}{\bar{z}_1} + \frac{t_3}{z_2} + \frac{t_4}{\bar{z}_2}, \\ \Lambda_1(x_1, x_2) &= \frac{t_5}{z_1} + \frac{t_6}{z_2} + \frac{t_7}{\bar{z}_2} + \frac{t_8 \bar{z}_1}{z_1^2} + \frac{1}{z_1} \left(w_1 \ln \frac{\bar{z}_1}{1 + \delta_1} + \right. \\ &\quad \left. + w_2 \ln \frac{z_2}{1 + \delta_2} + w_3 \ln \frac{\bar{z}_2}{1 + \delta_2} \right), \\ \Lambda_2(x_1, x_2) &= \frac{t_9 \bar{z}_2}{z_2^2} + \frac{1}{z_2} \left(w_4 \ln \frac{z_1}{1 + \delta_1} + w_5 \ln \frac{\bar{z}_1}{1 + \delta_1} + w_6 \ln \frac{\bar{z}_2}{1 + \delta_2} \right), \end{aligned} \right\} \quad (6.26)$$

while $t_1, \dots, t_9, w_1, \dots, w_6$ are parameters depending only on the elastic constants of second and third orders and on the Burgers vector, and whose explicit expressions are given in the Appendix.

From (6.19), (6.21), (6.24), and (6.25), it follows that

$$\frac{\partial F^{(2)}}{\partial \bar{z}}(x_1, x_2) = \sum_{\alpha} \{ \tau_{\alpha} [\omega'_{\alpha}(z_{\alpha}) + \Lambda_{\alpha}(x_1, x_2)] + \overline{\omega'_{\alpha}(z_{\alpha})} + \overline{\Lambda_{\alpha}(x_1, x_2)} \} \quad (6.27)$$

$$U^{(2)}(x_1, x_2) = \Lambda_0(x_1, x_2) + \sum_{\alpha} \{ \delta_{\alpha} [\omega'_{\alpha}(z_{\alpha}) + \Lambda_{\alpha}(x_1, x_2)] + \rho_{\alpha} [\overline{\omega'_{\alpha}(z_{\alpha})} + \overline{\Lambda_{\alpha}(x_1, x_2)}] \}. \quad (6.28)$$

Inspection of (6.26) shows that $\Lambda_0(x_1, x_2)$ is continuous across τ_0 , while $\Lambda_1(x_1, x_2)$ and $\Lambda_2(x_1, x_2)$ have the jumps

$$\Lambda_{\alpha}(x_1, 0^+) - \Lambda_{\alpha}(x_1, 0^-) = -2\pi i K_{\alpha}/x_1, \quad \alpha = 1, 2 \quad (6.29)$$

for $x_1 \in (-\infty, -r_0]$, where

$$K_1 = w_1 + w_3 - w_2, \quad K_2 = w_5 + w_6 - w_4. \quad (6.30)$$

In view of the continuity conditions (6.3) and (6.10), it may be shown that the part of the solution (6.27), (6.28) corresponding to the functions $\omega'_{\alpha}(z_{\alpha})$ must represent a generalized Somigliana dislocation of the type considered in [10], with variable displacement jump across the cut τ_0 and a distribution of non-equilibrated tractions acting on the cut faces. As shown in [10], the solution to this problem may be found by setting

$$\omega'_{\alpha}(z_{\alpha}) = \tilde{\omega}'_{\alpha}(z_{\alpha}) + \hat{\omega}'_{\alpha}(z_{\alpha}) \quad (6.31)$$

and requiring that the functions $\tilde{\omega}'_{\alpha}(z_{\alpha})$ satisfy the jump conditions on τ_0 and vanish at infinity, while $\hat{\omega}'_{\alpha}(z_{\alpha})$ must be

continuous across $\bar{\gamma}_0$, vanish at infinity, and fulfil the boundary conditions on $\bar{\Gamma}_0$, modified by the contribution of $\tilde{\omega}'_\alpha(z_\alpha)$. In our case, we may satisfy the jump conditions resulting for $\tilde{\omega}'_\alpha(z_\alpha)$ from (6.3), (6.10), and (6.27 - 30) by simply taking

$$\omega'_\alpha(z_\alpha) = \frac{K_\alpha}{z_\alpha} \ln \frac{z_\alpha}{1+\bar{\gamma}_\alpha}, \quad \alpha = 1, 2. \quad (6.32)$$

On the other hand, in agreement with the approximation adopted above, we shall take

$$\hat{\omega}'_\alpha(z_\alpha) = \frac{a_{1\alpha}^{(2)}}{z_\alpha}, \quad \alpha = 1, 2, \quad (6.33)$$

interpreting the coefficients $a_{1\alpha}^{(2)}$ as adjustable parameters.

Summarizing the above considerations, we conclude that the non-linear elastic displacement field is given up to terms of order $O(\varepsilon^2)$ and $O(\varepsilon^{-1})$ by the expression

$$U(x_1, x_2) = \sum_\alpha \left\{ \delta_\alpha \left[\left(\varepsilon \kappa_\alpha + \frac{\varepsilon^2 K_\alpha}{z_\alpha} \right) \ln \frac{z_\alpha}{1+\bar{\gamma}_\alpha} + \frac{A_\alpha}{z_\alpha} \right] + \right. \\ \left. + \vartheta_\alpha \left[\left(\varepsilon \bar{\kappa}_\alpha + \frac{\varepsilon^2 \bar{K}_\alpha}{\bar{z}_\alpha} \right) \ln \frac{\bar{z}_\alpha}{1+\bar{\gamma}_\alpha} + \frac{\bar{A}_\alpha}{\bar{z}_\alpha} \right] \right\} + \varepsilon^2 U_0(x_1, x_2) + u_0 + i v_0, \quad (6.34)$$

where

$A_\alpha = \varepsilon a_{1\alpha}^{(1)} + \varepsilon^2 a_{1\alpha}^{(2)}$, $u_0 = \varepsilon u_0^{(1)}$, $v_0 = \varepsilon v_0^{(1)}$, while κ_α , K_α , $U_0(x_1, x_2)$ are given by (5.34), (6.30), and (6.25), respectively. Since κ_1 and κ_2 are proportional to $b^{(1)}$, while K_1 , K_2 , and $U_0(x_1, x_2)$ are proportional to the square of $b^{(1)}$, and since $b = \varepsilon b^{(1)}$, the final expression (6.34) of the displacement field does not depend on the choice of the small parameter ε , as it should be.

The solution obtained depends linearly on two arbitrary complex constants, A_1 and A_2 . When using a semidiscrete method, these constants should be considered as adjustable parameters in the expression of the total potential energy, together with the positions of the atoms inside the dislocation core, and are to be calculated by minimizing

this energy. Finally, $u_0 + iv_0$ gives a rigid translation that can be determined by prescribing the displacement of an arbitrary point of the elastic medium.

APPENDIX

This appendix is devoted to the determination of the functions $\partial F_0 / \partial \bar{z}$ and U_0 . We follow the procedure employed by Seeger, Teodosiu, and Petrasch [7], taking advantage, however, of the simplifications brought about by the Eulerian formulation.

Let us first determine the explicit expressions of the functions Θ_0 and Φ_0 . By introducing the concised notation

$$u_{1,1}^{*(1)} = h_1, \quad u_{2,2}^{*(1)} = h_2, \quad u_{1,2}^{*(1)} = h_3, \quad u_{2,1}^{*(1)} = h_4, \quad (A.1)$$

we obtain ¹ from (6.8), (4.5), and (4.2)₃

$$\Theta_0 = A_{KR} h_K h_R, \quad \Phi_0 = B_{KR} h_K h_R \quad (A.2)$$

where the coefficients A_{KR} and B_{KR} , which satisfy the symmetry relations

$$A_{KR} = A_{RK} = \bar{A}_{KR}, \quad B_{KR} = B_{RK}, \quad (A.3)$$

are given by

¹ Throughout the Appendix capital Latin subscripts range over the values 1, 2, 3, 4 and the summation convention with respect to repeated such indices is being used.

$$A_{11} = \frac{1}{2}(5c_{11} + c_{12} + C_{111} + C_{112}), \quad A_{12} = \frac{1}{2}(-c_{11} + 2c_{12} - c_{22} + C_{112} + C_{122}),$$

$$A_{13} = \frac{1}{2}(5c_{16} + c_{26} + C_{116} + C_{126}), \quad A_{14} = \frac{1}{2}(4c_{16} + C_{116} + C_{126}),$$

$$A_{22} = \frac{1}{2}(c_{12} + 5c_{22} + C_{122} + C_{222}), \quad A_{23} = \frac{1}{2}(4c_{26} + C_{126} + C_{226}),$$

$$A_{24} = \frac{1}{2}(c_{16} + 5c_{26} + C_{126} + C_{226}), \quad A_{33} = \frac{1}{2}(c_{12} + c_{22} + 4c_{66} + C_{166} + C_{266}),$$

$$A_{34} = \frac{1}{2}(c_{11} + 2c_{12} + c_{22} + 4c_{66} + C_{166} + C_{266}),$$

$$A_{44} = \frac{1}{2}(c_{11} + c_{12} + 4c_{66} + C_{166} + C_{266}),$$

$$B_{11} = \frac{1}{2}(5c_{11} - c_{12} + C_{111} - C_{112}) + i(3c_{16} + C_{116}),$$

$$B_{12} = \frac{1}{2}(c_{22} - c_{11} + C_{112} - C_{126}) + iC_{126},$$

$$B_{13} = \frac{1}{2}(5c_{16} - c_{26} + C_{116} - C_{126}) + i(c_{12} + 2c_{66} + C_{166}),$$

$$B_{14} = \frac{1}{2}(C_{116} - C_{126}) + i(c_{11} + c_{66} + C_{166}),$$

$$B_{22} = \frac{1}{2}(c_{12} - 5c_{22} + C_{122} - C_{222}) + i(3c_{26} + C_{226}),$$

$$B_{23} = \frac{1}{2}(C_{126} - C_{226}) + i(c_{22} + c_{66} + C_{266}),$$

$$B_{24} = \frac{1}{2}(c_{16} - 5c_{26} + C_{126} - C_{226}) + i(c_{12} + 2c_{66} + C_{266}),$$

$$B_{33} = \frac{1}{2}(c_{12} - c_{22} + 4c_{66} + C_{166} - C_{266}) + i(3c_{26} + C_{266}),$$

$$B_{34} = \frac{1}{2}(c_{11} - c_{22} + C_{166} - C_{266}) + i(2c_{16} + 2c_{26} + C_{666}),$$

$$B_{44} = \frac{1}{2}(c_{11} - c_{12} - 4c_{66} + C_{166} - C_{266}) + i(3c_{16} + C_{666}).$$

The next step is the determination of h_K in terms of $\Omega'_\alpha(z_\alpha)$ by means of (A.1) and (5.20). As already mentioned in Sect. 6, we wish to determine the terms that are at most of the order $O(\varrho^{-1})$ for the displacements and $O(\varrho^{-2})$ for the stresses, as $\varrho \rightarrow \infty$. Inspection of equations (6.15) and (6.20) reveals that all terms of the expansion (6.24) but the logarithmic one lead to terms of order higher than $O(\varrho^{-2})$ in stresses, and hence can be disregarded in finding the functions $h(z_2, \bar{z}_2)$ and $\partial F_0 / \partial \bar{z}$. Consequently, we simplify (5.24) to

$$\Omega'_\alpha(z_\alpha) = \kappa_\alpha \ln \frac{z_\alpha}{1+\tau_\alpha},$$

whence, by (5.20),

$$\left. \begin{aligned} u_1^{*(1)} &= \operatorname{Re} \sum_\alpha (\delta_\alpha + \bar{\varrho}_\alpha) \kappa_\alpha \ln \frac{z_\alpha}{1+\tau_\alpha} + u_0^{(1)}, \\ u_2^{*(1)} &= \operatorname{Im} \sum_\alpha (\delta_\alpha - \bar{\varrho}_\alpha) \kappa_\alpha \ln \frac{z_\alpha}{1+\tau_\alpha} + v_0^{(1)}, \end{aligned} \right\} \quad (\text{A.4})$$

Next, introducing (A.4) into (A.1) and taking into account that

$$z_\alpha = z + \tau_\alpha \bar{z} = (1+\tau_\alpha) x_1 + i(1-\tau_\alpha) x_2,$$

we obtain

$$h_K = 2 \operatorname{Re} \sum_\alpha (E_{K\alpha} / z_\alpha), \quad (\text{A.5})$$

where

$$\begin{aligned} E_{1\alpha} &= \kappa_\alpha (\delta_\alpha + \bar{\varrho}_\alpha) (1+\tau_\alpha) / 2, & E_{2\alpha} &= \kappa_\alpha (\delta_\alpha - \bar{\varrho}_\alpha) (1-\tau_\alpha) / 2, \\ E_{3\alpha} &= i \kappa_\alpha (\delta_\alpha + \bar{\varrho}_\alpha) (1-\tau_\alpha) / 2, & E_{4\alpha} &= -i \kappa_\alpha (\delta_\alpha - \bar{\varrho}_\alpha) (1+\tau_\alpha) / 2. \end{aligned}$$

Finally, substituting (A.5) into (A.2), we find

$$\Theta_0 = \sum_{\alpha, \beta} \left(\frac{F_{\alpha\beta}}{z_\alpha z_\beta} + \frac{\bar{F}_{\alpha\beta}}{\bar{z}_\alpha \bar{z}_\beta} + \frac{2G_{\alpha\beta}}{z_\alpha \bar{z}_\beta} \right), \quad \Phi_0 = \sum_{\alpha, \beta} \left(\frac{I_{\alpha\beta}}{z_\alpha z_\beta} + \frac{L_{\alpha\beta}}{\bar{z}_\alpha \bar{z}_\beta} + \frac{2M_{\alpha\beta}}{z_\alpha \bar{z}_\beta} \right) \quad (\text{A.6})$$

with the notation

$$\left. \begin{aligned} F_{\alpha\beta} = F_{\beta\alpha} = A_{KR} E_{K\alpha} E_{R\beta}, \quad G_{\alpha\beta} = \bar{G}_{\beta\alpha} = A_{KR} E_{K\alpha} \bar{E}_{R\beta}, \\ I_{\alpha\beta} = I_{\beta\alpha} = B_{KR} E_{K\alpha} E_{R\beta}, \quad L_{\alpha\beta} = L_{\beta\alpha} = B_{KR} \bar{E}_{K\alpha} \bar{E}_{R\beta}, \\ M_{\alpha\beta} = B_{KR} E_{K\alpha} \bar{E}_{R\beta}. \end{aligned} \right\} \quad (A.7)$$

We proceed now to determining the functions $h(z_2, \bar{z}_2)$ and $\partial F_0 / \partial \bar{z}_1$. From (A.6) we deduce that

$$\begin{aligned} k_1 \Phi_0 + k_2 \Phi_0 + k_3 \bar{\Phi}_0 = \frac{m_1}{z_1^2} + \frac{m_2}{z_1 \bar{z}_1} + \frac{m_3}{z_1 \bar{z}_2} + \frac{m_4}{z_1 \bar{z}_2} + \frac{m_5}{\bar{z}_1^2} + \\ + \frac{m_6}{\bar{z}_1 \bar{z}_2} + \frac{m_7}{\bar{z}_1 \bar{z}_2} + \frac{m_8}{z_2^2} + \frac{m_9}{z_2 \bar{z}_2} + \frac{m_{10}}{\bar{z}_2^2}, \end{aligned} \quad (A.8)$$

where

$$\begin{aligned} m_1 &= k_1 F_{11} + k_2 I_{11} + k_3 \bar{L}_{11}, & m_2 &= 2(k_1 G_{11} + k_2 M_{11} + k_3 \bar{M}_{11}), \\ m_3 &= 2(k_1 F_{12} + k_2 I_{12} + k_3 \bar{L}_{12}), & m_4 &= 2(k_1 G_{12} + k_2 M_{12} + k_3 \bar{M}_{21}), \\ m_5 &= k_1 \bar{F}_{11} + k_2 L_{11} + k_3 \bar{I}_{11}, & m_6 &= 2(k_1 \bar{G}_{12} + k_2 M_{21} + k_3 \bar{M}_{12}), \\ m_7 &= 2(k_1 \bar{F}_{12} + k_2 L_{12} + k_3 \bar{I}_{12}), & m_8 &= k_1 F_{22} + k_2 I_{22} + k_3 \bar{L}_{22}, \\ m_9 &= 2(k_1 G_{22} + k_2 M_{22} + k_3 \bar{M}_{22}), & m_{10} &= k_1 \bar{F}_{22} + k_2 L_{22} + k_3 \bar{I}_{22}. \end{aligned}$$

Substituting (A.8) into (6.15) and using the formulae

$$z = \frac{z_2 - \delta_2 \bar{z}_2}{\nu_2}, \quad \bar{z} = \frac{-\bar{\delta}_2 z_2 + \bar{z}_2}{\nu_2}, \quad z_1 = \frac{\nu_3 z_2 + \nu_4 \bar{z}_2}{\nu_2}, \quad \bar{z}_1 = \frac{\bar{\nu}_4 z_2 + \bar{\nu}_3 \bar{z}_2}{\nu_2},$$

$$\int \frac{dz_2}{(az_2 + b\bar{z}_2)(cz_2 + d\bar{z}_2)} = \frac{1}{(ad-bc)\bar{z}_2} \left[\ln(az_2 + b\bar{z}_2) - \ln(cz_2 + d\bar{z}_2) \right] + \overline{\psi_2(z_2)}, \quad (A.9)$$

$$\begin{aligned} \int \frac{\ln(cz_2 + d\bar{z}_2) dz_2}{(az_2 + b\bar{z}_2)^2} = - \frac{\ln(cz_2 + d\bar{z}_2)}{a(az_2 + b\bar{z}_2)} + \\ + \frac{c}{a(ad-bc)\bar{z}_2} \left[\ln(az_2 + b\bar{z}_2) - \ln(cz_2 + d\bar{z}_2) \right] + \overline{\psi_3(z_2)}, \end{aligned} \quad (A.10)$$

where $ad-bc \neq 0$ and $\psi(z_2), \psi_3(z_2)$ denote two arbitrary analytic functions of z_2 , we obtain

$$h(z_2, \bar{z}_2) = \nu_2 \left(-\frac{m_1}{\nu_3 z_1} - \frac{m_5}{\nu_4 \bar{z}_1} - \frac{m_8}{\nu_2 z_2} + \frac{m_{10} z_2}{\nu_2 \bar{z}_2^2} + \right. \\ \left. + \frac{n_1}{\bar{z}_2} \ln \frac{z_1}{1+\delta_1} + \frac{n_2}{\bar{z}_2} + \frac{n_3}{\bar{z}_2} \ln \frac{\bar{z}_2}{1+\delta_2} \right), \quad (A.11)$$

where

$$n_1 = \frac{m_2}{\nu_1} - \frac{m_3}{\nu_4} + \frac{m_4}{\nu_3}, \quad n_2 = -\frac{m_2}{\nu_1} - \frac{m_6}{\nu_3} + \frac{m_7}{\nu_4}, \quad n_3 = \frac{m_3}{\nu_4} + \frac{m_6}{\nu_3} + \frac{m_9}{\nu_2}.$$

Finally, by introducing (A.6) and (A.11) into (6.20) and omitting terms in z_2^{-2} and \bar{z}_2^{-2} , which can be included in $\eta''(z_2)$ and $\overline{\eta''(z_2)}$, we find

$$\frac{\partial^2 F_0}{\partial z_1 \partial \bar{z}_1} = 2 \operatorname{Re} \left[\frac{r_1}{z_1^2} + \frac{r_2}{z_1 \bar{z}_1} + \frac{r_3}{z_1 z_2} + \frac{r_4}{z_1 \bar{z}_2} + \frac{r_5}{z_2 \bar{z}_2} - \frac{2m_{10} z_2}{\bar{z}_2^3} \right. \\ \left. - \frac{\nu_2}{\bar{z}_2^2} \left(\bar{n}_2 \ln \frac{z_1}{1+\delta_1} + \bar{n}_1 \ln \frac{\bar{z}_1}{1+\delta_1} + \bar{n}_3 \ln \frac{\bar{z}_2}{1+\delta_2} \right) \right],$$

where

$$r_1 = 2k_4 F_{11} + k_5 I_{11} + \bar{k}_5 \bar{L}_{11} + \frac{\nu_4 m_1}{\nu_3} + \frac{\nu_3 \bar{m}_5}{\nu_4},$$

$$r_2 = 2(k_4 G_{11} + k_5 M_{11}), \quad r_5 = 2(k_4 G_{22} + k_5 M_{22}),$$

$$r_3 = 2(2k_4 F_{12} + k_5 I_{12} + \bar{k}_5 \bar{L}_{12}) + \nu_3 \bar{n}_2,$$

$$r_4 = 2(2k_4 G_{12} + k_5 M_{12} + \bar{k}_5 \bar{M}_{21}) + \nu_4 n_1.$$

Using now again (A.9) and (A.10) with z_2 replaced by z_1 , and taking into account that

$$z = \frac{z_1 - \bar{\sigma}_1 \bar{z}_1}{\nu_1}, \quad \bar{z} = \frac{-\bar{\sigma}_1 z_1 + \bar{z}_1}{\nu_1}, \quad z_2 = \frac{\bar{\nu}_3 z_1 - \nu_4 \bar{z}_1}{\nu_1}, \quad \bar{z}_2 = \frac{-\bar{\nu}_4 z_1 + \nu_3 \bar{z}_1}{\nu_1},$$

we obtain

$$\begin{aligned} \frac{\partial F_0}{\partial \bar{z}_1} = & \nu_1 \left[-\frac{r_1}{\nu_1 z_1} - \frac{2\bar{\nu}_4 \bar{m}_{10}}{\bar{\nu}_3^2 z_2} + \frac{2\bar{\nu}_3 m_{10}}{\bar{\nu}_4^2 \bar{z}_2} + \frac{\bar{r}_1 z_1}{\nu_1 \bar{z}_1^2} - \frac{\nu_2 m_{10} \bar{z}_1}{\bar{\nu}_4^2 \bar{z}_2^2} + \frac{\nu_2 m_{10} \bar{z}_1}{\bar{\nu}_3^2 z_2^2} + \right. \\ & + \left(\frac{\lambda_1}{\bar{z}_1} + \frac{\nu_2 \bar{n}_2}{\bar{\nu}_3 z_2} - \frac{\nu_2 n_1}{\bar{\nu}_4 \bar{z}_2} \right) \ln \frac{z_1}{1+\bar{\sigma}_1} + \left(\frac{\nu_2 \bar{n}_1}{\bar{n}_3 z_2} - \frac{\nu_2 n_2}{\bar{\nu}_4 \bar{z}_2} \right) \ln \frac{\bar{z}_1}{1+\bar{\sigma}_1} + \\ & \left. + \left(\frac{\lambda_2}{\bar{z}_1} - \frac{\nu_2 n_3}{\bar{\nu}_4 \bar{z}_2} \right) \ln \frac{z_2}{1+\bar{\sigma}_2} + \left(\frac{\lambda_3}{\bar{z}_1} + \frac{\nu_2 \bar{n}_3}{\bar{\nu}_3 z_2} \right) \ln \frac{\bar{z}_2}{1+\bar{\sigma}_2} \right], \quad (A.12) \end{aligned}$$

where

$$\lambda_1 = \frac{r_2 + \bar{r}_2}{\nu_1} - \frac{r_3}{\nu_4} + \frac{r_4}{\nu_3} - \nu_5 n_1 - \bar{\nu}_5 n_2, \quad \nu_5 = -\frac{\nu_1 \nu_2}{\nu_3 \nu_4},$$

$$\lambda_2 = \frac{r_3}{\nu_4} + \frac{\bar{r}_4}{\bar{\nu}_3} + \frac{r_5 + \bar{r}_5}{\nu_2} + \bar{\nu}_5 \bar{n}_2 + \frac{\bar{\nu}_4 \bar{n}_3}{\bar{\nu}_3} + \frac{\bar{\nu}_3 n_3}{\bar{\nu}_4},$$

$$\lambda_3 = -\frac{\bar{r}_3}{\bar{\nu}_4} - \frac{r_4}{\nu_3} - \frac{r_5 + \bar{r}_5}{\nu_2} + \nu_5 n_1 - \frac{\bar{\nu}_3 n_3}{\bar{\nu}_4} - \frac{\bar{\nu}_4 \bar{n}_3}{\bar{\nu}_3}.$$

Finally, by taking into account that

$$\frac{\partial F_0}{\partial \bar{z}} = \bar{\sigma}_1 \frac{\partial F_0}{\partial z_1} + \frac{\partial F_0}{\partial \bar{z}_1} \quad (A.13)$$

and introducing (A.11) and (A.12) into (A.13) and (6.22), we find the expressions (6.24) and (6.25) given for $\partial F_0 / \partial \bar{z}$ and U_0 in the main text, with the notation

$$t_1 = -\frac{k_0}{\nu_2} \left(\frac{r_2 m_1}{\nu_3} + \frac{\bar{m}_5}{\nu_4} \right), \quad t_2 = -\frac{k_0}{\nu_2} \left(\frac{r_2 m_5}{\bar{\nu}_4} + \frac{\bar{m}_1}{\nu_3} \right), \quad t_3 = -\frac{k_0 r_2 m_8}{\nu_2^2}, \quad t_4 = -\frac{k_0 \bar{m}_8}{\bar{\nu}_2^2},$$

$$t_5 = -\bar{r}_1, \quad t_6 = \frac{\nu_1 \nu_3 \bar{m}_{10}}{\nu_4^2}, \quad t_7 = -\frac{\nu_1 \nu_4 m_{10}}{\bar{\nu}_3^2}, \quad t_8 = r_1, \quad t_9 = \nu_1 \bar{\nu}_5 \bar{m}_{10},$$

$$w_1 = \nu_1 \bar{\lambda}_1, \quad w_2 = \nu_1 \bar{\lambda}_3, \quad w_3 = \nu_1 \bar{\lambda}_2,$$

$$w_4 = \nu_1 \bar{\nu}_5 \bar{n}_2, \quad w_5 = \nu_1 \bar{\nu}_5 \bar{n}_1, \quad w_6 = \nu_1 \bar{\nu}_5 \bar{n}_3.$$

Using new basis (A.9) and (A.10) with \bar{z}_1 replaced by \bar{z}_1' and taking into account that

$$\bar{z}_1 = \frac{\bar{z}_1' - \bar{z}_1''}{\sqrt{2}}, \quad \bar{z}_2 = \frac{-\bar{z}_1' + \bar{z}_1''}{\sqrt{2}}, \quad \bar{z}_3 = \frac{\bar{z}_1' + \bar{z}_1''}{\sqrt{2}}, \quad \bar{z}_4 = \frac{-\bar{z}_1' - \bar{z}_1''}{\sqrt{2}},$$

we obtain

$$\begin{aligned} \frac{9F}{95} = \frac{1}{\sqrt{2}} \left[\frac{2}{\sqrt{2}} \frac{\pi}{2} + \frac{2}{\sqrt{2}} \frac{\pi}{2} - \frac{2}{\sqrt{2}} \frac{\pi}{2} + \frac{2}{\sqrt{2}} \frac{\pi}{2} + \frac{2}{\sqrt{2}} \frac{\pi}{2} + \frac{2}{\sqrt{2}} \frac{\pi}{2} + \frac{2}{\sqrt{2}} \frac{\pi}{2} + \frac{2}{\sqrt{2}} \frac{\pi}{2} \right] \\ + \left(\frac{2}{\sqrt{2}} \frac{\pi}{2} + \frac{2}{\sqrt{2}} \frac{\pi}{2} - \frac{2}{\sqrt{2}} \frac{\pi}{2} - \frac{2}{\sqrt{2}} \frac{\pi}{2} \right) \ln \left(\frac{2}{\sqrt{2}} \frac{\pi}{2} \right) + \left(\frac{2}{\sqrt{2}} \frac{\pi}{2} + \frac{2}{\sqrt{2}} \frac{\pi}{2} \right) \ln \left(\frac{2}{\sqrt{2}} \frac{\pi}{2} \right) \\ + \left(\frac{2}{\sqrt{2}} \frac{\pi}{2} - \frac{2}{\sqrt{2}} \frac{\pi}{2} \right) \ln \left(\frac{2}{\sqrt{2}} \frac{\pi}{2} \right) + \left(\frac{2}{\sqrt{2}} \frac{\pi}{2} - \frac{2}{\sqrt{2}} \frac{\pi}{2} \right) \ln \left(\frac{2}{\sqrt{2}} \frac{\pi}{2} \right) \end{aligned} \quad (A.12)$$

where

$$\begin{aligned} \bar{z}_1' &= \frac{\bar{z}_1 + \bar{z}_2}{\sqrt{2}} = \frac{\bar{z}_1}{\sqrt{2}} + \frac{\bar{z}_2}{\sqrt{2}} \\ \bar{z}_2' &= \frac{\bar{z}_1 - \bar{z}_2}{\sqrt{2}} = \frac{\bar{z}_1}{\sqrt{2}} - \frac{\bar{z}_2}{\sqrt{2}} \\ \bar{z}_3' &= \frac{\bar{z}_1 + \bar{z}_3}{\sqrt{2}} = \frac{\bar{z}_1}{\sqrt{2}} + \frac{\bar{z}_3}{\sqrt{2}} \\ \bar{z}_4' &= \frac{\bar{z}_1 - \bar{z}_3}{\sqrt{2}} = \frac{\bar{z}_1}{\sqrt{2}} - \frac{\bar{z}_3}{\sqrt{2}} \end{aligned}$$

Finally, by taking into account that

$$\frac{9F}{95} = \frac{9F}{95} + \frac{9F}{95} \quad (A.13)$$

and introducing (A.11) and (A.12) into (A.13) and (A.14), we find the expressions (6.7) and (6.8) given for $9F/95$ and U in

the main text, with the notation

$$\begin{aligned} \bar{z}_1' &= \frac{\bar{z}_1 + \bar{z}_2}{\sqrt{2}}, \quad \bar{z}_2' = \frac{\bar{z}_1 - \bar{z}_2}{\sqrt{2}}, \quad \bar{z}_3' = \frac{\bar{z}_1 + \bar{z}_3}{\sqrt{2}}, \quad \bar{z}_4' = \frac{\bar{z}_1 - \bar{z}_3}{\sqrt{2}}, \\ \bar{z}_1'' &= \frac{\bar{z}_1 + \bar{z}_4}{\sqrt{2}}, \quad \bar{z}_2'' = \frac{\bar{z}_1 - \bar{z}_4}{\sqrt{2}}, \quad \bar{z}_3'' = \frac{\bar{z}_1 + \bar{z}_5}{\sqrt{2}}, \quad \bar{z}_4'' = \frac{\bar{z}_1 - \bar{z}_5}{\sqrt{2}} \end{aligned}$$