MoDELib manual

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Preface

Acknowledgements

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Chapter 1

The elastic theory of discrete dislocations

The key aspect of the DDD method is that dislocation interactions are computed without resorting to expensive atomistic calculations. This is made possible by the elastic theory of dislocations, which provides semi-analytical expressions of the elastic fields (displacement, stress, strain…) generated by arbitrary dislocation loops within an infinite elastic medium. We now briefly summarize this theory, as a special case of Mura's linearized eigendistortion theory [Mura, 1987].

1.1 Eigendistortion theory in elastic media

1.1.1 Eigendistortion theory in infinite anisotropic media

Let us consider an elastic body occupying the infinite three-dimensional space $\mathbb{R}^3$, and let $\boldsymbol{u}(\boldsymbol{x})$ be its displacement field. We adopt here the linearized eigen-distortion framework of Mura [1987], in which the main kinematic assumption is that the displacement gradient is split additively into an elastic distortion $\boldsymbol{\beta}$, and an inelastic distortion $\boldsymbol{\beta}^\star$:

$$u_{i,j} = \beta_{ij} + \beta^\star_{ij}\,. \tag{1.1}$$

The elastic distortion describes the local stretching of the atomic bonds and is related to stress via Hookes law ($\sigma_{ij} = \mathbb{C}_{ijkl}\beta_{kl}$). On the other hand, the inelastic distortion is the *eigendistortion* of the material, and it may contain several (additive) contributions, including plastic deformation, thermal deformation, deformation due to point defects and diffusive species in the lattice, and more. The inelastic distortion is also referred to as an *eigendistortion*, because it is imagined to take place within a fictitious "intermediate" configuration where the body is allowed to deform with incompatibilities (separations and/or interpenetrations) in order to remain stress free. It is the subsequent elastic distortion which is responsible to develop the internal stress field necessary to remove the incompatibilities of the intermediate configuration. It will be shown that an eigendistortion field results in a state of self-stress if it is incompatible, that is if its (negative) curl

$$\alpha_{ij} = -\epsilon_{jkm}\beta^\star_{im,k} \tag{1.2}$$

is non vanishing. If the eigendistortion is due to dislocations, then $\boldsymbol{\alpha}$ can be interpreted as a tensorial density of dislocations, which is known as the Kröner-Nye dislocation density tensor.

In the presence of a body forces density $\boldsymbol{b}$, the static Lagrangian density of the classical linear elastic medium reads

$$\mathcal{L} = -\mathcal{W} - \mathcal{V} = -\frac{1}{2}\mathbb{C}_{ijkl}\beta_{ij}\beta_{kl} + u_i f_i\,,$$

where

$$\mathcal{V} = -u_i b_i \tag{1.3}$$

is the potential of the body force density $\boldsymbol{f}$, while

$$\mathcal{W} = \frac{1}{2}\mathbb{C}_{ijkl}\varepsilon_{ij}\varepsilon_{kl} \tag{1.4}$$

is the strain energy density, which is assumed to be quadratic in the elastic strain

$$\varepsilon_{ij} = \frac{1}{2}\left(\beta_{ij} + \beta_{ji}\right) \tag{1.5}$$

Here $\mathbb{C}_{ijkl}$ is the rank-4 tensor of elastic moduli. By virtue of the symmetries

$$\mathbb{C}_{ijkl} = \mathbb{C}_{jikl} = \mathbb{C}_{ijlk} = \mathbb{C}_{klij}\,, \tag{1.6}$$

it possesses up to 21 independent constants.

The condition of static equilibrium for displacement is expressed by the Euler-Lagrange equation

$$\frac{\delta\mathcal{L}}{\delta u_i} = \frac{\partial\mathcal{L}}{\partial u_i} - \partial_j\,\frac{\partial\mathcal{L}}{\partial(\partial_j u_i)} = -\sigma_{ij,j} - f_i = . \tag{1.7}$$

where

$$\sigma_{ij} = \frac{\partial W}{\partial\varepsilon_{ij}} = \mathbb{C}_{ijkl}\varepsilon_{kl} = \mathbb{C}_{ijkl}\beta_{kl} \tag{1.8}$$

is the Cauchy stress tensor. Using the additive decomposition (1.1), the equilibrium equation in terms of displacement takes the form of the following inhomogeneous Navier equation:

$$L_{ik}u_k = \mathbb{C}_{ijkl}\beta^{\star}_{kl,j}\,, \tag{1.9}$$

where

$$L_{ik} = \mathbb{C}_{ijkl}\partial_j\partial_l \tag{1.10}$$

is the Navier differential operator. This operator admits the well-known Green's tensor G_{im} given in Eq. (A.23). Because the Green's tensor G_{im} is the fundamental solution of the Navier operator, the particular solution of Eq. (1.9) can be obtained from it by convolution with the source term. In particular, for an infinite medium the displacement field reads [Mura, 1987]:

$$\begin{aligned} u_i &= -\mathbb{C}_{mnpq}G_{im} * \beta^{\star}_{pq,n} \\ &= -\mathbb{C}_{mnpq}G_{im,n} * \beta^{\star}_{pq} \qquad \text{(generalized Volterra equation)}\,. \end{aligned} \tag{1.11}$$

In Eq. (1.11) we have introduced the symbol $*$ to indicate convolution over the infinite three-dimensional space. With dislocation theory in mind, Eq. (1.11) can be considered a *generalized Volterra solution* valid for an arbitrary source of eigendistortion.

An expression for the displacement gradient split into elastic and plastic contributions is obtained using the Mura-Willis procedure:

$$\begin{aligned} u_{i,j} &= -\mathbb{C}_{mnpq}G_{im,n} * \beta^P_{pq,j} = -\mathbb{C}_{mnpq}G_{im,n} * \left(\beta^P_{pj,q} + \epsilon_{qjr}\alpha_{pr}\right) \\ &= -\mathbb{C}_{mnpq}G_{im,nq} * \beta^P_{pj} - \mathbb{C}_{mnpq}\epsilon_{qjr}G_{im,n} * \alpha_{pr} \\ &= -L_{pm}G_{im} * \beta^P_{pj} - \mathbb{C}_{mnpq}\epsilon_{qjr}G_{im,n} * \alpha_{pr} = \delta_{ip}\delta * \beta^P_{pj} - \mathbb{C}_{mnpq}\epsilon_{qjr}G_{im,n} * \alpha_{pr} \\ &= \beta^P_{ij} + \mathbb{C}_{mnpq}\epsilon_{jqr}G_{im,n} * \alpha_{pr} \end{aligned} \tag{1.12}$$

From (1.12), the elastic distortion follows immediately as

$$\beta_{ij} = \mathbb{C}_{mnpq}\epsilon_{jqr}G_{im,n} * \alpha_{pr}\,. \qquad \text{(Mura-Willis equation)} \tag{1.13}$$

Clearly, the Cauchy stress field σ_{ij} can be obtained from (1.13) using the Hooke's law (1.8).

$$\sigma_{ij} = \mathbb{C}_{ijkl}\mathbb{C}_{mnpq}\epsilon_{lqr}G_{km,n} * \alpha_{pr} \qquad \text{(anisotropic Peach-Koehler stress equation)}\,. \tag{1.14}$$

Note that elastic distortion (1.13) and stress (1.14) depend on the eigendistortion $\boldsymbol{\beta}^\star$ only through its curl $\boldsymbol{\alpha}$, and therefore they vanish is $\boldsymbol{\beta}^\star$ is compatible.

We are now interested in obtaining an alternative expression of the displacement field (1.11) where the contribution of elastic and plastic distortions appear in separate additive terms. Following [Lazar and Kirchner, 2013], we first take the derivative of Eq. (1.1) with respect to x_j in order to obtain the Poisson equation:

$$\Delta u_i = u_{i,jj} = \beta_{ij,j} + \beta^\star_{ij,j}\ , \tag{1.15}$$

where $\Delta = \partial_j\partial_j$ is the Laplace operator. Second we "invert" Eq. (1.15) using the Green's function[1] of the Laplace operator G^Δ:

$$u_i = \left(\beta^\star_{ij,j} + \beta_{ij,j}\right) * G^\Delta = \beta^\star_{ij} * G^\Delta_{,j} + \beta_{ij,j} * G^\Delta\,. \tag{1.17}$$

It will be clearer in the following sections that Eq. (1.17) can be considered as a *generalized Burgers equation*. In fact, although Eq. (1.17) is valid for an arbitrary source of eigendistortion in an anisotropic medium, its name is well-justified in the case of dislocation loops because the term $\beta^\star_{ij} * G^\Delta_{,j}$ corresponds to the contribution of the solid angle subtended by a loop, which was first isolated by Burgers [Burgers, 1939a,b] in the classical isotropic case. Substituting Eq. (1.13) in (1.17), we find the generalized Burgers solution for the displacement field (see also Lazar and Kirchner [2013]):

$$u_i = G^\Delta_{,j} * \beta^\star_{ij} - \mathbb{C}_{mnpq}\epsilon_{jqr}F_{jnim} * \alpha_{pr} \qquad \text{(generalized Burgers equation)}\,. \tag{1.18}$$

Note that, following **?** and Lazar and Kirchner [2013], in Eq. (1.18) we have introduced the fourth-rank tensor F_{jnim} defined as:

$$F_{jnim} = -G_{im,jn} * G^\Delta\,. \tag{1.19}$$

Similar to the Green's tensor, also the "$\boldsymbol{F}$-tensor" has an explicit form, which is given in Eq. (A.26).

The $\boldsymbol{F}$-tensor is also useful in deriving a compact expression for the interaction energy between two sources of eigendistortion. In fact, using the identity

$$G_{im,j} = G_{im,jnn} * G^\Delta = -F_{jnim,n}\,, \tag{1.20}$$

the interaction energy W_{AB} between two between two sources of eigendistortion, labeled A and B respectively,

[1] The three-dimensional Green's function of the Laplace operator is [Vladimirov, 1971]

$$G^\Delta(\boldsymbol{R}) = -\frac{1}{4\pi R} \tag{1.16}$$

where $R = \sqrt{\boldsymbol{R}\cdot\boldsymbol{R}}$ is the Euclidean norm of $\boldsymbol{R}$.

can be obtained as follows [Po et al., 2018]:

$$
\begin{aligned}
W_{AB} &= \int_{\mathbb{R}^3} \sigma_{il}^{(A)}\, \beta_{il}^{(B)}\, \mathrm{d}V = \int_{\mathbb{R}^3} \mathbb{C}_{ilmn}\epsilon_{npq}\mathbb{C}_{rstp} \left(G_{mr,s} * \alpha_{tq}^{(A)}\right) \beta_{il}^{(B)}\, \mathrm{d}V \\
&= -\int_{\mathbb{R}^3} \mathbb{C}_{ilmn}\epsilon_{npq}\mathbb{C}_{rstp} \left(F_{skmr,k} * \alpha_{tq}^{(A)}\right) \beta_{il}^{(B)}\, \mathrm{d}V = \int_{\mathbb{R}^3} \mathbb{C}_{ilmn}\epsilon_{npq}\mathbb{C}_{rstp} \left(F_{skmr} * \alpha_{tq}^{(A)}\right) \beta_{il,k}^{(B)}\, \mathrm{d}V \\
&= \int_{\mathbb{R}^3} \mathbb{C}_{ilmn}\epsilon_{npq}\mathbb{C}_{rstp} \left(F_{skmr} * \alpha_{tq}^{(A)}\right) \left(\beta_{ik,l}^{(B)} + \epsilon_{jkl}\alpha_{ij}^{(B)}\right) \mathrm{d}V \\
&= -\int_{\mathbb{R}^3} \underbrace{\mathbb{C}_{ilmn}\epsilon_{npq}\mathbb{C}_{rstp} \left(G_{mr,skl} * \alpha_{tq}^{(A)}\right)}_{\sigma_{il,lk}=0} * G^{\Delta}\, \beta_{ik}^{(B)}\, \mathrm{d}V \\
&+ \int_{\mathbb{R}^3} \epsilon_{jkl}\mathbb{C}_{ilmn}\epsilon_{npq}\mathbb{C}_{rstp} \left(F_{skmr} * \alpha_{tq}^{(A)}\right) \alpha_{ij}^{(B)}\, \mathrm{d}V \\
&= \int_{\mathbb{R}^3} \epsilon_{jkl}\mathbb{C}_{ilmn}\epsilon_{npq}\mathbb{C}_{rstp} \left(F_{skmr} * \alpha_{tq}^{(A)}\right) \alpha_{ij}^{(B)}\, \mathrm{d}V \quad \text{(generalized Blin's interaction energy equation)}\,.
\end{aligned}
\tag{1.21}
$$

This result shows that the interaction energy between two sources of eigendistortion depends only on their curls. Therefore it can be regarded as an anisotropic generalization of Blin's equation [Blin, 1955], valid for arbitrary sources of eigendistortion[2].

while the configurational force exerted on the eigendistortion can be computed from the divergence of Eshelby's stress tensor. This gives the Peach-Koehler force on the eigendistortion:

$$
\mathcal{F}_k = \int_{\mathbb{R}^3} \left(W\delta_{kj} - \sigma_{ij}\beta_{ik}\right)_{,j}\, \mathrm{d}V = \int_{\mathbb{R}^3} \epsilon_{kjm}\sigma_{ij}\alpha_{im}\, \mathrm{d}V\,. \tag{1.22}
$$

1.1.2 Eigendistortion theory in infinite isotropic media

In the isotropic case: Starting from (1.18)

$$
c_{mnpq} = \mu\left(\frac{2\nu}{1-2\nu}\delta_{mn}\delta_{pq} + \delta_{mp}\delta_{nq} + \delta_{mq}\delta_{np}\right) \tag{1.23}
$$

and

$$
G_{im,n}(\boldsymbol{x}) = \frac{1}{16\pi\mu(1-\nu)}\left[2(1-\nu)\delta_{im}\partial_n\Delta - \partial_n\partial_i\partial_m\right] R(\boldsymbol{x}) \tag{1.24}
$$

where $R(\boldsymbol{x}) = \sqrt{\boldsymbol{x}\cdot\boldsymbol{x}}$ is the distance function. Therefore

$$
c_{mnpq}G_{im,n} = \frac{1}{8\pi(1-\nu)}\left[\nu\delta_{pq}\partial_i\Delta + (1-\nu)\left(\delta_{ip}\partial_q\Delta + \delta_{iq}\partial_p\Delta\right) - \partial_i\partial_p\partial_q\right] R(\boldsymbol{x}) \tag{1.25}
$$

and obtain

$$
\begin{aligned}
u_i &= -\frac{b_i\Omega}{4\pi} - \frac{1}{8\pi(1-\nu)}\left[(1-\nu)\Delta R * \epsilon_{kip}\alpha_{pk} - \partial_i\partial_q R * \epsilon_{kqp}\alpha_{pk}\right] \\
&= -\frac{b_i\Omega}{4\pi} - \frac{1}{8\pi}\epsilon_{kqp}\left[\delta_{iq}\Delta - \frac{1}{1-\nu}\partial_i\partial_q\right] R * \alpha_{pk} \\
&= -\frac{b_i\Omega}{4\pi} - \frac{1}{8\pi}\epsilon_{lmk}\left[\delta_{im}\Delta - \frac{1}{1-\nu}\partial_i\partial_m\right] R * \alpha_{kl} \\
&= -\frac{b_i\Omega}{4\pi} - U_{ikl}R * \alpha_{kl}
\end{aligned}
\tag{1.26}
$$

[2] Surprisingly, such fundamental result has long been missing in anisotropic eigendistortion theory, and it was found only recently by Lazar and Kirchner [2013] using the method of stress functions.

The operator U_{ill} is:

$$U_{ikl} = \frac{1}{8\pi}\epsilon_{klm}\left[\delta_{im}\Delta - \frac{1}{1-\nu}\partial_i\partial_m\right] \tag{1.27}$$

In order to find a compact expression for the displacement gradient we define the function

$$B_{ijkl}(\boldsymbol{x}) = \mathbb{C}_{mnkq}\epsilon_{jql}G_{im,n}(\boldsymbol{x}) = \frac{1}{8\pi}\left[\left(-\delta_{ik}\epsilon_{jlm}\partial_m + \epsilon_{ilk}\partial_j\right)\Delta + \frac{1}{1-\nu}\epsilon_{klm}\partial_i\partial_j\partial_m\right]R(\boldsymbol{x}) \tag{1.28}$$

With this definition we obtain the displacement gradient as

$$u_{i,j} = \beta^P_{ij} + \mathbb{C}_{mnkq}\epsilon_{jql}G_{im,n} * \alpha_{kl} = \beta^P_{ij} + B_{ijkl} * \alpha_{kl} \tag{1.29}$$

which corresponds to the result of de Wit p 264.

Elastic distortion

$$\beta^E_{ij} = u_{i,j} - \beta^P_{ij} = B_{ijkl}R * \alpha_{kl} \tag{1.30}$$

Elastic strain

$$\varepsilon^E_{ij} = \frac{1}{2}\left(\beta^E_{ij} + \beta^E_{ji}\right) = E_{ijkl}R * \alpha_{kl} \tag{1.31}$$

$$\begin{aligned}
E_{ijkl} &= \frac{1}{2}\left(B_{ijkl} + B_{jikl}\right) \\
&= \frac{1}{16\pi}\left[\left(-\delta_{ik}\epsilon_{jlm}\partial_m - \delta_{jk}\epsilon_{ilm}\partial_m + \epsilon_{ilk}\partial_j + \epsilon_{jlk}\partial_i\right)\Delta + \frac{2}{1-\nu}\epsilon_{klm}\partial_i\partial_j\partial_m\right] \\
&= \frac{1}{16\pi}\left[\left(-\delta_{ik}\epsilon_{jlm}\delta_{mr} - \delta_{jk}\epsilon_{ilm}\delta_{mr} + \epsilon_{ilk}\delta_{jr} + \epsilon_{jlk}\delta_{ir}\right)\partial_r\Delta + \frac{2}{1-\nu}\epsilon_{klm}\partial_i\partial_j\partial_m\right] \\
&= \frac{1}{16\pi}\left[\left(\epsilon_{ilk}\delta_{jr} - \delta_{jk}\epsilon_{ilm}\delta_{mr} + \epsilon_{jlk}\delta_{ir} - \delta_{ik}\epsilon_{jlm}\delta_{mr}\right)\partial_r\Delta + \frac{2}{1-\nu}\epsilon_{klm}\partial_i\partial_j\partial_m\right] \\
&= \frac{1}{16\pi}\left[\left(\epsilon_{ilm}(\delta_{mk}\delta_{jr} - \delta_{jk}\delta_{mr}) + \epsilon_{jlm}(\delta_{mk}\delta_{ir} - \delta_{ik}\delta_{mr})\right)\partial_r\Delta + \frac{2}{1-\nu}\epsilon_{klm}\partial_i\partial_j\partial_m\right] \\
&= \frac{1}{16\pi}\left[\left(\epsilon_{ilm}\epsilon_{smj}\epsilon_{skr} + \epsilon_{jlm}\epsilon_{smi}\epsilon_{skr}\right)\partial_r\Delta + \frac{2}{1-\nu}\epsilon_{klm}\partial_i\partial_j\partial_m\right] \\
&= \frac{1}{16\pi}\left[\epsilon_{skr}\left(\epsilon_{mil}\epsilon_{mjs} + \epsilon_{mjl}\epsilon_{mis}\right)\partial_r\Delta + \frac{2}{1-\nu}\epsilon_{klm}\partial_i\partial_j\partial_m\right] \\
&= \frac{1}{16\pi}\left[\epsilon_{skr}\left(\delta_{ij}\delta_{ls} - \delta_{is}\delta_{lj} + \delta_{ij}\delta_{ls} - \delta_{js}\delta_{il}\right)\partial_r\Delta + \frac{2}{1-\nu}\epsilon_{klm}\partial_i\partial_j\partial_m\right] \\
&= \frac{1}{16\pi}\left[\left(2\epsilon_{lkm}\delta_{ij} - \epsilon_{ikm}\delta_{lj} - \epsilon_{jkm}\delta_{il}\right)\partial_m\Delta + \frac{2}{1-\nu}\epsilon_{klm}\partial_i\partial_j\partial_m\right]
\end{aligned} \tag{1.32}$$

same as de Wit p 264.

Stress

$$\sigma_{pq} = c_{pqij}\beta^E_{ij} = \mu\left(\frac{2\nu}{1-2\nu}\delta_{pq}\delta_{ij} + \delta_{pi}\delta_{qj} + \delta_{pj}\delta_{qi}\right) E_{ijkl} R * \alpha_{kl} = S_{pqkl} * \alpha_{kl} \tag{1.33}$$

$$S_{ijkl} = \frac{\mu}{8\pi}\left[\left(\delta_{il}\epsilon_{jmk} + \delta_{jl}\epsilon_{imk}\right)\partial_m\Delta + \frac{2}{1-\nu}\epsilon_{klm}\left(\partial_i\partial_j\partial_m - \delta_{ij}\partial_m\Delta\right)\right] \tag{1.34}$$

1.1.3 Eigendistortion theory in finite media: the superposition principle

So far we have discussed the DDD method in the infinite elastic medium. However, many applications in micro-plasticity, such as micro indentation and micro-pillar compression, require that the dislocation network be embedded in a finite domain subject to prescribed boundary conditions. In order to extend the DDD method to finite domains, let us consider the eigenstrain problem in a finite domain $\mathcal{B}$. In this case, the displacement field u_k must satisfy the following boundary value problem (BVP) :

$$\begin{cases} \sigma_{ij} = c_{ijkl}\left(u_{k,l} - \beta^{\star}_{kl}\right) & \text{in } \mathcal{B} \\ \sigma_{ij,j} = 0 & \text{in } \mathcal{B} \\ \sigma_{ij}\hat{n}_j = p_i & \text{on } \partial_N\mathcal{B} \\ u_i = \overline{u}_i & \text{on } \partial_D\mathcal{B} \end{cases} \tag{1.35}$$

where p_i is the prescribed traction on the portion of the boundary $\partial_N\mathcal{B}$, and $\overline{u}_i$ is the prescribed displacement on the portion of the boundary $\partial_D\mathcal{B}$. Ideally, the BVP (1.35) could be solved at each DDD step by incrementally updating β^P_{ij} using its rate from eq. (1.41). In a finite element framework this would provide the nodal displacements, from which the total stress could be computed and used to drive the discrete dislocation system inside $\mathcal{B}$. Practically, however, this approach is unfeasible because stresses, obtained as derivatives of displacement shape functions, would result in smooth fields which fail to capture sharp gradients in proximity of dislocation lines. In order to overcome this issue, an alternative formulation has been sought (c.f. Eshelby [1979], Lubarda et al. [1993], Van der Giessen and Needleman [1995], Deng et al. [2008], Weygand et al. [2002]), where the problem is decomposed into two auxiliary problems. The first problem, with infinite domain $\mathbb{R}^3$, consists in finding u^∞_i such that:

$$\begin{cases} \sigma^\infty_{ij} = c_{ijkl}(u^\infty_{k,l} - \beta^P_{kl}) & \text{in } \mathbb{R}^3 \\ \sigma^\infty_{ij,j} = 0 & \text{in } \mathbb{R}^3 \end{cases} \tag{1.36}$$

The second is a purely elastic "correction" problem, with domain $\mathcal{B}$ consisting in finding u^c_i such that:

$$\begin{cases} \sigma^c_{ij} = c_{ijkl}u^c_{k,l} & \text{in } \mathcal{B} \\ \sigma^c_{ij,j} = 0 & \text{in } \mathcal{B} \\ \sigma^c_{ij}\hat{n}_j = p_i - \sigma^\infty_{ij}\hat{n}_j & \text{on } \partial_N\mathcal{B} \\ u^c_i = \overline{u}_i - u^\infty_i & \text{on } \partial_D\mathcal{B} \end{cases} \tag{1.37}$$

The rationale behind this decomposition is clearly that (1.36) is the standard dislocation eigenstrain problem in an infinite medium that we already solved in the previous sections. The total solution is clearly obtained as a sum: $u_i = u^\infty_i + u^c_i$ and the total stress field $\sigma_{ij} = \sigma^\infty_{ij} + \sigma^c_{ij}$ is used to drive dislocations in the finite-domain version of DDD.

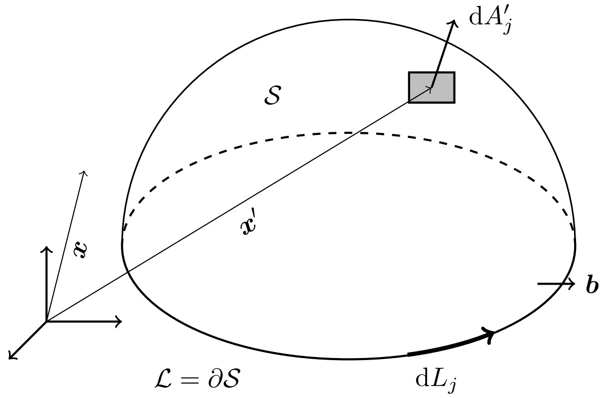


Figure 1.1: The plastic distortion is concentrated on the surface $\mathcal{S}$, which is bounded by the dislocation line $\mathcal{L} = \partial\mathcal{S}$.

1.2 Discrete dislocation loops

1.2.1 Discrete dislocation loops in infinite anisotropic media

Let us know assume that the eigendistortion $\boldsymbol{\beta}^\star$ is only due to plastic deformation cause by dislocations, that is

$$\boldsymbol{\beta}^\star = \boldsymbol{\beta}^P \tag{1.38}$$

The key equations of classical dislocation theory are now obtained by prescribing the form of the eigendistortion tensor $\boldsymbol{\beta}^P$. For a dislocation extending over a surface $\mathcal{S}$, the classical plastic eigendistortion tensor is taken in following form:

$$\beta^P_{kl}(\boldsymbol{x}) = -\int_{\mathcal{S}} \delta(\boldsymbol{x} - \boldsymbol{x}') b_k \,\mathrm{d}A'_l \,, \tag{1.39}$$

where δ is the Dirac delta function, and b_i is the displacement jump across $\mathcal{S}$, or Burgers vector. For a Volterra dislocation, as opposed to a Somigliana dislocation, the Burgers vector is constant. In this case, the tensor $\alpha_{ij} = -\epsilon_{jkm}\beta^P_{im,k}$ turns out to be concentrated on the dislocation line, that is the closed line $\mathcal{L} = \partial\mathcal{S}$ bounding the surface $\mathcal{S}$, and it is known as the *dislocation density tensor*:

$$\alpha_{ij}(\boldsymbol{x}) = \oint_{\mathcal{L}} \delta(\boldsymbol{x} - \boldsymbol{x}') b_i \,\mathrm{d}L'_j \,. \tag{1.40}$$

The rate of plastic distortion can be written in terms of the local dislocation velocity w_k as

$$\dot{\beta}^P_{ij}(\boldsymbol{x}) = -\oint_{\mathcal{L}} \delta(\boldsymbol{x} - \boldsymbol{x}') b_i \epsilon_{jkm} w_k(\boldsymbol{x}') \,\mathrm{d}L'_m \,. \tag{1.41}$$

Using the special forms (1.39) and (1.40) in the results obtained in the previous section we find all the key equations of classical dislocation theory in the anisotropic case. Letting $\boldsymbol{R} = \boldsymbol{x} - \boldsymbol{x}'$, these are:

$$u_i(\boldsymbol{x}) = -\frac{b_i\,\Omega(\boldsymbol{x})}{4\pi} - \oint_{\mathcal{L}} \mathbb{C}_{mnpq}\epsilon_{jqr}b_pF_{jnim}(\boldsymbol{R})\,\mathrm{d}L'_r \qquad \text{(anisotropic Burgers equation)} \tag{1.42a}$$

$$\beta_{ij}(\boldsymbol{x}) = \oint_{\mathcal{L}} \mathbb{C}_{mnpq}\epsilon_{jqr}G_{im,n}(\boldsymbol{R})b_p\,\mathrm{d}L'_r \qquad \text{(Mura-Willis equation)} \tag{1.42b}$$

$$\sigma_{ij}(\boldsymbol{x}) = \oint_{\mathcal{L}} \mathbb{C}_{ijkl}\mathbb{C}_{mnpq}\epsilon_{lqr}G_{km,n}(\boldsymbol{R})b_p\,\mathrm{d}L'_r \qquad \text{(anisotropic Peach-Koehler stress equation)} \tag{1.42c}$$

$$W_{AB} = \oint_{\mathcal{L}_A}\oint_{\mathcal{L}_B} \epsilon_{jkl}\mathbb{C}_{ilmn}\epsilon_{npq}\mathbb{C}_{rstp}F_{skmr}(\boldsymbol{R})\,b^A_t b^B_i\,\mathrm{d}L^A_q\,\mathrm{d}L^B_j \qquad \text{(anisotropic Blin's formula)} \tag{1.42d}$$

$$\mathcal{F}_k = \oint_{\mathcal{L}} \epsilon_{kjm}\sigma_{ij}b_i\,\mathrm{d}L_m \qquad \text{(Peach-Koehler force)} \tag{1.42e}$$

Note that, in the Burgers equation, we have introduced the solid angle $\Omega(\boldsymbol{x})$ subtended by the loop from the relationship $G^{\Delta}_{,j} * \beta^P_{ij} = -b_i\,\Omega/4\pi$, which yields:

$$\Omega(\boldsymbol{x}) = 4\pi\int_{\mathcal{S}} G^{\Delta}_{,j}\,\mathrm{d}A'_j = \int_{\mathcal{S}} \frac{R_j}{R^3}\,\mathrm{d}A'_j\,. \tag{1.43}$$

The kernel of Eq. (**??**)

1.2.2 Discrete dislocation loops in infinite isotropic media

complete steps here

$$\boldsymbol{u} = -\frac{\boldsymbol{b}\Omega}{4\pi} - \frac{1}{4\pi}\oint\left[\frac{\boldsymbol{b}\times\boldsymbol{\xi}}{R} + \frac{\lambda+\mu}{\lambda+2\mu}\left(\frac{\boldsymbol{\xi}\times\boldsymbol{b}}{R} - \frac{(\boldsymbol{b}\times\boldsymbol{R})\cdot\boldsymbol{\xi}}{R^3}\boldsymbol{R}\right)\right]dl \tag{1.44}$$

where

$$\Omega = \int\frac{R_k\hat{n}_k}{R^3}dS = -\frac{1}{2}\int R_{,ppk}\hat{n}_k dS \tag{1.45}$$

When using the line integral expression of the solid angle (A.9), eq. (1.44) becomes:

$$\begin{aligned}\boldsymbol{u} &= \frac{1}{4\pi}\oint\left[\frac{(\boldsymbol{s}\times\boldsymbol{R})\cdot\boldsymbol{\xi}}{R(R+\boldsymbol{s}\cdot\boldsymbol{R})}\boldsymbol{b} + \frac{\boldsymbol{\xi}\times\boldsymbol{b}}{R} + \frac{1}{2(1-\nu)}\left(\frac{\boldsymbol{b}\times\boldsymbol{\xi}}{R} + \frac{(\boldsymbol{b}\times\boldsymbol{R})\cdot\boldsymbol{\xi}}{R^3}\boldsymbol{R}\right)\right]dl \\ &= \underbrace{\frac{1}{8\pi(1-\nu)}}_{c_4}\oint\frac{1}{R}\left[2\underbrace{(1-\nu)}_{c1}\frac{(\boldsymbol{s}\times\boldsymbol{R})\cdot\boldsymbol{\xi}}{R+\boldsymbol{s}\cdot\boldsymbol{R}}\boldsymbol{b} + \underbrace{(1-2\nu)}_{c_3}\boldsymbol{\xi}\times\boldsymbol{b} + \frac{(\boldsymbol{\xi}\times\boldsymbol{b})\cdot\boldsymbol{R}}{R^2}\boldsymbol{R}\right]dl\end{aligned} \tag{1.46}$$

Stress field

$$\sigma_{ij}(\boldsymbol{F}) = \frac{\mu b_n}{8\pi}\int_{\mathcal{S}}\left[R_{,mpp}\left(\in_{jmn}\xi_i + \in_{imn}\xi_j\right) + \frac{2}{1-\nu}\in_{kmn}\left(R_{,ijm} - \delta_{ij}R_{,ppm}\right)\xi_k\right]dl^s \tag{1.47}$$

where $\boldsymbol{R} = \boldsymbol{F} - \boldsymbol{S}$ is the vector connecting the source point to the field point and $\xi = \frac{d\boldsymbol{S}}{dl^s}$ s the unit tangent along the source dislocation.

Substituting

$$R_{,ijk} = -\frac{\delta_{ij}R_k + \delta_{jk}R_i + \delta_{ki}R_j}{R^3} + \frac{3R_iR_jR_k}{R^5} \qquad R_{,ipp} = -\frac{2R_i}{R^3} \tag{1.48}$$

$$\sigma_{ij}(\boldsymbol{F}) = \frac{\mu b_n}{4\pi}\int_{\mathcal{S}}\left[-\frac{R_m}{R^3}\left(\in_{jmn}\xi_i + \in_{imn}\xi_j\right) + \frac{1}{1-\nu}\in_{kmn}\left(\frac{\delta_{ij}R_m - \delta_{jm}R_i - \delta_{mi}R_j}{R^3} + \frac{3R_iR_jR_m}{R^5}\right)\xi_k\right] dl^s \tag{1.49}$$

or in dyadic form:

$$\begin{aligned}\frac{d\boldsymbol{\sigma}}{dl} &= \frac{\mu}{4\pi R^2}\Big\{\hat{\boldsymbol{\xi}}\otimes(\boldsymbol{b}\times\hat{\boldsymbol{R}}) + (\boldsymbol{b}\times\hat{\boldsymbol{R}})\otimes\hat{\boldsymbol{\xi}} \\ &+ \frac{1}{1-\nu}\Big[\hat{\boldsymbol{R}}\otimes(\hat{\boldsymbol{\xi}}\times\boldsymbol{b}) + (\hat{\boldsymbol{\xi}}\times\boldsymbol{b})\otimes\hat{\boldsymbol{R}} + \Big[(\hat{\boldsymbol{R}}\times\boldsymbol{b})\cdot\hat{\boldsymbol{\xi}}\Big]\Big(\boldsymbol{I}+3\hat{\boldsymbol{R}}\otimes\hat{\boldsymbol{R}}\Big)\Big]\Big\}\end{aligned} \tag{1.50}$$

more efficient to compute

$$\begin{aligned}\frac{d\boldsymbol{\sigma}}{dl} &= \frac{\mu}{4\pi(1-\nu)R^2}\Big\{(1-\nu)\Big[\hat{\boldsymbol{\xi}}\otimes(\boldsymbol{b}\times\hat{\boldsymbol{R}}) + (\boldsymbol{b}\times\hat{\boldsymbol{R}})\otimes\hat{\boldsymbol{\xi}}\Big] \\ &+ \hat{\boldsymbol{R}}\otimes(\hat{\boldsymbol{\xi}}\times\boldsymbol{b}) + (\hat{\boldsymbol{\xi}}\times\boldsymbol{b})\otimes\hat{\boldsymbol{R}} \\ &+ \Big[(\hat{\boldsymbol{R}}\times\boldsymbol{b})\cdot\hat{\boldsymbol{\xi}}\Big]\Big(\boldsymbol{I}+3\hat{\boldsymbol{R}}\otimes\hat{\boldsymbol{R}}\Big)\Big\}\end{aligned} \tag{1.51}$$

or factoring the symmetric part

$$\frac{d\boldsymbol{\sigma}}{dl} = \frac{\mu}{2\pi(1-\nu)R^2}\Big\{(1-\nu)\hat{\boldsymbol{\xi}}\otimes(\boldsymbol{b}\times\hat{\boldsymbol{R}}) + \hat{\boldsymbol{R}}\otimes(\hat{\boldsymbol{\xi}}\times\boldsymbol{b}) + \frac{1}{2}\Big[(\hat{\boldsymbol{R}}\times\boldsymbol{b})\cdot\hat{\boldsymbol{\xi}}\Big]\Big(\boldsymbol{I}+3\hat{\boldsymbol{R}}\otimes\hat{\boldsymbol{R}}\Big)\Big\}_{sym} \tag{1.52}$$

where $\boldsymbol{x}_{\text{sym}} = \frac{1}{2}(\boldsymbol{x}+\boldsymbol{x}^T)$

1.2.3 Line-integral representation of the solid angle subtended by a loop

$$\boldsymbol{u}^0(\boldsymbol{x}) = -\frac{\boldsymbol{b}\Omega^0}{4\pi} - \frac{1}{8\pi(1-\nu)}\oint_{\mathcal{L}}\frac{1}{R}\Big\{\,(1-2\nu)\,\boldsymbol{b}\times\hat{\boldsymbol{\xi}}' + \Big[\hat{\boldsymbol{R}}\cdot\Big(\boldsymbol{b}\times\hat{\boldsymbol{\xi}}'\Big)\Big]\,\hat{\boldsymbol{R}}\Big\}\,\mathrm{d}L' \tag{1.53}$$

$$\begin{aligned}\boldsymbol{\sigma}^0(\boldsymbol{x}) = \frac{\mu}{4\pi(1-\nu)}\oint_{\mathcal{L}}\frac{1}{R^2}\Big\{(1-\nu)\Big[\hat{\boldsymbol{\xi}}'\otimes(\boldsymbol{b}\times\hat{\boldsymbol{R}}) + (\boldsymbol{b}\times\hat{\boldsymbol{R}})\otimes\hat{\boldsymbol{\xi}}'\Big] + \Big[(\hat{\boldsymbol{\xi}}'\times\boldsymbol{b})\otimes\hat{\boldsymbol{R}} + \hat{\boldsymbol{R}}\otimes(\hat{\boldsymbol{\xi}}'\times\boldsymbol{b})\Big] \\ +\hat{\boldsymbol{R}}\cdot(\boldsymbol{b}\times\hat{\boldsymbol{\xi}}')\Big[3\hat{\boldsymbol{R}}\otimes\hat{\boldsymbol{R}}+\boldsymbol{I}\Big]\Big\}\,\mathrm{d}L'\end{aligned} \tag{1.54}$$

Numerical implementation

$$\mathbf{u}(\boldsymbol{x}) = -\frac{\mathbf{b}\Omega(\mathbf{x})}{4\pi} - \frac{1}{8\pi(1-\nu)}\oint_{\mathcal{L}}\frac{1}{R}\Big\{\,(1-2\nu)\,\mathbf{b}\times\hat{\xi}' + \Big[\hat{\mathbf{R}}\cdot\Big(\mathbf{b}\times\hat{\xi}'\Big)\Big]\,\hat{\mathbf{R}}\Big\}\,\mathrm{d}L' \tag{1.55}$$

where $\mathbf{R} = \mathbf{x} - \mathbf{x}'$, and $\Omega(\mathbf{x})$ is the solid angle subtended by the surface $\mathcal{S}$:

$$\Omega(\mathbf{x}) = \int_{\mathcal{S}}\left(-\frac{1}{2}\partial_k\Delta R\right)\,dA'_k = \int_{\mathcal{S}} v_k(\mathbf{R})\,dA'_k \qquad\qquad v_k(\mathbf{y}) = \frac{y_k}{y^3} \tag{1.56}$$

In order to transform the solid angle into a line integral, we need to introduce a fictitious vector field $v^f_k(\mathbf{R})$ with the property $v^f_{k,k} = -v_{k,k}$. In this way we can find a vector potential $\Psi_m(\mathbf{R})$ for the divergence-less sum $v_k + v_k^f$. The vector potential satisfies both $v_k + v_k^f = \epsilon_{klm}\Psi_{m,l}$, and $\Psi_{k,k} = 0$. Therefore, using Stokes theorem, we can write

$$
\begin{aligned}
\Omega(\mathbf{x}) &= \int_{\mathcal{S}} \left(\epsilon_{klm}\Psi_{m,l} - v_k^f\right)\ dA'_k = \int_{\mathcal{S}} \left(-\epsilon_{klm}\Psi_{m,l'} - v_k^f\right)\ dA'_k \\
&= -\oint_{\mathcal{L}} \Psi_m\ dL'_m - \int_{\mathcal{S}} v_k^f\ dA'_k = -\oint_{\mathcal{L}} \Psi_i\ dL'_i - \Omega^f
\end{aligned}
\tag{1.57}
$$

Note that there is an error in Po-Lazar 2014, where the first term in the last equation has the wrong sign. We now need to find the vector potential Ψ_i and the fictitious vector field v_i^f. To do this we consider the auxiliary curve (Dirac string) $\mathcal{D}$, starting from $\mathbf{x}$ and ending at a point at infinity. Using the Dirac string, the fictitious vector can be found as

$$
v_k^f(\mathbf{R}) = \int_{\mathcal{D}} v_{m,m}(\mathbf{R}+\mathbf{s})ds_k = \int_{\mathcal{D}} \left(-\frac{1}{2}\Delta\Delta|\mathbf{x}+\mathbf{s}|\right) ds_k = 4\pi \int_{\mathcal{D}} \delta(\mathbf{R}+\mathbf{s})ds_k \tag{1.58}
$$

The aforementioned property of $\mathbf{v}^f$ can be verified as follows:

$$
\begin{aligned}
v_{k,k}^f(\mathbf{R}) &= \frac{\partial}{\partial x_k}\int_{\mathcal{D}} v_{m,m}(\mathbf{R}+\mathbf{s})ds_k = \int_{\mathcal{D}} \frac{\partial}{\partial x_k} v_{m,m}(\mathbf{R}+\mathbf{s})ds_k \\
&= \int_{\mathcal{D}} \frac{\partial}{\partial s_k} v_{m,m}(\mathbf{R}+\mathbf{s})ds_k = \left[v_{m,m}(\mathbf{R}+\mathbf{s})\right]_{\mathbf{0}}^{\infty} = -v_{m,m}(\mathbf{R})
\end{aligned}
\tag{1.59}
$$

Knowing the fictitious vector, the vector potential can be found observing that

$$
-\Delta\Psi_i = \epsilon_{ijk}(v_k + v_k^f)_{,j} = \epsilon_{ijk} v_{k,j}^f = -\epsilon_{ijk}\partial_j \int_{\mathcal{D}} \frac{1}{2}\Delta\Delta|\mathbf{R}+\mathbf{s}|ds_k \tag{1.60}
$$

Therefore

$$
\Psi_i(\mathbf{R}) = \epsilon_{ijk}\int_{\mathcal{D}} \frac{1}{2}\partial_j\Delta|\mathbf{R}+\mathbf{s}|ds_k = -\epsilon_{ijk}\int_{\mathcal{D}} \frac{R_j + s_j}{|\mathbf{R}+\mathbf{s}|^3} ds_k \tag{1.61}
$$

Choosing the Dirac string to be a straight line with unit direction $\hat{\mathbf{s}}$, the expression above becomes:

$$
\begin{aligned}
\Psi_i(\mathbf{R}) &= -\epsilon_{ijk}\int_0^{\infty} \frac{R_j + \alpha\hat{s}_j}{|\mathbf{R}+\alpha\hat{\mathbf{s}}|^3}\hat{s}_k\ d\alpha = -\epsilon_{ijk}R_j\hat{s}_k \int_0^{\infty} \frac{1}{|\mathbf{R}+\alpha\hat{\mathbf{s}}|^3}\ d\alpha \\
&= -\epsilon_{ijk}R_j\hat{s}_k \left[\frac{\alpha + \mathbf{R}\cdot\hat{\mathbf{s}}}{(R^2 - (\mathbf{R}\cdot\hat{\mathbf{s}})^2)\,|\mathbf{R}+\alpha\hat{\mathbf{s}}|}\right]_0^{\infty} \\
&= -\epsilon_{ijk}R_j\hat{s}_k \left[\frac{1}{R^2 - (\mathbf{R}\cdot\hat{\mathbf{s}})^2} - \frac{\mathbf{R}\cdot\hat{\mathbf{s}}}{(R^2 - (\mathbf{R}\cdot\hat{\mathbf{s}})^2)\,R}\right] \\
&= -\epsilon_{ijk}R_j\hat{s}_k \frac{R - \mathbf{R}\cdot\hat{\mathbf{s}}}{(R^2 - (\mathbf{R}\cdot\hat{\mathbf{s}})^2)\,R} = -\frac{\epsilon_{ijk}R_j\hat{s}_k}{R\,(R + \mathbf{R}\cdot\hat{\mathbf{s}})}
\end{aligned}
\tag{1.62}
$$

In vector form this reads

$$
\mathbf{\Psi}(\mathbf{x}) = -\frac{\mathbf{R}\times\hat{\mathbf{s}}}{R\,(R + \mathbf{R}\cdot\hat{\mathbf{s}})} \tag{1.63}
$$

Finally, the Burgers equation becomes

$$
\begin{aligned}
\mathbf{u}(\mathbf{x}) &= -\frac{\mathbf{b}}{4\pi}\left(-\oint_{\mathcal{L}} \Psi_i(\mathbf{R})\ dL_i' - \Omega^f\right) - \frac{1}{8\pi(1-\nu)}\oint_{\mathcal{L}} \frac{1}{R}\left\{\ (1-2\nu)\,\mathbf{b}\times\hat{\xi}' + \left[\hat{\mathbf{R}}\cdot\left(\mathbf{b}\times\hat{\xi}'\right)\right]\hat{\mathbf{R}}\right\}\mathrm{d}L' \\
&= \frac{\mathbf{b}\Omega^f}{4\pi} - \frac{\mathbf{b}}{4\pi}\oint_{\mathcal{L}} \frac{(\mathbf{R}\times\hat{\mathbf{s}})\cdot\hat{\xi}'}{R\,(R+\mathbf{R}\cdot\hat{\mathbf{s}})}\ dL' - \frac{1}{8\pi(1-\nu)}\oint_{\mathcal{L}} \frac{1}{R}\left\{\ (1-2\nu)\,\mathbf{b}\times\hat{\xi}' + \left[\hat{\mathbf{R}}\cdot\left(\mathbf{b}\times\hat{\xi}'\right)\right]\hat{\mathbf{R}}\right\}\mathrm{d}L' \\
&= \mathbf{b}^f(\mathbf{x}) - \frac{1}{8\pi(1-\nu)}\oint_{\mathcal{L}} \frac{1}{R}\left\{\ \frac{2(1-\nu)(\hat{\mathbf{R}}\times\hat{\mathbf{s}})\cdot\hat{\xi}'}{1+\hat{\mathbf{R}}\cdot\hat{\mathbf{s}}}\mathbf{b} + (1-2\nu)\,\mathbf{b}\times\hat{\xi}' + \left[\hat{\mathbf{R}}\cdot\left(\mathbf{b}\times\hat{\xi}'\right)\right]\hat{\mathbf{R}}\right\}\mathrm{d}L' \\
&= \mathbf{b}^f(\mathbf{x}) + \frac{1}{8\pi(1-\nu)}\oint_{\mathcal{L}} \frac{1}{R}\left\{\ \frac{2(1-\nu)(\hat{\mathbf{s}}\times\hat{\mathbf{R}})\cdot\hat{\xi}'}{1+\hat{\mathbf{R}}\cdot\hat{\mathbf{s}}}\mathbf{b} + (1-2\nu)\,\hat{\xi}'\times\mathbf{b} + \left[\hat{\mathbf{R}}\cdot\left(\hat{\xi}'\times\mathbf{b}\right)\right]\hat{\mathbf{R}}\right\}\mathrm{d}L'
\end{aligned}
\tag{1.64}
$$

Notice that

$$
\begin{aligned}
\mathbf{b}^f(\mathbf{x}) = \frac{\mathbf{b}\Omega^f}{4\pi} &= \frac{\mathbf{b}}{4\pi}\int_{\mathcal{S}} v_k^f(\mathbf{R})\ dA_k' = \frac{\mathbf{b}}{4\pi}\int_{\mathcal{S}} 4\pi\int_{\mathcal{D}} \delta(\mathbf{R}+\mathbf{s})ds_k\ dA_k' \\
&= \begin{cases} +\mathbf{b} & \text{if the Dirac string crosses the slip surface positively} \\ -\mathbf{b} & \text{if the Dirac string crosses the slip surface negatively} \\ \mathbf{0} & \text{if the Dirac string does not cross the slip surface} \end{cases}
\end{aligned}
\tag{1.65}
$$

1.2.4 Multipole expansion

Stress field

$$
\sigma_{ij} = \oint_{\mathcal{L}} S_{ijkl}R(\mathbf{x}-\mathbf{x}')b_k'\xi_l'\ dL' \tag{1.66}
$$

Now let $\mathbf{x}' = \mathbf{x}^c - \tilde{\mathbf{x}}$, then

$$
\sigma_{ij} = \oint_{\mathcal{L}} S_{ijkl}R(\mathbf{x}-\mathbf{x}^c+\tilde{\mathbf{x}})b_k'\xi_l'\ dL' \tag{1.67}
$$

Now assume

$$
|\tilde{\mathbf{x}}| \ll |\mathbf{x}-\mathbf{x}^c| \tag{1.68}
$$

then, expanding R for $\tilde{\mathbf{x}} \to 0$ yields

$$
R(\mathbf{x}-\mathbf{x}^c+\tilde{\mathbf{x}}) \approx R(\mathbf{x}-\mathbf{x}^c) + \partial_p R(\mathbf{x}-\mathbf{x}^c)\tilde{x}_p + \dots \tag{1.69}
$$

and

$$
\sigma_{ij} = S_{ijkl}R(\mathbf{x}-\mathbf{x}^c)\oint_{\mathcal{L}} b_k'\xi_l'\ dL' + S_{ijkl}\partial_p R(\mathbf{x}-\mathbf{x}^c)\oint_{\mathcal{L}} \tilde{x}_p b_k'\xi_l' + \dots \tag{1.70}
$$

First order expansion:

$$
\begin{aligned}
\boldsymbol{\sigma}^0(\boldsymbol{x}) = \frac{\mu}{4\pi(1-\nu)R^2}&\Big\{(1-\nu)\left[\hat{\boldsymbol{\xi}}'\otimes(\boldsymbol{b}\times\hat{\boldsymbol{R}}) + (\boldsymbol{b}\times\hat{\boldsymbol{R}})\otimes\hat{\boldsymbol{\xi}}'\right] + \left[(\hat{\boldsymbol{\xi}}'\times\boldsymbol{b})\otimes\hat{\boldsymbol{R}} + \hat{\boldsymbol{R}}\otimes(\hat{\boldsymbol{\xi}}'\times\boldsymbol{b})\right] \\
&+\hat{\boldsymbol{R}}\cdot(\boldsymbol{b}\times\hat{\boldsymbol{\xi}}')\left[3\hat{\boldsymbol{R}}\otimes\hat{\boldsymbol{R}}+\boldsymbol{I}\right]\Big\}
\end{aligned}
\tag{1.71}
$$

Letting

$$(\boldsymbol{b} \times \hat{\boldsymbol{R}}) \otimes \hat{\boldsymbol{\xi}})_{ij} = \epsilon_{ikm} b_k R_m \xi_j = \epsilon_{ikm} R_m \alpha_{kj} = \mathbf{S} \cdot \alpha \tag{1.72}$$

$$\mathbf{S} = \begin{bmatrix} 0 & R_3 & -R_2 \\ -R_3 & 0 & R_1 \\ R_2 & -R_1 & 0 \end{bmatrix} \tag{1.73}$$

$$\boldsymbol{b} \times \hat{\boldsymbol{\xi}}' = \epsilon_{ikm} b_k \xi_m = a_i \tag{1.74}$$

$$\mathbf{a} = \begin{bmatrix} \alpha_{23} - \alpha_{32} \\ \alpha_{31} - \alpha_{13} \\ \alpha_{12} - \alpha_{21} \end{bmatrix} \tag{1.75}$$

we obtain

$$\begin{aligned} \boldsymbol{\sigma}^0(\boldsymbol{x}) = \frac{\mu}{4\pi(1-\nu)R^2} \Big\{ (1-\nu) \left[(\mathbf{S} \cdot \alpha)^T + \mathbf{S} \cdot \alpha \right] - \Big[\mathbf{a} \otimes \hat{\boldsymbol{R}} + \hat{\boldsymbol{R}} \otimes \mathbf{a} \Big] \\ + (\hat{\boldsymbol{R}} \cdot \boldsymbol{a}) \Big[3\hat{\boldsymbol{R}} \otimes \hat{\boldsymbol{R}} + \boldsymbol{I} \Big] \Big\} \end{aligned} \tag{1.76}$$

Displacement field

$$\mathbf{u}(\mathbf{x}) = \mathbf{b}^f(\mathbf{x}) + \frac{1}{8\pi(1-\nu)} \frac{1}{R} \left\{ \boldsymbol{\alpha} \cdot \frac{2(1-\nu)(\hat{\mathbf{s}} \times \hat{\mathbf{R}})}{1 + \hat{\mathbf{R}} \cdot \hat{\mathbf{s}}} - (1-2\nu)\, \boldsymbol{a} - \left(\hat{\mathbf{R}} \cdot \boldsymbol{a} \right) \hat{\mathbf{R}} \right\} \tag{1.77}$$

Interaction Energy

$$\begin{aligned} E_I = -\frac{\mu}{4\pi(1-\nu)} \oint_{\mathcal{L}_2} \oint_{\mathcal{L}_1} \frac{1}{R} \Big\{ \Big[(1-\nu) \left(\boldsymbol{b}_1 \cdot \hat{\boldsymbol{\xi}}_1 \right) \left(\boldsymbol{b}_2 \cdot \hat{\boldsymbol{\xi}}_2 \right) + 2\nu \left(\boldsymbol{b}_1 \cdot \hat{\boldsymbol{\xi}}_2 \right) \left(\boldsymbol{b}_2 \cdot \hat{\boldsymbol{\xi}}_1 \right) - 2 \left(\boldsymbol{b}_1 \cdot \boldsymbol{b}_2 \right) \left(\hat{\boldsymbol{\xi}}_1 \cdot \hat{\boldsymbol{\xi}}_2 \right) \Big] \\ + \left(\hat{\boldsymbol{\xi}}_1 \cdot \hat{\boldsymbol{\xi}}_2 \right) \Big[(\boldsymbol{b}_1 \cdot \boldsymbol{b}_2) - \left(\boldsymbol{b}_1 \cdot \hat{\boldsymbol{R}} \right) \left(\boldsymbol{b}_2 \cdot \hat{\boldsymbol{R}} \right) \Big] \Big\} dL_1 dL_2 \end{aligned} \tag{1.78}$$

$$\begin{aligned} E_I = -\frac{\mu}{4\pi(1-\nu)} \oint_{\mathcal{L}_2} \oint_{\mathcal{L}_1} \frac{1}{R} \Big\{ (1-\nu) \left(\boldsymbol{b}_1 \cdot \hat{\boldsymbol{\xi}}_1 \right) \left(\boldsymbol{b}_2 \cdot \hat{\boldsymbol{\xi}}_2 \right) + 2\nu \left(\boldsymbol{b}_1 \cdot \hat{\boldsymbol{\xi}}_2 \right) \left(\boldsymbol{b}_2 \cdot \hat{\boldsymbol{\xi}}_1 \right) - \left(\boldsymbol{b}_1 \cdot \boldsymbol{b}_2 \right) \left(\hat{\boldsymbol{\xi}}_1 \cdot \hat{\boldsymbol{\xi}}_2 \right) \\ - \left(\hat{\boldsymbol{\xi}}_1 \cdot \hat{\boldsymbol{\xi}}_2 \right) \left(\boldsymbol{b}_1 \cdot \hat{\boldsymbol{R}} \right) \left(\boldsymbol{b}_2 \cdot \hat{\boldsymbol{R}} \right) \Big\} dL_1 dL_2 \end{aligned} \tag{1.79}$$

1.2.5 Plastic strain rate

For conservative motion (glide) $\boldsymbol{v} \cdot \hat{\boldsymbol{n}} = 0$, therefore, from (A.4):

$$\dot{\beta}^p_{ij}(\boldsymbol{x}) = -b_i \int_{\boldsymbol{A}}^{\boldsymbol{B}} \delta(\boldsymbol{x} - \boldsymbol{x}') \epsilon_{jkm} v_k dl'_m \tag{1.80}$$

1.2.6 Discrete dislocations in finite media

From a numerical viewpoint, it is interesting to ask; what is the distribution of β^P_{ij} outside $\mathcal{B}$ in (1.36)? We shall call this quantity β^{P*}_{ij}. In fact, although the solution to the problems (1.36) and (1.37) depend individually on β^{P*}_{ij}, it is easy to see that the total solution is independent of β^{P*}_{ij}. Therefore β^{P*}_{ij} can be chosen arbitrarily[3]. The arbitrariness of β^{P*}_{ij} can be exploited in the numerical implementation. To see how, we can cast (1.37) in its corresponding Galerkin weak form

$$\int_{\mathcal{B}} c_{ijkl} u^c_{k,l} \tilde{u}_{i,j} d\mathcal{V} = \int_{\partial_N \mathcal{B}} \left(p_i - \sigma^\infty_{ij} \hat{n}_j\right) \tilde{u}_i d\mathcal{A} \tag{1.81}$$

and notice that the RHS involves a surface integral of the stress field σ^∞_{ij} induced by the dislocation network. When a dislocation segment reaches the domain boundary, the numerical evaluation of this integral becomes challenging. This numerical difficulty can be overcome using the construction shown in Fig. **??**. In fact, because β^{P*}_{ij} is arbitrary, it is possible to add an external loop with the same Burgers vector of the boundary segment and opposite line direction, constructed so that one side of the loop overlaps with the boundary segment, and the opposite side is pushed to infinity along the direction of the boundary normal vector. In this way, because the contributions of the overlapping segments cancel out, the line integral involved in the calculation of σ^∞_{ij} can be limited to the portion of the dislocation configuration strictly inside the domain, and the virtual straight dislocation lines extending from the domain boundary to infinity. Notice that this construction unambiguously defines β^{P*}_{ij} and the surface over which it extends, a fundamental requirement for the calculation of u^∞_i needed to satisfy displacement boundary conditions in the BVP (1.37).

1.2.7 Force vector of a triangular element due to a straight segments

We would like to compute the force vector of a triangular boundary element due to a straight segment. The weak form involved in the FEM problem is

$$\int_{\mathcal{T}} \tilde{u}_i t_i \mathrm{d}A = \sum_n \tilde{u}^n_i \int_{\mathcal{T}} N^n \sigma_{ij} \hat{n}_j \mathrm{d}A \tag{1.82}$$

where N^n is the shape function of the n-th node of the triangle, and $\tilde{u}^n_i$ its test displacement. The stress field generated by the dislocaiton loops is

$$\sigma_{ij}(\boldsymbol{x}) = \tilde{S}_{ijl}\left[q_l(\boldsymbol{x})\right] \tag{1.83}$$

where

$$q_l(\boldsymbol{x}) = \oint_{\mathcal{L}} R_a(\boldsymbol{x} - \boldsymbol{x}')\ d\ell'_l \tag{1.84}$$

and $\tilde{S}$ is the the third-order dislocation stress differential operator, which is defined as

$$\tilde{S}_{ijl}[\cdot] = \frac{\mu b_k}{8\pi}\left[\left(\delta_{il}\epsilon_{jmk} + \delta_{jl}\epsilon_{imk}\right)\partial_m \Delta + \frac{2}{1-\nu}\epsilon_{klm}\left(\partial_i\partial_j\partial_m - \delta_{ij}\partial_m\Delta\right)\right] \tag{1.85}$$

Note that this operator can be rewritten as

$$\tilde{S}_{ijl}[\cdot] = \partial_m \hat{S}_{ijlm}[\cdot] \tag{1.86}$$

where the auxiliary second-order differential operator $\hat{S}_{ijlm}[\cdot]$ is

$$\tilde{S}_{ijlm}[\cdot] = \frac{\mu b_k}{8\pi}\left[\left(\delta_{il}\epsilon_{jmk} + \delta_{jl}\epsilon_{imk}\right)\Delta + \frac{2}{1-\nu}\epsilon_{klm}\left(\partial_i\partial_j - \delta_{ij}\Delta\right)\right] \tag{1.87}$$

[3] We observe that the arbitrariness of β^{P*}_{ij} implies that also its bounding curve (or virtual dislocation line) is arbitrary, in agreement with the "mirror image construction" of Weygand et al. [2002] and the "independence of the total stress on the choice of virtual segments" mentioned in Weinberger et al. [2009].

Let us focus on the integral

$$
\begin{aligned}
F_i^{(n)} &= \int_{\mathcal{T}} N^{(n)} \sigma_{ij} \mathrm{d}A_j = \int_{\mathcal{T}} N^n \partial_m \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \mathrm{d}A_j \\
&= \int_{\mathcal{T}} \partial_m \left\{ N^n \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \right\} \mathrm{d}A_j - \int_{\mathcal{T}} N^n_{,m} \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \mathrm{d}A_j
\end{aligned} \tag{1.88}
$$

We now apply Stokes theorem (A.2) to the first term of (1.89) to find

$$
\begin{aligned}
F_i^{(n)} &= \oint_{\partial\mathcal{T}} \epsilon_{kjm} N^{(n)} \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \mathrm{d}\ell_k + \int_{\mathcal{T}} \partial_j \left\{ N^n \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \right\} \mathrm{d}A_m - \int_{\mathcal{T}} N^n_{,m} \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \mathrm{d}A_j \\
&= \oint_{\partial\mathcal{T}} \epsilon_{kjm} N^{(n)} \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \mathrm{d}\ell_k + \int_{\mathcal{T}} N^n \partial_j \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \mathrm{d}A_m \\
&+ \int_{\mathcal{T}} N^n_{,j} \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \ \mathrm{d}A_m - \int_{\mathcal{T}} N^n_{,m} \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] \mathrm{d}A_j
\end{aligned} \tag{1.89}
$$

Note that in the expression above, the only third-order differential operator is $\partial_j \hat{S}_{ijlm}$. However a closer inspection reveals that

$$
\begin{aligned}
\partial_j \hat{S}_{ijlm} \left[q_l(\boldsymbol{x}) \right] &= \frac{\mu b_k}{8\pi} \left[\left(\delta_{il} \epsilon_{jmk} + \delta_{jl} \epsilon_{imk} \right) \partial_j \Delta + \frac{2}{1-\nu} \epsilon_{klm} \cancel{\left(\partial_i \partial_j \partial_j - \delta_{ij} \partial_j \Delta \right)} \right] \left[q_l(\boldsymbol{x}) \right] \\
&= \frac{\mu b_k}{8\pi} \left(\epsilon_{jmk} \Delta \partial_j \left[q_i(\boldsymbol{x}) \right] + \epsilon_{imk} \Delta \left[\oint_{\mathcal{L}} \frac{\partial}{\partial x_l} R_a(\boldsymbol{x} - \boldsymbol{x}') \ d\ell'_l \right] \right) \\
&= \frac{\mu b_k}{8\pi} \left(\epsilon_{jmk} \Delta \partial_j \left[q_i(\boldsymbol{x}) \right] - \epsilon_{imk} \Delta \left[\cancel{\oint_{\mathcal{L}} \frac{\partial}{\partial x'_l} R_a(\boldsymbol{x} - \boldsymbol{x}')} \ d\ell'_l \right] \right)
\end{aligned}
$$

The first term is zero if the Burgers vector is aligned with the surface normal (not very useful). Moreover

$$
\begin{aligned}
\epsilon_{kjm} \tilde{S}_{ijlm} &= \frac{\mu b_p}{8\pi} \left[\left(\delta_{il} \epsilon_{kjm} \epsilon_{jmp} + \delta_{jl} \epsilon_{mkj} \epsilon_{mpi} \right) \Delta + \frac{2}{1-\nu} \epsilon_{mkj} \epsilon_{mpl} \left(\partial_i \partial_j - \delta_{ij} \Delta \right) \right] \\
&= \frac{\mu b_p}{8\pi} \left[\left(\delta_{il} 2 \delta_{kp} + \delta_{jl} \left(\delta_{kp} \delta_{ij} - \delta_{ik} \delta_{jp} \right) \right) \Delta + \frac{2}{1-\nu} \left(\delta_{kp} \delta_{jl} - \delta_{kl} \delta_{jp} \right) \left(\partial_i \partial_j - \delta_{ij} \Delta \right) \right] \\
&= \frac{\mu b_p}{8\pi} \left[\left(2 \delta_{il} \delta_{kp} + \delta_{kp} \delta_{il} - \delta_{ik} \delta_{lp} \right) \Delta + \frac{2}{1-\nu} \left(\delta_{kp} \delta_{jl} - \delta_{kl} \delta_{jp} \right) \left(\partial_i \partial_j - \delta_{ij} \Delta \right) \right]
\end{aligned} \tag{1.90}
$$

1.2.8 Discrete dislocations in periodic media

Chapter 2

Discrete Dislocation Dynamics in MoDELib

2.1 Topology of dislocation networks

2.1.1 Topological operations

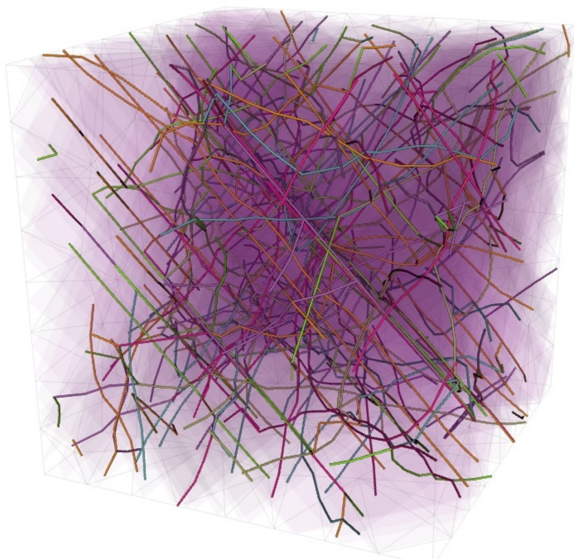
The objective of this chapter is to give an overview of the DDD method, and to describe its implementation in the MoDELib library.

DDD is a simulation method to study the plastic deformation of crystalline materials due to the motion of dislocations. It is a hybrid discrete-continuum simulation method, which in the multiscale modeling framework bridges atomistic methods (e.g. Molecular Dynamics) and continuum methods (e.g. Finite Element Crystal Plasticity). Its hybrid character is due to the fact that crystal dislocations are represented discretely (individually), although their interactions are computed semi-analytically using continuum elasticity and without atomistic degrees of freedom.

DDD simulation typically take place in a spatial domain representing either a finite or a periodic material volume. Fig. 2.1a shows a snapshot of a typical MoDELib DDD simulation, where individual dislocation lines are colored according to their Burgers vector, and the intensity of the shaded background represents the local slip due to their motion. A minimal DDD algorithm is reported in Fig. 2.1b.

During the initialization phase a mesh of the simulation domain is prepared, material properties are selected, and an initial dislocation microstructure is generated. In. MoDELib, these processes are automated as explained in section **??**. During the main simulation loop the mutual interaction forces between dislocations are computed using semi-analytical expressions derived from the elastic theory of dislocations described in section 1. This is typically the most time-consuming part of a single simulation step. External loads and possibly other stress sources are then added to determine the total force on each line element of a dislocation. Overdamped dynamics is then invoked to compute the local dislocation velocity given the local force, using special functions called *mobility laws*. A Finite Element (FE) scheme is then employed to find the velocity of the discretization points (nodes) which determine the dislocation configuration. Once ta new configuration is obtained through a simple time-marching scheme, a series of processes takes place to update the dislocation topology due to discrete physical events such as collisions, cross slip, etc.

In the remainder of this chapter we develop the necessary theoretical background necessary to understand the DDD method. We then proceed to the description of the MoDELib implementation.



(a) sample configuration

initialization:
  simulation domain;
  material properties and slip systems;
  initial dislocation configuration;
end
main loop
  compute mutual dislocation stress;
  add other stress sources;
  compute line velocities from local stress;
  compute nodal velocities;
  update nodal positions;
  perform discrete events:
  - junctions
  - cross-slip
  - network remeshing
  - nucleation
end

(b) minimal DDD algorithm

Figure 2.1: typical DDD simulation in MoDELib.

Appendix A

Review of tensor calculus

A.1 Mathematical preliminaries

A.1.1 Kelvin-Stokes Theorem

Theorem 1. *(Kelvin-Stokes Theorem)*

$$\int_{\mathcal{S}} \epsilon_{ikl} f_{,l} \hat{n}_k ds = \oint_{\partial \mathcal{S}} f dl_i \tag{A.1}$$

Theorem 2. *(Corollary)*

$$\int_{\mathcal{S}} \left(f_{,q} \hat{n}_p - f_{,p} \hat{n}_q \right) ds = \oint_{\partial \mathcal{S}} \epsilon_{ipq} f dl_i \tag{A.2}$$

A.1.2 Surface Divergence Theorem

In this section we recall some useful theorems in surface integration. **?**, **?**.

See Slattery et al. [2006] p. 669.

Theorem 3. *(Surface Divergence Theorem) fdsfsd*

A.1.3 Surface Transport Theorem

Theorem 4. *(Surface Transport Theorem)*

$$\frac{d}{dt} \int_{\mathcal{S}_x = \boldsymbol{\varphi}(\mathcal{S}_X)} \alpha \hat{n}_i ds = \int_{\mathcal{S}_x} \left(\frac{\partial \alpha}{\partial t} + \left(\alpha \dot{\varphi}_k \right)_{,k} \right) \hat{n}_i ds - \int_{\mathcal{S}_x} \alpha \dot{\varphi}_{k,i} \hat{n}_k ds \tag{A.3}$$

Proof. From Scovazzi and Hughes [2007]. □

Theorem 5. *(Surface Transport Theorem (alternative form))*

$$\frac{d}{dt} \int_{\mathcal{S}_x} \alpha ds = \int_{\mathcal{S}_x} \frac{\partial \alpha}{\partial t} \hat{n}_i ds + \oint \epsilon_{ikm} \alpha v_k dl_m + \int_{\mathcal{S}_x} \alpha_{,i} v_k \hat{n}_k ds \tag{A.4}$$

Proof. Consider the second term on the r.h.s. of A.3 and use (A.2):

$$\int_{\mathcal{S}_x} \left(\alpha \dot{\varphi}_k \right)_{,k} \hat{n}_i ds = \int_{\mathcal{S}_x} \left(\alpha \dot{\varphi}_k \right)_{,i} \hat{n}_k ds + \oint \epsilon_{mik} \alpha v_k dl_m \tag{A.5}$$

Now consider the third term on the r.h.s. of A.3

$$\int_{\mathcal{S}_x} \alpha \dot{\varphi}_{k,i} \hat{n}_k ds = \int_{\mathcal{S}_x} (\alpha v_k)_{,i} \hat{n}_k ds - \int_{\mathcal{S}_x} \alpha_{,i} v_k \hat{n}_k ds \tag{A.6}$$

Subtract to obtain result □

Theorem 6. *(Surface Transport Theorem (alternative form))*

$$\frac{d}{dt} \int_{\mathcal{S}_x = \boldsymbol{\varphi}(\mathcal{S}_X)} \alpha ds = \tag{A.7}$$

Proof. See Slattery et al. [2006] p 61. □

A.1.4 Solid angles and line integration

Theorem 7. *(Surface to Line integration) Let $\mathcal{S}$ be a surface bounded by the closed contour Γ. Then let $\boldsymbol{R} = \boldsymbol{R}_s - \boldsymbol{R}_f$ where $\boldsymbol{R}_f$ is the field point and $\boldsymbol{R}_s$ is the source point on $\mathcal{S}$. If $\boldsymbol{s}$ is a unit vector applied at $\boldsymbol{R}_f$ such that the direction containing it never intersects $\mathcal{S}$ nor Γ, then:*

$$-\int \frac{\boldsymbol{R}}{R^3} \cdot \hat{n} dS = \oint \frac{\boldsymbol{s} \times \boldsymbol{R}}{R(R - \boldsymbol{s} \cdot \boldsymbol{R})} \cdot d\boldsymbol{l} \tag{A.8}$$

Obviously if $\boldsymbol{R}$ has opposite definition, i.e. $\boldsymbol{R} = \boldsymbol{R}_f - \boldsymbol{R}_s$ then

$$\int \frac{\boldsymbol{R}}{R^3} \cdot \hat{n} dS = -\oint \frac{\boldsymbol{s} \times \boldsymbol{R}}{R(R + \boldsymbol{s} \cdot \boldsymbol{R})} \cdot d\boldsymbol{l} \tag{A.9}$$

Note that for unit vector $\boldsymbol{s}$ we have $(\boldsymbol{R} - R\boldsymbol{s})^2 = R^2 + R^2 - 2R\boldsymbol{R} \cdot \boldsymbol{s} = 2R(R - \boldsymbol{R} \cdot \boldsymbol{s})$. This means that $2R(R - \boldsymbol{R} \cdot \boldsymbol{s}) = 0$ only when $\boldsymbol{R}$ is aligned with $\boldsymbol{s}$.

Proof. From Stokes theorem:

$$\oint \frac{\boldsymbol{s} \times \boldsymbol{R}}{R(R - \boldsymbol{s} \cdot \boldsymbol{R})} \cdot d\boldsymbol{l} = \int \nabla \times \left[\frac{\boldsymbol{s} \times \boldsymbol{R}}{R(R - \boldsymbol{s} \cdot \boldsymbol{R})} \right] ds \tag{A.10}$$

Now exapand the curl

$$
\begin{aligned}
\nabla \times \left[\frac{\boldsymbol{s} \times \boldsymbol{R}}{R(R - \boldsymbol{s} \cdot \boldsymbol{R})}\right] &= \epsilon_{ijk}\partial_j \left[\frac{\epsilon_{kmn} s_m R_n}{R(R - s_p R_p)}\right] = (\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm})\,\partial_j \left[\frac{s_m R_n}{R(R - s_p R_p)}\right] \\
&= (\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}) \left[\frac{s_m R_{n,j}}{R(R - s_p R_p)} - \frac{s_m R_n \left[R_{,j}(R - s_p R_p) + R(R_{,j} - s_p R_{p,j})\right]}{R^2 (R - s_p R_p)^2}\right] \\
&= (\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}) \left[\frac{s_m \delta_{nj}}{R(R - s_p R_p)} - \frac{s_m R_n \left[\frac{R_j}{R}(R - s_p R_p) + R(\frac{R_j}{R} - s_p \delta_{pj})\right]}{R^2 (R - s_p R_p)^2}\right] \\
&= (\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}) \left[\frac{s_m \delta_{nj}}{R(R - s_p R_p)} - \frac{s_m R_n \left[\frac{R_j}{R}(R - s_p R_p) + (R_j - R s_j)\right]}{R^2 (R - s_p R_p)^2}\right] \\
&= \left[\frac{\delta_{im}\delta_{jn} s_m \delta_{nj}}{R(R - s_p R_p)} - \frac{\delta_{im}\delta_{jn} s_m R_n \left[\frac{R_j}{R}(R - s_p R_p) + (R_j - R s_j)\right]}{R^2 (R - s_p R_p)^2}\right] \\
&- \left[\frac{\delta_{in}\delta_{jm} s_m \delta_{nj}}{R(R - s_p R_p)} - \frac{\delta_{in}\delta_{jm} s_m R_n \left[\frac{R_j}{R}(R - s_p R_p) + (R_j - R s_j)\right]}{R^2 (R - s_p R_p)^2}\right] \\
&= \left[\frac{3 s_i}{R(R - s_p R_p)} - \frac{s_i \left[R(R - s_p R_p) + R(R - R_j s_j)\right]}{R^2 (R - s_p R_p)^2}\right] \\
&- \left[\frac{s_i}{R(R - s_p R_p)} - \frac{R_i \left[\frac{R_j s_j}{R}(R - s_p R_p) + (R_j s_j - R)\right]}{R^2 (R - s_p R_p)^2}\right] \\
&= \frac{3 s_i}{R(R - s_p R_p)} - \frac{2 s_i}{R(R - s_p R_p)} \\
&- \frac{s_i}{R(R - s_p R_p)} + R_i \frac{\left[-R - \frac{R_j s_j s_p R_p}{R} + 2 R_j s_j\right]}{R^2 (R^2 + s_p R_p s_j R_j - 2 R s_p R_p)} \\
&= -\frac{R_i}{R^3}
\end{aligned}
\tag{A.11}
$$

□

A.2 OLD NOTES: Elastic Energy of a Dislocation Loop

A.2.1 Volume to Surface

(Eshelby) Let's consider a body delimited by a closed surface S_0 having a source of eigenstress[1] I enclosed within the surface S and a source of stress II outside S.

[1] no external surface traction

$$
\begin{aligned}
E &= \frac{1}{2}\int_V \sigma_{ij}\epsilon_{ij} dV = \frac{1}{2}\int_V \left(\sigma^I_{ij}+\sigma^{II}_{ij}\right)\left(\epsilon^I_{ij}+\epsilon^{II}_{ij}\right) dV \\
&= \frac{1}{2}\int_V \sigma^I_{ij}\epsilon^I_{ij} dV + \frac{1}{2}\int_V \sigma^{II}_{ij}\epsilon^{II}_{ij} dV + \underbrace{\frac{1}{2}\int_V \sigma^I_{ij}\epsilon^{II}_{ij} dV + \frac{1}{2}\int_V \sigma^{II}_{ij}\epsilon^I_{ij} dV}_{\text{equal for reciprocity theorem}} \\
&= \underbrace{\frac{1}{2}\int_V \sigma^I_{ij}\epsilon^I_{ij} dV}_{E_I} + \underbrace{\frac{1}{2}\int_V \sigma^{II}_{ij}\epsilon^{II}_{ij} dV}_{E_{II}} + \underbrace{\int_V \sigma^I_{ij}\epsilon^{II}_{ij} dV}_{E_{int}} \qquad \text{(A.12)}
\end{aligned}
$$

Away from their respective sources strains are gradients of displacement fields therefore $\epsilon^I_{ij} = \frac{1}{2}\left(u^I_{i,j}+u^I_{j,i}\right)$ in V_{II} and $\epsilon^{II}_{ij} = \frac{1}{2}\left(u^{II}_{i,j}+u^{II}_{j,i}\right)$ in V_I, but not conversely.

$$
\begin{aligned}
E_{int} &= \int_{V_I} \sigma^I_{ij} u^{II}_{i,j} dV_I + \int_{V_{II}} \sigma^{II}_{ij} u^I_{i,j} dV_{II} \qquad \text{(A.13)} \\
&= \oint_S \sigma^I_{ij} u^{II}_i \hat{n}_j dS - \underbrace{\int_{V_I} \sigma^I_{i,j} u^{II}_i dV_I}_{\text{equilibrium}} \\
&+ \oint_{S_0} \sigma^{II}_{ij} u^I_i \hat{n}_j dS - \oint_S \sigma^{II}_{ij} u^I_i \hat{n}_j dS + \underbrace{\int_{V_{II}} \sigma^{II}_{i,j} u^I_i dV_{II}}_{\text{equilibrium}} \\
&= \oint_S \left(\sigma^I_{ij} u^{II}_i - \sigma^{II}_{ij} u^I_i\right) \hat{n}_j dS + \underbrace{\oint_{S_0} t^{II}_i u^I_i dS}_{\text{no surface tractions}} \qquad \text{(A.14)}
\end{aligned}
$$

the end result is

$$
E_{int} = b_i \int_{\mathcal{S}} \sigma^{II}_{ij} \hat{n}_j dS \qquad \text{(A.15)}
$$

A.3 Convolution integrals

Throughout this document, the symbol $*$ stands for the convolution operator over the infinite three-dimensional space $\mathbb{R}^3$:

$$
f * g = \int_{\mathbb{R}^3} f(\boldsymbol{x}-\boldsymbol{x}')g(\boldsymbol{x}')\,\mathrm{d}V' \qquad \text{(A.16)}
$$

Convolution enjoys the following properties

$$
f * g = \int_{\mathbb{R}^3} f(\boldsymbol{x}-\boldsymbol{x}')g(\boldsymbol{x}')\,\mathrm{d}V' = -\int_{-\mathbb{R}^3} f(\boldsymbol{x}'')g(\boldsymbol{x}-\boldsymbol{x}'')\,\mathrm{d}V'' = g * f \qquad \text{(A.17)}
$$

$$
(f * g)_{,i} = \int_{\mathbb{R}^3} f_{,i}(\boldsymbol{x}-\boldsymbol{x}')g(\boldsymbol{x}')\,\mathrm{d}V' = f_{,i} * g = f * g_{,i} \qquad \text{(A.18)}
$$

$$
(f * g) * h = f * (g * h) \qquad \text{(A.19)}
$$

Figure A.1: The unit sphere in Fourier space. The unit vector $\boldsymbol{\kappa}(\theta, \phi)$ is defined by the azimuth angle ϕ, and the zenith angle θ measured from the axis $\hat{\boldsymbol{e}}_3 = \boldsymbol{R}/R$.

A.4 The nabla operator

A.5 The Green's tensor and the F-tensor in classical anisotropic elasticity

In classical elasticity, the Green's tensor of the anisotropic Navier operator G^0_{ij} satisfies the following inhomogeneous PDE:

$$L_{ik}G^0_{kj} + \delta_{ij}\delta = 0 \,. \tag{A.20}$$

In Fourier space[2] this reads:

$$\hat{G}^0_{ik}(\boldsymbol{k}) = \frac{1}{k^2}\,\hat{L}^{-1}_{ik}(\boldsymbol{\kappa}) \,. \tag{A.22}$$

where $\hat{L}_{ik}(\boldsymbol{\kappa}) = \mathbb{C}_{ijkl}\kappa_j\kappa_l$, $\boldsymbol{\kappa} = \boldsymbol{k}/k$, and $k = \sqrt{\boldsymbol{k}\cdot\boldsymbol{k}}$. The Green's tensor in real space is obtained by inverse Fourier transform. Expressing the elementary volume element in Fourier space as $\mathrm{d}\hat{V} = k^2\,\mathrm{d}k\,\mathrm{d}\omega$, where $\mathrm{d}\omega$ is an elementary surface element of the unit sphere $\mathcal{S}$, we obtain:

$$G^0_{ik}(\boldsymbol{R}) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\frac{\hat{L}^{-1}_{ik}(\boldsymbol{\kappa})}{k^2}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,\mathrm{d}\hat{V} = \frac{1}{(2\pi)^3}\int_{\mathcal{S}}\hat{L}^{-1}_{kl}(\boldsymbol{\kappa})\int_0^\infty\cos(k\boldsymbol{\kappa}\cdot\boldsymbol{R})\,\mathrm{d}k\,\mathrm{d}\omega = \frac{1}{8\pi^2 R}\int_{\mathcal{S}}\hat{L}^{-1}_{kl}(\boldsymbol{\kappa})\,\delta(\boldsymbol{\kappa}\cdot\boldsymbol{R})\,\mathrm{d}\omega \,.$$

Choosing a reference system with $\hat{\boldsymbol{e}}_3$ aligned with $\boldsymbol{R}$, as shown in Fig. A.1, and using the sifting property of the Dirac δ-function, we finally obtain the expression for the Green tensor as:

$$G^0_{ik}(\boldsymbol{R}) = \frac{1}{8\pi^2 R}\int_0^{2\pi}\hat{L}^{-1}_{ik}(\boldsymbol{n})\,\mathrm{d}\phi \,. \tag{A.23}$$

Here, $\boldsymbol{n}$ indicates a unit vector on the equatorial plane of the unit sphere in Fourier space. This result was first obtained by **?** and **?**.

The classical $\boldsymbol{F}$-tensor, introduced by **?**, is defined by Eq. (1.19), which in Fourier space reads:

$$\hat{F}^0_{ijkl} = -\hat{G}^0_{kl}\,k_ik_j\,\hat{G}^\Delta = -\frac{1}{k^2}\,\hat{L}^{-1}_{kl}(\boldsymbol{\kappa})\,k_ik_j\,\frac{1}{k^2} = -\frac{1}{k^2}\,\hat{L}^{-1}_{kl}(\boldsymbol{\kappa})\,\kappa_i\kappa_j \,. \tag{A.24}$$

The classical $\boldsymbol{F}$-tensor in real space is obtained by inverse Fourier transform:

$$\begin{aligned} F^0_{ijkl}(\boldsymbol{R}) &= -\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\frac{1}{k^2}\,\hat{L}^{-1}_{kl}(\boldsymbol{\kappa})\,\kappa_i\kappa_j\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\,\mathrm{d}\hat{V} = -\frac{1}{(2\pi)^3}\int_{\mathcal{S}}\hat{L}^{-1}_{kl}(\boldsymbol{\kappa})\,\kappa_i\kappa_j\int_0^\infty\cos(k\boldsymbol{\kappa}\cdot\boldsymbol{R})\,\mathrm{d}k\,\mathrm{d}\omega \\ &= -\frac{1}{8\pi^2 R}\int_{\mathcal{S}}\hat{L}^{-1}_{kl}(\boldsymbol{\kappa})\,\kappa_i\kappa_j\,\delta(\boldsymbol{\kappa}\cdot\boldsymbol{R})\,\mathrm{d}\omega \,. \end{aligned} \tag{A.25}$$

In the reference system of Fig. A.1, we finally obtain:

$$F^0_{ijkl}(\boldsymbol{R}) = -\frac{1}{8\pi^2 R}\int_0^{2\pi}\hat{L}^{-1}_{kl}(\boldsymbol{n})\,n_in_j\;\mathrm{d}\phi \,. \tag{A.26}$$

[2] The Fourier transform and its inverse are defined as, respectively [Vladimirov, 1971]:

$$\hat{f}(\boldsymbol{k}) = \int_{\mathbb{R}^3} f(\boldsymbol{x})\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,\mathrm{d}V \,, \qquad f(\boldsymbol{x}) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\hat{f}(\boldsymbol{k})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,\mathrm{d}\hat{V} \,. \tag{A.21}$$

Appendix B

Elastic fields of piecewise-straight dislocations loop

B.0.1 Straight segments

For a straight segment starting at $\boldsymbol{A}$ and ending at $\boldsymbol{B}$, it is useful to preliminary compute the function

$$q(\boldsymbol{x}) = \int_{\boldsymbol{A}}^{\boldsymbol{B}} R_a \, d\ell' \tag{B.1}$$

where $R_a = \sqrt{\boldsymbol{R}\cdot\boldsymbol{R}+a^2}$, $\boldsymbol{R} = \boldsymbol{x}-\boldsymbol{x}'$. Integration is performed on the primed variable along the segment $\boldsymbol{AB}$. This can be parametrized as a function of a scalar variable u as

$$\boldsymbol{x}'(u) = \boldsymbol{A}(1-u)+\boldsymbol{B}u = \boldsymbol{A}+(\boldsymbol{B}-\boldsymbol{A})u \qquad u\in[0,1] \tag{B.2}$$

Therefore

$$\begin{aligned} q(\boldsymbol{x}) &= L\int_0^1 \sqrt{[(\boldsymbol{A}-\boldsymbol{x})+(\boldsymbol{B}-\boldsymbol{A})u]^2+a^2}\; du \\ &= L\int_0^1 \sqrt{(\boldsymbol{B}-\boldsymbol{A})^2u^2+2(\boldsymbol{A}-\boldsymbol{x})\cdot(\boldsymbol{B}-\boldsymbol{A})u+(\boldsymbol{A}-\boldsymbol{x})^2+a^2}\; du \end{aligned} \tag{B.3}$$

Now

$$\int \sqrt{du^2+bu+c}\; du = \left(\frac{b}{4d}+\frac{u}{2}\right)\sqrt{du^2+bu+c}+\frac{4dc-b^2}{8d^{\frac{3}{2}}}\ln\left(\frac{2du+b}{\sqrt{d}}+2\sqrt{du^2+bu+c}\right) \tag{B.4}$$

So

$$\int_0^1 \sqrt{du^2+bu+c}\; du = \frac{2d+b}{4d}\sqrt{d+b+c}-\frac{b}{4d}\sqrt{c}+\frac{4dc-b^2}{8d^{\frac{3}{2}}}\ln\left(\frac{\frac{2d+b}{\sqrt{d}}+2\sqrt{d+b+c}}{\frac{b}{\sqrt{d}}+2\sqrt{c}}\right) \tag{B.5}$$

Note that in our case

$$
\begin{aligned}
d &= (\boldsymbol{B}-\boldsymbol{A})^2 = L^2 && \text{(B.6)}\\
b &= 2(\boldsymbol{A}-\boldsymbol{x})\cdot(\boldsymbol{B}-\boldsymbol{A}) = 2L(\boldsymbol{A}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}} && \text{(B.7)}\\
c &= (\boldsymbol{A}-\boldsymbol{x})^2 + a^2 && \text{(B.8)}\\
d+b+c &= (\boldsymbol{B}-\boldsymbol{x})^2 + a^2 && \text{(B.9)}\\
2d+b &= 2(\boldsymbol{B}-\boldsymbol{x})\cdot(\boldsymbol{B}-\boldsymbol{A}) = 2L(\boldsymbol{B}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}} && \text{(B.10)}\\
4dc-b^2 &= 4(\boldsymbol{B}-\boldsymbol{A})^2(\boldsymbol{A}-\boldsymbol{x})^2 - [2(\boldsymbol{A}-\boldsymbol{x})\cdot(\boldsymbol{B}-\boldsymbol{A})]^2 + 4da^2\\
&= 4L^2[(\boldsymbol{A}-\boldsymbol{x})^2 - ((\boldsymbol{A}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}})^2 + a^2]\\
&= 4L^2[(\boldsymbol{A}-\boldsymbol{B}+\boldsymbol{B}-\boldsymbol{x})^2 - ((\boldsymbol{A}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}})^2 + a^2]\\
&= 4L^2[(\boldsymbol{A}-\boldsymbol{B})^2 + 2(\boldsymbol{A}-\boldsymbol{B})\cdot(\boldsymbol{B}-\boldsymbol{x}) + (\boldsymbol{B}-\boldsymbol{x})^2 - ((\boldsymbol{A}-\boldsymbol{B})\cdot\hat{\boldsymbol{\xi}} + (\boldsymbol{B}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}})^2 + a^2]\\
&= 4L^2[L^2 - 2L\hat{\boldsymbol{\xi}}\cdot(\boldsymbol{B}-\boldsymbol{x}) + (\boldsymbol{B}-\boldsymbol{x})^2 - (-L + (\boldsymbol{B}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}})^2 + a^2]\\
&= 4L^2[L^2 - 2L\hat{\boldsymbol{\xi}}\cdot(\boldsymbol{B}-\boldsymbol{x}) + (\boldsymbol{B}-\boldsymbol{x})^2 - L^2 + 2L(\boldsymbol{B}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}} - ((\boldsymbol{B}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}})^2 + a^2]\\
&= 4L^2[(\boldsymbol{B}-\boldsymbol{x})^2 - ((\boldsymbol{B}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}})^2 + a^2]\\
&= 4L^2\rho_a^2 && \text{(B.11)}
\end{aligned}
$$

where

$$\rho_a^2 = (\boldsymbol{B}-\boldsymbol{x})^2 - ((\boldsymbol{B}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}})^2 + a^2 = (\boldsymbol{A}-\boldsymbol{x})^2 - ((\boldsymbol{A}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}})^2 + a^2 \quad \text{(B.12)}$$

ρ^2 is the regularized distance of $\boldsymbol{x}$ from the line passing through $\boldsymbol{A}$ and $\boldsymbol{B}$.

Therefore

$$
\begin{aligned}
\int_0^1 \sqrt{du^2+bu+c}\,du =& \frac{(\boldsymbol{B}-\boldsymbol{x})\cdot(\boldsymbol{B}-\boldsymbol{A})}{2(\boldsymbol{B}-\boldsymbol{A})^2}\sqrt{(\boldsymbol{B}-\boldsymbol{x})^2+a^2} - \frac{(\boldsymbol{A}-\boldsymbol{x})\cdot(\boldsymbol{B}-\boldsymbol{A})}{2(\boldsymbol{B}-\boldsymbol{A})^2}\sqrt{(\boldsymbol{A}-\boldsymbol{x})^2+a^2}\\
&+ \frac{4dc-b^2}{8L^3}\ln\left(\frac{\frac{2(\boldsymbol{B}-\boldsymbol{x})\cdot(\boldsymbol{B}-\boldsymbol{A})}{\sqrt{d}} + 2\sqrt{(\boldsymbol{B}-\boldsymbol{x})^2+a^2}}{\frac{2(\boldsymbol{A}-\boldsymbol{x})\cdot(\boldsymbol{B}-\boldsymbol{A})}{\sqrt{d}} + 2\sqrt{(\boldsymbol{A}-\boldsymbol{x})^2+a^2}}\right)\\
=& \frac{(\boldsymbol{B}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}}}{2L}\sqrt{(\boldsymbol{B}-\boldsymbol{x})^2+a^2} - \frac{(\boldsymbol{A}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}}}{2L}\sqrt{(\boldsymbol{A}-\boldsymbol{x})^2+a^2}\\
&+ \frac{\rho_a^2}{2L}\ln\left(\frac{(\boldsymbol{B}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}} + \sqrt{(\boldsymbol{B}-\boldsymbol{x})^2+a^2}}{(\boldsymbol{A}-\boldsymbol{x})\cdot\hat{\boldsymbol{\xi}} + \sqrt{(\boldsymbol{A}-\boldsymbol{x})^2+a^2}}\right) \quad \text{(B.13)}
\end{aligned}
$$

If we define

$$
\begin{aligned}
f(\boldsymbol{z}) &= \frac{\boldsymbol{z}\cdot\hat{\boldsymbol{\xi}}}{2}z_a + \frac{\rho_a^2}{2}\ln\left(\boldsymbol{z}\cdot\hat{\boldsymbol{\xi}} + z_a\right)\\
&= \frac{\boldsymbol{z}\cdot\hat{\boldsymbol{\xi}}}{2}z_a + \frac{\rho_a^2}{2}\ln\left(\boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}\right) \quad \text{(B.14)}
\end{aligned}
$$

and

$$
\begin{aligned}
\boldsymbol{Y}_a &= \boldsymbol{z} + z_a\hat{\boldsymbol{\xi}} && \text{(B.15)}\\
\rho_a^2 &= \boldsymbol{\rho}_a\cdot\boldsymbol{\rho}_a = z^2 - (\boldsymbol{z}\cdot\hat{\boldsymbol{\xi}})^2 + a^2 && \text{(B.16)}\\
\boldsymbol{\rho}_a &= \boldsymbol{z} - (\boldsymbol{z}\cdot\hat{\boldsymbol{\xi}} \pm a)\hat{\boldsymbol{\xi}} && \text{(B.17)}
\end{aligned}
$$

then we have

$$q(\boldsymbol{x}) = f(\boldsymbol{B}-\boldsymbol{x}) - f(\boldsymbol{A}-\boldsymbol{x}) \quad \text{(B.18)}$$

Now consider the following identities:

$$\boldsymbol{\rho}_a \cdot \hat{\boldsymbol{\xi}} = \mp a \tag{B.19}$$

$$\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}} = \boldsymbol{z} \cdot \hat{\boldsymbol{\xi}} + z_a \tag{B.20}$$

$$Y_a^2 = 2z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}} - a^2 \tag{B.21}$$

$$\frac{\partial \rho_{ai}}{\partial z_j} = \delta_{ij} - \hat{\xi}_i \hat{\xi}_j \tag{B.22}$$

$$\frac{\partial \rho_a^2}{\partial z_i} = 2\rho_{ak} \frac{\partial \rho_{ak}}{\partial z_i} = 2\rho_{ak} \left(\delta_{ki} - \hat{\xi}_i \hat{\xi}_k\right) = 2(\underbrace{z_i - (\boldsymbol{z} \cdot \hat{\boldsymbol{\xi}})\hat{\xi}_i}_{\rho_i}) = 2\rho_i \tag{B.23}$$

$$\frac{\partial \rho_i}{\partial z_j} = \delta_{ij} - \hat{\xi}_i \hat{\xi}_j \tag{B.24}$$

$$\frac{\partial Y_{ai}}{\partial z_j} = \delta_{ij} + \frac{z_j \hat{\xi}_i}{z_a} \tag{B.25}$$

$$\frac{\partial (\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})}{\partial z_i} = \frac{Y_{ai}}{z_a} \tag{B.26}$$

$$\frac{\partial}{\partial z_i} \ln(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}) = \frac{Y_{ai}}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \tag{B.27}$$

First derivative

$$\begin{aligned}
\frac{\partial f}{\partial z_i} &= \frac{z_a \hat{\xi}_i}{2} + \frac{z_p \hat{\xi}_p z_i}{2z_a} + \rho_i \ln(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}) + \frac{\rho_a^2}{2} \frac{Y_{ai}}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \\
&= \frac{z_a \hat{\xi}_i}{2} + \frac{z_p \hat{\xi}_p z_i}{2z_a} + \rho_i \ln(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}) + \frac{(z^2 - (z_q \hat{\xi}_q)^2 + a^2)}{2} \frac{Y_{ai}}{z_a(z_a + z_p \hat{\xi}_p)} \\
&= \frac{z_a \hat{\xi}_i}{2} + \frac{z_p \hat{\xi}_p z_i}{2z_a} + \rho_i \ln(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}) + \frac{(z_a - z_q \hat{\xi}_q)}{2} \frac{Y_{ai}}{z_a} \\
&= \frac{z_a^2 \hat{\xi}_i + z_p \hat{\xi}_p z_i + (z_a - z_q \hat{\xi}_q)(z_i + z_a \hat{\xi}_i)}{2z_a} + \rho_i \ln(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}) \\
&= \frac{\rho_i}{2} + z_a \hat{\xi}_i + \rho_i \ln(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})
\end{aligned} \tag{B.28}$$

Second derivative

$$\begin{aligned}
\frac{\partial^2 f}{\partial z_i \partial z_j} &= \frac{\rho_{i,j}}{2} + \frac{z_j}{z_a} \hat{\xi}_i + \rho_{i,j} \ln\left(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}\right) + \frac{\rho_i Y_{aj}}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \\
&= \frac{\delta_{ij} - \hat{\xi}_i \hat{\xi}_j}{2} + \frac{z_j}{z_a} \hat{\xi}_i + (\delta_{ij} - \hat{\xi}_i \hat{\xi}_j) \ln\left(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}\right) + \frac{\rho_i Y_{aj}}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \\
&= \frac{\delta_{ij} - \hat{\xi}_i \hat{\xi}_j}{2} + (\delta_{ij} - \hat{\xi}_i \hat{\xi}_j) \ln\left(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}\right) + \frac{\rho_i Y_{aj} + z_j \hat{\xi}_i \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \\
&= \frac{\delta_{ij} - \hat{\xi}_i \hat{\xi}_j}{2} + (\delta_{ij} - \hat{\xi}_i \hat{\xi}_j) \ln\left(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}\right) + \frac{1}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \left(\frac{z_i z_j}{z_a} + z_i \hat{\xi}_j + z_j \hat{\xi}_i - z_q \hat{\xi}_q \hat{\xi}_i \hat{\xi}_j\right)
\end{aligned} \tag{B.29}$$

$$
\begin{aligned}
\frac{\partial^2 f}{\partial z_p \partial z_p} &= 1 + 2\ln\left(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}\right) + \frac{1}{\mathbf{Y}_a \cdot \hat{\boldsymbol{\xi}}}\left(\frac{z^2}{z_a} + \boldsymbol{z}\cdot\hat{\boldsymbol{\xi}}\right) \\
&= 1 + 2\ln\left(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}\right) + \frac{1}{\mathbf{Y}_a \cdot \hat{\boldsymbol{\xi}}}\left(z_a + \boldsymbol{z}\cdot\hat{\boldsymbol{\xi}} - \frac{a^2}{z_a}\right) \\
&= 2 + 2\ln\left(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}\right) - \frac{a^2}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \qquad \text{(B.30)}
\end{aligned}
$$

Third derivative

$$
\begin{aligned}
\frac{\partial^3 f}{\partial z_i \partial z_j z_m} &= \frac{\delta_{jm} Y_{ai} + \delta_{im} Y_{aj} + \delta_{ij} Y_{am}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})} && \text{(B.31)} \\
&+ \frac{1}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}\left(\frac{\boldsymbol{z}\cdot\hat{\boldsymbol{\xi}}}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} - 2\right)\hat{\xi}_i \hat{\xi}_j \hat{\xi}_m && \text{(B.32)} \\
&- \frac{1}{z_a^2 \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}\left(\frac{1}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} + \frac{1}{z_a}\right) z_i z_j z_m && \text{(B.33)} \\
&- \frac{\hat{\xi}_i z_m Y_{aj} + \hat{\xi}_j z_i Y_{am} + \hat{\xi}_m z_j Y_{ai}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} && \text{(B.34)} \\
& && \text{(B.35)}
\end{aligned}
$$

Letting $i = j$

$$\frac{\partial^3 f}{\partial z_p \partial z_p z_m} = \frac{5Y_{am}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})} \tag{B.36}$$

$$+ \frac{1}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \left(\frac{\boldsymbol{z} \cdot \hat{\boldsymbol{\xi}}}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} + \frac{a^2}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} - 2 \right) \hat{\xi}_m \tag{B.37}$$

$$- \frac{1}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \left(\frac{1}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} + \frac{1}{z_a} \right) \left(1 - \frac{a^2}{z_a^2} \right) z_m \tag{B.38}$$

$$- \frac{z_a + 2(\boldsymbol{z} \cdot \hat{\boldsymbol{\xi}})}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} Y_{am}$$

$$= \frac{5Y_{am}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})} \tag{B.39}$$

$$- \frac{z^2 + z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} \hat{\xi}_m \tag{B.40}$$

$$- \frac{z_a + \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} \left(1 - \frac{a^2}{z_a^2} \right) z_m \tag{B.41}$$

$$- \frac{z_a + 2(\boldsymbol{z} \cdot \hat{\boldsymbol{\xi}})}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} Y_{am} \tag{B.42}$$

$$= \frac{5Y_{am}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})} \tag{B.43}$$

$$- \frac{z^2 + z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}{z_a^2(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} Y_{am} + \frac{a^2}{z_a^3 \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} z_m$$

$$- \frac{z_a + 2(\boldsymbol{z} \cdot \hat{\boldsymbol{\xi}})}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} Y_{am}$$

$$= \left(\frac{2}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} + \frac{a^2}{z_a^2(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} \right) Y_{am} + \frac{a^2}{z_a^3 \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} z_m \tag{B.44}$$

Since $\epsilon_{klm}\hat{\xi}_l\hat{\xi}_m = 0$, then $\epsilon_{klm}\hat{\xi}_l Y_m = \epsilon_{klm}\hat{\xi}_l Y_{am} = \epsilon_{klm}\hat{\xi}_l \rho_m = \epsilon_{klm}\hat{\xi}_l z_m$. Therefore

$$\epsilon_{klm}\hat{\xi}_l \frac{\partial^3 f}{\partial z_i \partial z_j z_m} = \frac{\epsilon_{klj}\hat{\xi}_l Y_{ai} + \epsilon_{kli}\hat{\xi}_l Y_{aj} + \epsilon_{klm}\hat{\xi}_l \delta_{ij} Y_{am}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})} \tag{B.45}$$

$$- \epsilon_{klm}\hat{\xi}_l \frac{1}{z_a^2 \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \left(\frac{1}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} + \frac{1}{z_a} \right) z_i z_j Y_{am} \tag{B.46}$$

$$- \frac{\epsilon_{klm}\hat{\xi}_l \hat{\xi}_i Y_{am} Y_{aj} + \epsilon_{klm}\hat{\xi}_l \hat{\xi}_j z_i Y_{am}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} \tag{B.47}$$

and

$$\epsilon_{klm}\hat{\xi}_l \frac{\partial^3 f}{\partial z_p \partial z_p z_m} = \epsilon_{klm}\hat{\xi}_l \left(\frac{2}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} + \frac{a^2}{z_a^2(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} + \frac{a^2}{z_a^3 \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \right) Y_{am} \tag{B.48}$$

Simplifying:

$$\begin{aligned}\epsilon_{klm}\hat{\xi}_l \frac{\partial^3 f}{\partial z_i \partial z_j z_m} &= \frac{\epsilon_{klj}\hat{\xi}_l Y_{ai} + \epsilon_{kli}\hat{\xi}_l Y_{aj}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})} \\ &\quad + \frac{\epsilon_{klm}\hat{\xi}_l Y_{am}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})}\left[\delta_{ij} - \frac{z_a + \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}{z_a^2 \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} z_i z_j - \frac{\hat{\xi}_i z_j + \hat{\xi}_j z_i + z_a \hat{\xi}_i \hat{\xi}_j}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}\right] \end{aligned} \tag{B.49}$$

(B.50)

B.0.2 Stress field of a straight segment

The stress field of the segment $\boldsymbol{A} \to \boldsymbol{B}$ is

$$\sigma_{ij}(\boldsymbol{x}) = b_k \int_{\boldsymbol{A}}^{\boldsymbol{B}} S_{ijkl} R_a \, d\ell'_l \tag{B.51}$$

$$S_{ijkl} = \frac{\mu}{8\pi}\left[(\delta_{il}\epsilon_{jmk} + \delta_{jl}\epsilon_{imk})\,\partial_m \Delta + \frac{2}{1-\nu}\epsilon_{klm}\,(\partial_i \partial_j \partial_m - \delta_{ij}\partial_m \Delta)\right] \tag{B.52}$$

Now notice that differentiation is in $\boldsymbol{x}$, while integration is in $\boldsymbol{x}'$. Therefore they commute.

$$\begin{aligned}\sigma_{ij}(\boldsymbol{x}) &= b_k \hat{\xi}_l S_{ijkl} q(\boldsymbol{x}) \\ &= \hat{\xi}_l b_k \frac{\mu}{8\pi}\left[(\delta_{il}\epsilon_{jmk} + \delta_{jl}\epsilon_{imk})\,\partial_m \Delta + \frac{2}{1-\nu}\epsilon_{klm}\,(\partial_i \partial_j \partial_m - \delta_{ij}\partial_m \Delta)\right][f(\boldsymbol{B}-\boldsymbol{x}) - f(\boldsymbol{A}-\boldsymbol{x})] \\ &= \hat{\xi}_l b_k \frac{\mu}{8\pi}\left[(\delta_{il}\epsilon_{jmk} + \delta_{jl}\epsilon_{imk})\,\partial_m \Delta + \frac{2}{1-\nu}\epsilon_{klm}\,(\partial_i \partial_j \partial_m - \delta_{ij}\partial_m \Delta)\right][f(\boldsymbol{z})]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}} \\ &= \frac{\mu}{4\pi(1-\nu)}\left[\frac{1-\nu}{2}\left(\hat{\xi}_i b_k \epsilon_{jmk} + \hat{\xi}_j b_k \epsilon_{imk}\right)\frac{\partial^3 f}{\partial z_p \partial z_p \partial z_m} + \epsilon_{klm}\hat{\xi}_l b_k\left(\frac{\partial^3 f}{\partial z_i \partial z_j \partial z_m} - \delta_{ij}\frac{\partial^3 f}{\partial z_p \partial z_p \partial z_m}\right)\right]_{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}\end{aligned} \tag{B.53}$$

Plugging back in (B.53) we obtain

$$\begin{aligned}\sigma_{ij}(\boldsymbol{x}) = \frac{\mu}{4\pi(1-\nu)}&\left[\frac{1-\nu}{2}\left(\hat{\xi}_i b_k \epsilon_{jmk} + \hat{\xi}_j b_k \epsilon_{imk}\right)\left[\left(\frac{2}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} + \frac{a^2}{z_a^2 (\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2}\right) Y_{am} + \frac{a^2}{z_a^3 \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} z_m\right]\right. \\ &+ \frac{\epsilon_{klj} b_k \hat{\xi}_l Y_{ai} + \epsilon_{kli} b_k \hat{\xi}_l Y_{aj}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})} \\ &+ \frac{\epsilon_{klm} b_k \hat{\xi}_l Y_{am}}{z_a(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})}\left(\delta_{ij} - \frac{z_a + \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}{z_a^2 \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} z_i z_j - \frac{\hat{\xi}_i z_j + \hat{\xi}_j z_i + z_a \hat{\xi}_i \hat{\xi}_j}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}\right) \\ &\left. - \epsilon_{klm} b_k \hat{\xi}_l Y_{am} \delta_{ij}\left(\frac{2}{z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} + \frac{a^2}{z_a^2 (\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}})^2} + \frac{a^2}{z_a^3 \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}\right)\right]_{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}\end{aligned} \tag{B.54}$$

Factoring the term $z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}} = (Y_a^2 + a^2)/2$ we obtain

$$\begin{aligned}\sigma_{ij}(\boldsymbol{x}) = \frac{\mu}{4\pi(1-\nu)}&\left[\frac{2}{Y_a^2 + a^2}\left\{(1-\nu)\left(\hat{\xi}_i b_k \epsilon_{jmk} + \hat{\xi}_j b_k \epsilon_{imk}\right)\left[\left(1 + \frac{a^2}{Y_a^2 + a^2}\right) Y_{am} + \frac{a^2}{2 z_a^2} z_m\right]\right.\right. \\ &+ \epsilon_{klj} b_k \hat{\xi}_l Y_{ai} + \epsilon_{kli} b_k \hat{\xi}_l Y_{aj} \\ &\left.\left. - \epsilon_{klm} b_k \hat{\xi}_l Y_{am}\left(\left(1 + 2\frac{a^2}{Y_a^2 + a^2} + \frac{a^2}{z_a^2}\right)\delta_{ij} + 2\frac{z_a + \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}{z_a (Y_a^2 + a^2)} z_i z_j + \frac{\hat{\xi}_i z_j + \hat{\xi}_j z_i + z_a \hat{\xi}_i \hat{\xi}_j}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}\right)\right\}\right]_{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}\end{aligned} \tag{B.55}$$

Inverting the order of evaluation, and changing the sign within the square bracket we have

$$
\begin{aligned}
\sigma_{ij}(\boldsymbol{x}) = \frac{\mu}{4\pi(1-\nu)} \Bigg[\frac{2}{Y_a^2+a^2} \bigg\{ &(1-\nu) \left(\hat{\xi}_i b_k \epsilon_{jkm} + \hat{\xi}_j b_k \epsilon_{ikm} \right) \left[\left(1 + \frac{a^2}{Y_a^2+a^2} \right) Y_{am} + \frac{a^2}{2z_a^2} z_m \right] \\
&- \left(Y_{ai} \epsilon_{jkl} b_k \hat{\xi}_l + \epsilon_{ikl} b_k \hat{\xi}_l Y_{aj} \right) \\
&- \epsilon_{klm} b_k Y_{al} \hat{\xi}_m \left(\left(1 + 2\frac{a^2}{Y_a^2+a^2} + \frac{a^2}{z_a^2} \right) \delta_{ij} + 2\frac{z_a + \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}{z_a(Y_a^2+a^2)} z_i z_j + \frac{\hat{\xi}_i z_j + \hat{\xi}_j z_i + z_a \hat{\xi}_i \hat{\xi}_j}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \right) \bigg\} \Bigg]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}}
\end{aligned}
\tag{B.56}
$$

It is more efficient to compute the stress field as

$$
\boldsymbol{\sigma}(\boldsymbol{x}) = \frac{\mu}{4\pi(1-\nu)} \left(\boldsymbol{s}(\boldsymbol{x}) + \boldsymbol{s}^T(\boldsymbol{x}) \right) \tag{B.57}
$$

where

$$
\boldsymbol{s}(\boldsymbol{x}) = \tilde{\boldsymbol{s}}(\boldsymbol{B}-\boldsymbol{x}) - \tilde{\boldsymbol{s}}(\boldsymbol{A}-\boldsymbol{x}) \tag{B.58}
$$

and

$$
\begin{aligned}
\tilde{\boldsymbol{s}}(\boldsymbol{z}) = \frac{2}{Y_a^2+a^2} \bigg\{ &(1-\nu) \left(1 + \frac{a^2}{Y_a^2+a^2} \right) \hat{\boldsymbol{\xi}} \otimes (\boldsymbol{b} \times \boldsymbol{Y}_a) \\
&+ (1-\nu) \frac{a^2}{2z_a^2} \hat{\boldsymbol{\xi}} \otimes (\boldsymbol{b} \times \boldsymbol{z}) \\
&- \boldsymbol{Y}_a \otimes \left(\boldsymbol{b} \times \hat{\boldsymbol{\xi}} \right) \\
&- \frac{\left[(\boldsymbol{b} \times \boldsymbol{Y}_a) \cdot \hat{\boldsymbol{\xi}} \right]}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}} \otimes \boldsymbol{z} \\
&- \frac{\left[(\boldsymbol{b} \times \boldsymbol{Y}_a) \cdot \hat{\boldsymbol{\xi}} \right]}{2} \left(\left(1 + 2\frac{a^2}{Y_a^2+a^2} + \frac{a^2}{z_a^2} \right) \boldsymbol{I} + 2\frac{z_a + \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}}{z_a(Y_a^2+a^2)} \boldsymbol{z} \otimes \boldsymbol{z} + \frac{z_a}{\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}} \otimes \hat{\boldsymbol{\xi}} \right) \bigg\}
\end{aligned}
\tag{B.59}
$$

with

$$
\boldsymbol{Y}_a(\boldsymbol{z}) = \boldsymbol{z} + z_a \hat{\boldsymbol{\xi}} \tag{B.60}
$$

$$
Y_a^2(\boldsymbol{z}) = 2 z_a \boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}} - a^2 \tag{B.61}
$$

Note that

$$
\left(Y_a^2 + a^2 \right)^2 = 4 z_a^2 \left(\boldsymbol{Y}_a \cdot \hat{\boldsymbol{\xi}} \right)^2 = 4 z_a^2 \left(\boldsymbol{z} \cdot \hat{\boldsymbol{\xi}} + z_a \right)^2 \tag{B.62}
$$

Stress of a straight segment on a distant point

Suppose that we want to compute the stress field of a segment $\boldsymbol{AB}$ at a point $\boldsymbol{x}$, which is located at distance d from the center $\boldsymbol{C}$ of the segment. Let the length of the segment be $AB = 2L$, then

$$
\boldsymbol{B} - \boldsymbol{x} = \boldsymbol{C} - \boldsymbol{x} + \boldsymbol{C} - \boldsymbol{B} = \boldsymbol{C} - \boldsymbol{x} - L\hat{\boldsymbol{\xi}} = d \left(\hat{\boldsymbol{r}}_c - \frac{L}{d} \hat{\boldsymbol{\xi}} \right) \tag{B.63}
$$

$$
\boldsymbol{A} - \boldsymbol{x} = \boldsymbol{C} - \boldsymbol{x} + \boldsymbol{C} - \boldsymbol{A} = \boldsymbol{C} - \boldsymbol{x} + L\hat{\boldsymbol{\xi}} = d \left(\hat{\boldsymbol{r}}_c + \frac{L}{d} \hat{\boldsymbol{\xi}} \right) \tag{B.64}
$$

where $\hat{\boldsymbol{r}}_c = (\boldsymbol{C} - \boldsymbol{x})/\|\boldsymbol{C} - \boldsymbol{x}\| = (\boldsymbol{C} - \boldsymbol{x})/d$. Therefore we have

$$\boldsymbol{s}(\boldsymbol{x}) = \tilde{\boldsymbol{s}}\left(d\left(\hat{\boldsymbol{r}}_c - \frac{L}{d}\hat{\boldsymbol{\xi}}\right)\right) - \tilde{\boldsymbol{s}}\left(d\left(\hat{\boldsymbol{r}}_c + \frac{L}{d}\hat{\boldsymbol{\xi}}\right)\right) \tag{B.65}$$

If d is large compared to the segment length, that is

$$\frac{L}{d} \ll 1 \tag{B.66}$$

then the difference above can be approximated as

$$\boldsymbol{s}(\boldsymbol{x}) \approx \left.\frac{\partial \tilde{\boldsymbol{s}}(\boldsymbol{z})}{\partial \boldsymbol{z}}\right|_{\boldsymbol{z}=\boldsymbol{C}-\boldsymbol{x}} \cdot (-2L\hat{\boldsymbol{\xi}}) \tag{B.67}$$

Note that

$$\frac{\partial Y_i}{\partial z_j}\hat{\xi}_j = \frac{\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}}{z}\hat{\xi}_i \tag{B.68}$$

then

$$
\begin{aligned}
\frac{\partial \tilde{\boldsymbol{s}}(\boldsymbol{z})}{\partial \boldsymbol{z}} = \frac{\partial}{\partial \boldsymbol{z}} \Bigg[\frac{2}{Y^2} \Big\{ & (1-\nu)\hat{\boldsymbol{\xi}} \otimes (\boldsymbol{b} \times \boldsymbol{Y}) \\
& - \boldsymbol{Y} \otimes \left(\boldsymbol{b} \times \hat{\boldsymbol{\xi}}\right) \\
& - \frac{\left[(\boldsymbol{b} \times \boldsymbol{Y}) \cdot \hat{\boldsymbol{\xi}}\right]}{\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}} \otimes \boldsymbol{z} \\
& - \frac{\left[(\boldsymbol{b} \times \boldsymbol{Y}) \cdot \hat{\boldsymbol{\xi}}\right]}{2} \left(\boldsymbol{I} + 2\frac{z + \boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}}{zY^2} \boldsymbol{z} \otimes \boldsymbol{z} + \frac{z}{\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}} \otimes \hat{\boldsymbol{\xi}} \right) \Big\} \Bigg] \cdot (-2L\hat{\boldsymbol{\xi}}) \\
& = \left[-\frac{2}{Y} \frac{\partial Y}{\partial \boldsymbol{z}} \cdot \left(-2L\hat{\boldsymbol{\xi}}\right) \right] \tilde{\boldsymbol{s}}(\boldsymbol{z}) \\
& + \frac{2}{Y^2} \Bigg[\frac{\partial}{\partial \boldsymbol{z}} \Big\{ (1-\nu)\hat{\boldsymbol{\xi}} \otimes (\boldsymbol{b} \times \boldsymbol{Y}) \\
& - \boldsymbol{Y} \otimes \left(\boldsymbol{b} \times \hat{\boldsymbol{\xi}}\right) \\
& - \frac{\left[(\boldsymbol{b} \times \boldsymbol{Y}) \cdot \hat{\boldsymbol{\xi}}\right]}{\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}} \otimes \boldsymbol{z} \\
& - \frac{\left[(\boldsymbol{b} \times \boldsymbol{Y}) \cdot \hat{\boldsymbol{\xi}}\right]}{2} \left(\boldsymbol{I} + 2\frac{z + \boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}}{zY^2} \boldsymbol{z} \otimes \boldsymbol{z} + \frac{z}{\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}} \otimes \hat{\boldsymbol{\xi}} \right) \Big\} \Bigg] \cdot (-2L\hat{\boldsymbol{\xi}}) \\
& = \frac{4L}{zY^2} \left(\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}\right)^2 \tilde{\boldsymbol{s}}(\boldsymbol{z}) \\
& - \frac{4L}{Y^2} \Bigg[\Big\{ (1-\nu) \frac{\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}}{z} \hat{\boldsymbol{\xi}} \otimes \left(\boldsymbol{b} \times \hat{\boldsymbol{\xi}}\right) \\
& - \frac{\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}}{z} \hat{\boldsymbol{\xi}} \otimes \left(\boldsymbol{b} \times \hat{\boldsymbol{\xi}}\right) \\
& + \frac{\left[(\boldsymbol{b} \times \boldsymbol{Y}) \cdot \hat{\boldsymbol{\xi}}\right]}{z\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}} \otimes \boldsymbol{z} - \frac{\left[(\boldsymbol{b} \times \boldsymbol{Y}) \cdot \hat{\boldsymbol{\xi}}\right]}{\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}} \otimes \hat{\boldsymbol{\xi}} \\
& - \left[(\boldsymbol{b} \times \boldsymbol{Y}) \cdot \hat{\boldsymbol{\xi}}\right] \left(\frac{z + \boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}}{zY^2} \boldsymbol{z} \otimes \boldsymbol{z} \right) \cdot \hat{\boldsymbol{\xi}} \Big\} \Bigg] \\
& - \frac{\left[(\boldsymbol{b} \times \boldsymbol{Y}) \cdot \hat{\boldsymbol{\xi}}\right]}{2} \frac{\partial}{\partial \boldsymbol{z}} \left(\frac{z}{\boldsymbol{Y} \cdot \hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}} \otimes \hat{\boldsymbol{\xi}} \right) \cdot \hat{\boldsymbol{\xi}} \Big\} \Bigg]
\end{aligned}
\tag{B.69}
$$

Now let C be the center of the segment $\boldsymbol{AB}$, so that

Stress of a straight segment in the neighborhood of a far point

Suppose that we want to compute the stress field of segment $\boldsymbol{AB}$ at a point $\boldsymbol{x}$ which is in the neighborhood of a point $\boldsymbol{x}_0$. Let the distance from $\boldsymbol{x}_0$ to the segment $\boldsymbol{AB}$ be d. Then we work under the assumption $AB \ll d$ and $\|\boldsymbol{x} - \boldsymbol{x}_0\| \ll d$.

B.0.3 Straight Displacement

$$\begin{aligned}
u_i &= -\frac{b_i\Omega}{4\pi} - b_k\hat{\xi}_l U_{ikl}\oint_{\mathcal{L}} R_a dL' \\
&= -\frac{b_i\Omega}{4\pi} - b_k\hat{\xi}_l \frac{1}{8\pi}\epsilon_{klm}\left[\delta_{im}\Delta - \frac{1}{1-\nu}\partial_i\partial_m\right][f(\boldsymbol{B}-\boldsymbol{x}) - f(\boldsymbol{A}-\boldsymbol{x})) \\
&= -\frac{b_i\Omega}{4\pi} - b_k\hat{\xi}_l \frac{1}{8\pi}\epsilon_{klm}\left[\delta_{im}\frac{\partial^2 f}{\partial z_p \partial z_p} - \frac{1}{1-\nu}\frac{\partial^2 f}{\partial z_i \partial z_m}\right]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}} \\
&= -\frac{b_i\Omega}{4\pi} + \epsilon_{ilk}\hat{\xi}_l b_k \frac{1}{8\pi}\left[\frac{\partial^2 f}{\partial z_p \partial z_p}\right]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}} + \frac{1}{8\pi}\frac{1}{1-\nu}\epsilon_{klm} b_k\hat{\xi}_l\left[\frac{\partial^2 f}{\partial z_i \partial z_m}\right]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}}
\end{aligned} \tag{B.70}$$

From Eq. (B.30)

$$\begin{aligned}
u_i = &-\frac{b_i\Omega}{4\pi} \\
&+ \epsilon_{ilk}\hat{\xi}_l b_k \frac{1}{8\pi}\left[2 + 2\ln\left(\boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}\right) - \frac{a^2}{z_a \boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}}\right]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}} \\
&+ \frac{1}{8\pi}\frac{1}{1-\nu}\epsilon_{klm} b_k\hat{\xi}_l\left[\frac{\delta_{im} - \hat{\xi}_i\hat{\xi}_m}{2} + (\delta_{im} - \hat{\xi}_i\hat{\xi}_m)\ln\left(\boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}\right) + \frac{1}{\boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}}\left(\frac{z_i z_m}{z_a} + z_i\hat{\xi}_m + z_m\hat{\xi}_i - z_q\hat{\xi}_q\hat{\xi}_i\hat{\xi}_m\right)\right]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}}
\end{aligned} \tag{B.71}$$

Dropping vanishing terms of containing $\epsilon_{klm} b_k\hat{\xi}_l\hat{\xi}_m$

$$\begin{aligned}
u_i = &-\frac{b_i\Omega}{4\pi} \\
&+ \epsilon_{ilk}\hat{\xi}_l b_k \frac{1}{8\pi}\left[2 + 2\ln\left(\boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}\right) - \frac{a^2}{z_a \boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}}\right]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}} \\
&+ \frac{1}{8\pi}\frac{1}{1-\nu}\epsilon_{klm} b_k\hat{\xi}_l\left[\frac{\delta_{im}}{2} + \delta_{im}\ln\left(\boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}\right) + \frac{1}{\boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}}\left(\frac{z_i z_m}{z_a} + z_m\hat{\xi}_i\right)\right]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}}
\end{aligned} \tag{B.72}$$

Factoring common terms

$$\begin{aligned}
u_i = &-\frac{b_i\Omega}{4\pi} \\
&- \epsilon_{ikl} b_k\hat{\xi}_l \frac{1}{8\pi}\left[2 - \frac{1}{2}\frac{1}{1-\nu} + \left(2 - \frac{1}{1-\nu}\right)\ln\left(\boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}\right) - \frac{a^2}{z_a \boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}}\right]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}} \\
&+ \frac{1}{8\pi}\frac{1}{1-\nu}\epsilon_{klm} b_k\hat{\xi}_l\left[\frac{z_m}{\boldsymbol{Y}_a\cdot\hat{\boldsymbol{\xi}}}\frac{Y_{ai}}{z_a}\right]_{\boldsymbol{z}=\boldsymbol{A}-\boldsymbol{x}}^{\boldsymbol{z}=\boldsymbol{B}-\boldsymbol{x}}
\end{aligned} \tag{B.73}$$

Straight Solid Angle

$$\Omega = -\oint \frac{\epsilon_{ijk}\hat{s}_j R_k}{R(R + \hat{s}_p R_p)} dL'_k \tag{B.74}$$

where $\boldsymbol{R} = \boldsymbol{x} - \boldsymbol{x}'$. We'll follow the integration method proposed by **?**. To do this we work with $\boldsymbol{Y} = -\boldsymbol{R}$ and $\hat{\boldsymbol{Y}} = \boldsymbol{Y}/Y$ to obtain

$$\Omega = \oint \frac{\epsilon_{ijk}\hat{s}_j Y_k}{Y(Y - \hat{s}_p Y_p)} dL'_k = \oint \frac{\epsilon_{ijk}\hat{s}_j \hat{Y}_k}{Y(1 - \hat{s}_p \hat{Y}_p)} dL'_k \tag{B.75}$$

This integral can be evaluated by summing over straight segments. Each segment can be evaluated on unit sphere where $Y = 1$, therefore

$$\Omega_n = \int_0^{\alpha_n} \frac{\epsilon_{ijk}\hat{s}_j\hat{Y}_k}{(1-\hat{s}_p\hat{Y}_p)}\hat{t}'_k d\alpha \tag{B.76}$$

where $\cos\alpha_n = \boldsymbol{Y}_n \cdot \boldsymbol{Y}_{n+1}$. If we let

$$\hat{\boldsymbol{e}}_1 = \hat{\boldsymbol{Y}}_n \qquad \hat{\boldsymbol{e}}_3 = \frac{\hat{\boldsymbol{Y}}_n \times \hat{\boldsymbol{Y}}_{n+1}}{|\hat{\boldsymbol{Y}}_n \times \hat{\boldsymbol{Y}}_{n+1}|} \qquad \hat{\boldsymbol{e}}_2 = \hat{\boldsymbol{e}}_3 \times \hat{\boldsymbol{e}}_1 \tag{B.77}$$

then

$$\hat{\boldsymbol{Y}}(\alpha) = \cos\alpha\,\hat{\boldsymbol{e}}_1 + \sin\alpha\,\hat{\boldsymbol{e}}_2 \tag{B.78}$$

$$\hat{\boldsymbol{t}}(\alpha) = -\sin\alpha\,\hat{\boldsymbol{e}}_1 + \cos\alpha\,\hat{\boldsymbol{e}}_2 \tag{B.79}$$

$$\hat{\boldsymbol{s}} = s_1\hat{\boldsymbol{e}}_1 + s_2\hat{\boldsymbol{e}}_2 + s_3\hat{\boldsymbol{e}}_3 \tag{B.80}$$

Substituting

$$\Omega_n = \int_0^{\alpha_n} \frac{s_3}{1 - s_1\cos\alpha - s_2\sin\alpha} d\alpha \tag{B.81}$$

This integral is evaluated using the transformation

$$\alpha = 2\tan^{-1} w \qquad \cos\alpha = \frac{1-w^2}{1+w^2} \qquad \sin\alpha = \frac{2w}{1+w^2} \qquad d\alpha = \frac{2dw}{1+w^2} \tag{B.82}$$

which gives

$$\begin{aligned}
\Omega_n &= 2s_3\int_0^{w^*} \frac{1}{1+w^2 - s_1(1-w^2) - s_2 2w} d\alpha = 2s_3\int_0^{w^*} \frac{1}{(1+s_1)w^2 - 2s_2 w + 1 - s_1} d\alpha \\
&= 2s_3\left[\frac{2}{\sqrt{4-4s_1^2-4s_2^2}}\tan^{-1}\left(\frac{2(1+s_1)w - 2s_2}{\sqrt{4-4s_1^2-4s_2^2}}\right)\right]_0^{w^*} \\
&= 2\frac{s_3}{|s_3|}\left[\tan^{-1}\left(\frac{(1+s_1)w - s_2}{|s_3|}\right)\right]_0^{w^*} \\
&= 2\frac{s_3}{|s_3|}\tan^{-1}\left(\frac{\frac{(1+s_1)w^*-s_2}{|s_3|} + \frac{s_2}{|s_3|}}{1 + \frac{(1+s_1)w^*-s_2}{|s_3|}\frac{-s_2}{|s_3|}}\right) \\
&= 2\frac{s_3}{|s_3|}\tan^{-1}\left(\frac{(1+s_1)w^*}{|s_3| - s_2\frac{(1+s_1)w^*-s_2}{|s_3|}}\right) \\
&= 2\frac{s_3}{|s_3|}\tan^{-1}\left(\frac{|s_3|(1+s_1)w^*}{s_3^2 - s_2((1+s_1)w^* - s_2)}\right) \\
&= 2\frac{s_3}{|s_3|}\tan^{-1}\left(\frac{|s_3|w^*}{1 - s_1 - s_2 w^*}\right) \\
&= 2\tan^{-1}\left(\frac{s_3 w^*}{1 - s_1 - s_2 w^*}\right)
\end{aligned} \tag{B.83}$$

where

$$w^* = \sqrt{\frac{1 - \boldsymbol{Y}_n \cdot \boldsymbol{Y}_{n+1}}{1 + \boldsymbol{Y}_n \cdot \boldsymbol{Y}_{n+1}}} \tag{B.84}$$

Non-singular Straight Solid Angle

$$\Omega = -\oint \frac{\epsilon_{ijk}\hat{s}_j R_k}{R_a(R_a + \hat{s}_p R_p)} dL'_k = \oint \frac{\epsilon_{ijk}\hat{s}_j Y_k}{Y_a(Y_a - \hat{s}_p Y_p)} dL'_k \tag{B.85}$$

If we now evaluate this expression on the unit sphere where $Y = 1$ and $Y_a = \sqrt{1+a^2}$ we have

$$\Omega_n = \int_0^{\alpha_n} \frac{\epsilon_{ijk}\hat{s}_j \hat{Y}_k}{\sqrt{1+a^2}(\sqrt{1+a^2} - \hat{s}_p \hat{Y}_p)} \hat{t}'_k d\alpha \tag{B.86}$$

We can then proceed as before and finally find

$$\Omega_n = \frac{2}{\sqrt{1+a^2}\sqrt{s_3^2+a^2}} \tan^{-1}\left(\frac{\sqrt{s_3^2+a^2}w^*}{\sqrt{1+a^2} - s_1 - s_2 w^*}\right) \tag{B.87}$$

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