New explicit expressions of the Hill polarization tensor for general anisotropic elastic solids

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Abstract

Except for particular cases, the classical expressions of the Eshelby or Hill polarization tensors, depend, respectively, on a simple or double integral for a fully anisotropic two-dimensional or three-dimensional elastic body. When the body is two-dimensional, we take advantage of Cauchy's theory of residues to derive a new explicit expression which depends on the two pairs of complex conjugate roots of a quartic equation. If the body exhibits orthotropic symmetry, these roots are explicitly given as a function of the independent components of the elasticity tensor. Similarly, the double integral is reduced to a simple one when the body is three-dimensional. The corresponding integrand depends on the three pairs of complex conjugate roots of a sextic equation which reduces to a cubic one for orthotropic symmetry. This new expression improves significantly the computation times when the degree of anisotropy is high. For both two and three-dimensional bodies, degenerate cases are also studied to yield valid expressions in any events.

Keywords: Eshelby problem; Anisotropic elasticity; Hill's polarization tensor; Inclusion

1. Introduction

Consider an infinite uniform elastic body with moduli denoted by the fourth-order tensor $\boldsymbol{C}$. If an ellipsoidal part Ω of this infinite body is submitted to a uniform stress free strain $\boldsymbol{\varepsilon}^{\mathbf{0}}$, the resulting strain $\boldsymbol{\varepsilon}$ is uniform throughout Ω (Eshelby, 1961) and equals to $\boldsymbol{S} : \boldsymbol{\varepsilon}^0$ ($\varepsilon_{ij} = S_{ijkl}\varepsilon^0_{kl}$ with summation on repeated indices) where $\boldsymbol{S}$ denotes the Eshelby fourth-order tensor (S_{ijkl} its components in a Cartesian coordinates system). The Eshelby $\boldsymbol{S}$-tensor displays minor symmetry $S_{ijkl} = S_{jikl} = S_{ijlk}$ but does not obey major (diagonal) symmetry in general. Alternatively, the Hill polarization $\boldsymbol{P}$-tensor (Hill, 1965) defined by $\boldsymbol{S} = \boldsymbol{P} : \boldsymbol{C}$ obeys both minor and major symmetries. Considering a fully anisotropic three-dimensional body, the algebraic expression of Hill's polarization tensor depend on a double integral (Mura, 1982). Various numerical procedures have been developed to evaluate theses tensors. Ghahremani (1977) proposed a double Gaussian quadrature to compute the Hill polarization $\boldsymbol{P}$-tensor while Gavazzi and Lagoudas (1990) applied a similar numerical method to compute the Eshelby $\boldsymbol{S}$-tensor. These latest authors studied different practical situations and reported that strongly anisotropic situations require a high number of Gaussian points (up to 1000 in some cases) to reach a satisfactory accuracy. More recently, Brenner et al. (2004) compared the accuracy achieved with the double Gaussian quadrature with respect to a Romberg's algorithm based on the extended trapezoidal rule. This latest method turns to be efficient when a low accuracy is required.

The homogeneous inclusion problem has been used to derive well known bounds (Hashin and Shtrikman, 1963; Ponte Castañeda and Willis, 1995) or estimates (Kröner, 1958; Mori and Tanaka, 1973) of the effective behaviour of linear elastic heterogeneous media. In many cases, this homogeneous inclusion problem is related to an isotropic elastic body and spherical or spheroidal inclusions. Under these assumptions, the Hill polarization tensor may be computed explicitly (see Ponte Castañeda and Willis, 1995 for spheroidal inclusions). However, many other situations lead to more sophisticated homogeneous inclusion problems. In addition, the homogenization of nonlinear heterogeneous media generally proceeds by linearization of the nonlinear constitutive laws to define a Linear Composite Material (Ponte Castañeda, 1991) which is often taken similar to the one of the nonlinear media. The various linearization procedures proposed to derive this Linear Composite Material (see Rekik et al., 2007) often yield fully anisotropic elastic moduli. If we consider a tangent linearization (Molinari et al., 1987; Lebensohn and Tomé, 1993; Rougier et al., 1994; Ponte Castañeda, 1996) of an isotropic nonlinear constitutive law, the linearized moduli tensor should at the best exhibit a transversely isotropic symmetry. In this specific case, the double integral can be reduced to a simple one (Kneer, 1965) with corrections in Hutchinson (1976), see (Lin and Mura, 1973) for a similar reduction when a spheroidal inclusion is embedded in a cubic material). However, phases of the Linear Composite Material would mostly exhibit a more general anisotropy (textured polycrystals, anisotropic composites, ...).

Should it be possible to derive explicit expressions of Hill's polarization tensor for a fully anisotropic body? Mura (1982) suggested to take advantage of the Cauchy theory of residues to reduce the double integral to a simple one. Ting and Lee (1997) applied this method to derive explicit expressions of the elastic Green function in terms of the poles of the integrand (the Stroh eigenvalues). Alternatively, Suvorov and Dvorak (2002) derived explicit expressions of the Hill polarization tensor for disk-shaped and cylindrical inclusions in anisotropic solids (see also Gruescu et al., 2005).

In this work, we aim at applying the Cauchy theory of residues to derive new and simpler expressions of the Hill polarization tensor whatever the shape of the ellipsoidal inclusion and the material symmetry may be. Two-dimensional and three-dimensional body are, respectively, considered in Sections 2 and 3.

2. Explicit expressions of Hill's polarization tensor for two-dimensional bodies

We consider in this section a two-dimensional elastic body. Let Ω_{2d} be an elliptical region specified by:

$$\left(\frac{x_1}{a_1}\right)^2 + \left(\frac{x_2}{a_2}\right)^2 = 1.$$

Let C_{ijkl} denote the components of the moduli tensor in these axis. This tensor is definite positive and satisfies the full symmetry.

In this two-dimensional case, the Hill polarisation $\boldsymbol{P}$-tensor reads:

$$P_{(2d)ijkl} = \frac{1}{2\pi}\int_0^{2\pi} M_{(2d)ijkl}(\theta)\,\mathrm{d}\theta,$$

with $\left(x_1 = \frac{\cos(\theta)}{a_1} \text{ and } x_2 = \frac{\sin(\theta)}{a_2}\right)$:

$$M_{(2d)ijkl} = \frac{1}{4}\left(A^{-1}_{(2d)jk}x_i x_l + A^{-1}_{(2d)ik}x_j x_l + A^{-1}_{(2d)jl}x_i x_k + A^{-1}_{(2d)il}x_j x_k\right) \tag{1}$$

and $\boldsymbol{A}^{-1}_{2d}$ denotes the inverse of $A_{(2d)ik} = C_{ijkl}x_j x_l$:

$$\boldsymbol{A}^{-1}_{2d} = \frac{1}{\det(\boldsymbol{A}_{2d})}\begin{pmatrix} A_{(2d)22} & -A_{(2d)12} \\ -A_{(2d)12} & A_{(2d)11}\end{pmatrix}. \tag{2}$$

It is clear that $\boldsymbol{A}_{2d}$ is the acoustic tensor in the case of a circular inclusion. $\boldsymbol{C}$ being a positive definite fourth-order tensor, the determinant of $\boldsymbol{A}_{2d}$ $(\det(\boldsymbol{A}_{2d}))$ exhibits complex conjugate roots which are the Stroh eigenvalues for this two-dimensional anisotropic body.

2.1. Stroh eigenvalues for two-dimensional anisotropic body

The fourth components of the acoustic tensor read:

$$\begin{aligned}
A_{(2d)11} &= \frac{1}{a_1^2}C_{11}\cos^2(\theta) + \frac{1}{a_2^2}C_{33}\sin^2(\theta) + \frac{2}{a_1a_2}C_{13}\cos(\theta)\sin(\theta),\\
A_{(2d)22} &= \frac{1}{a_1^2}C_{33}\cos^2(\theta) + \frac{1}{a_2^2}C_{22}\sin^2(\theta) + \frac{2}{a_1a_2}C_{23}\cos(\theta)\sin(\theta),\\
A_{(2d)12} &= A_{(2d)21} = \frac{1}{a_1^2}C_{13}\cos^2(\theta) + \frac{1}{a_2^2}C_{23}\sin^2(\theta) + \frac{1}{a_1a_2}(C_{12}+C_{33})\cos(\theta)\sin(\theta),
\end{aligned} \tag{3}$$

(with the use of contracted notations $C_{IJ(I,J=1,2,3)}$ for the moduli tensor C_{ijkl}: for instance $C_{23}=C_{2212}$) while the determinant of the tensor $\boldsymbol{A}_{2d}$ reads $\left(\rho=\frac{a_2}{a_1}\right)$:

$$[\det(\boldsymbol{A}_{2d})](\theta) = \frac{\cos^4(\theta)}{a_1^4}q_{(2d)}\left(\frac{tg(\theta)}{\rho}\right), \tag{4}$$

where $q_{(2d)}(z)$ denotes a polynomial function of degree 4: $q_{(2d)}(z)=\sum_{i=0}^{i=4}q_{i(2d)}z^i$.

For a full symmetric moduli tensor, the coefficients of the polynomial function $q_{(2d)}$ reduce to:

$$\begin{aligned}
&q_{0(2d)} = C_{11}C_{33}-C_{13}^2, \quad q_{1(2d)} = 2(C_{11}C_{23}-C_{12}C_{13}),\\
&q_{2(2d)} = 2(C_{13}C_{23}-C_{12}C_{33}) + C_{11}C_{22}-C_{12}^2,\\
&q_{3(2d)} = 2(C_{13}C_{22}-C_{12}C_{23}), \quad q_{4(2d)} = C_{22}C_{33}-C_{23}^2.
\end{aligned} \tag{5}$$

The roots of the quartic equation

$$q_{(2d)}(z)=0 \tag{6}$$

are denoted by $(z_1,z_2,\bar{z}_1,\bar{z}_2)$ hereafter ($\bar{z}$ denotes the complex conjugate of any complex number z), (z_1,z_2) having a positive imaginary part. The explicit expressions of these roots are reported in Appendix A when the $\boldsymbol{C}$ moduli tensor exhibits orthotropic or quadratic symmetries.

2.2. Explicit expressions of Hill's *P*-tensor

It is noted that $M_{(2d)ijkl}(\theta)$ is periodic in θ with periodicity π. It follows that:

$$P_{(2d)ijkl} = \frac{1}{2\pi}\int_0^{2\pi}M_{(2d)ijkl}(\theta)\,\mathrm{d}\theta = \frac{1}{\pi}\int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}}M_{(2d)ijkl}(\theta)\,\mathrm{d}\theta.$$

Substituting relations (2)–(4) in (1) yields:

$$P_{(2d)ijkl} \underbrace{=}_{t=\frac{tg(\theta)}{\rho}} \frac{1}{\pi}\int_{-\infty}^{+\infty}\rho\frac{p_{(2d)ijkl}(t)}{(1+(\rho t)^2)q_{2d}(t)}\,\mathrm{d}t,$$

where the fourth-order tensor $p_{2d}(t)$ is defined as (contracted notations):

$$\begin{pmatrix}
C_{22}t^2+2C_{23}t+C_{33} & -(C_{13}t+C_{23}t^3+(C_{12}+C_{33})t^2) & \frac{1}{2}(C_{22}t^3+C_{23}t^2-C_{12}t-C_{13})\\
\dots & t^2(C_{33}t^2+2C_{13}t+C_{11}) & \frac{1}{2}(C_{11}t+C_{13}t^2-C_{12}t^3-C_{23}t^4)\\
\dots & \dots & \frac{1}{4}(C_{11}-2C_{12}t^2+C_{22}t^4)
\end{pmatrix}. \tag{7}$$

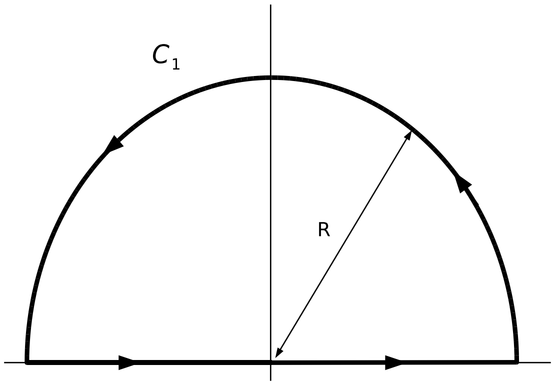

Fig. 1. Contour integral of Eq. (8).

We consider the closed path C_1 over the upper half of the complex plane (see Fig. 1). In the limit, as the radius of the path R approaches infinity, the integral over the outer circle vanishes (Jordan's lemma), leaving us with:

$$\int_{-\infty}^{+\infty} \frac{p_{(2d)ijkl}(t)}{(1+(\rho t)^2)q_{2d}(t)}\,\mathrm{d}t = \int_{C_1} \frac{p_{(2d)ijkl}(z)}{(1+(\rho z)^2)q_{2d}(z)}\,\mathrm{d}z. \tag{8}$$

Using Cauchy's theory of residues (see, for instance, Carrier et al. (1966)), the right term of the latest equation reduces to $2\imath\pi$ ($\imath^2=-1$) times the sum of the residues of the following function of the complex variable (z):

$$z \longrightarrow \frac{p_{(2d)ijkl}(z)}{(1+(\rho z)^2)q_{2d}(z)}$$

at poles $\frac{\imath}{\rho}, z_1, z_2$. As a result, we derive the following new expression of the Hill polarization $\boldsymbol{P}$-tensor:

$$P_{(2d)ijkl} = \frac{p_{(2d)ijkl}\left(\frac{\imath}{\rho}\right)}{q_{2d}\left(\frac{\imath}{\rho}\right)} + \frac{2\imath}{\rho}\sum_{u=1}^{u=2} \frac{p_{(2d)ijkl}(z_u)}{\left(\frac{1}{\rho^2}+z_u^2\right)q'_{2d}(z_u)}. \tag{9}$$

In this explicit relation:

- $q_{(2d)}$ and $p_{(2d)ijkl}$ are polynomial functions of degree 4 whose coefficients are given by relations (5) and (7) as a function of the elastic moduli $\boldsymbol{C}$ tensor ($q'_{2d}(z)$ denotes the derivative of $q_{2d}(z)$),
- the two complex numbers (z_1, z_2) are the roots with a positive imaginary part of the quartic equation $q_{2d}(z)=0$,
- $\rho = \frac{a_2}{a_1}$ is the aspect ratio of the elliptical inclusion.

2.3. Additional results (degenerate cases) for two-dimensional bodies

General expression (9) is no longer valid for the following degenerate cases. When $z_1 = z_2 \neq \frac{\imath}{\rho}$, the residues theorem gives ($z_1 - \bar{z}_1 = 2\imath\beta_1$):

$$P_{(2d)ijkl} = \frac{p_{(2d)ijkl}\left(\frac{\imath}{\rho}\right)}{q_{2d}\left(\frac{\imath}{\rho}\right)} + \frac{\imath}{\rho}\,\frac{\left(2\beta_1 z_1 - \imath\left(\frac{1}{\rho^2}+z_1^2\right)\right)p_{(2d)ijkl}(z_1) - \beta_1 p'_{(2d)ijkl}(z_1)\left(\frac{1}{\rho^2}+z_1^2\right)}{2\beta_1^3 q_{4(2d)}\left(\frac{1}{\rho^2}+z_1^2\right)^2}, \tag{10}$$

($p'_{(2d)ijkl}(z)$ denotes the derivative of $p_{(2d)ijkl}(z)$) while if $z_1 = z_2 = \frac{\imath}{\rho}$, it yields:

$$P_{(2d)ijkl} = \frac{\rho^4}{8q_{4(2d)}}\left(3p_{(2d)ijkl}\left(\frac{\imath}{\rho}\right) - \frac{3\imath}{\rho}p'_{(2d)ijkl}\left(\frac{\imath}{\rho}\right) - \frac{1}{\rho^2}p''_{(2d)ijkl}\left(\frac{\imath}{\rho}\right)\right),$$

($p''_{(2d)ijkl}(z)$ denotes the second derivative of $p_{(2d)ijkl}(z)$) which may be simplified further (contracted notations):

$$\frac{1}{8(C_{22}C_{33}-C_{23}^2)}\begin{pmatrix} \rho^2(C_{22}+3\rho^2C_{33}) & -\rho^2(C_{12}+C_{33}) & \frac{\rho^2}{2}(C_{23}-3\rho^2C_{13}) \\ \dots & 3C_{33}+\rho^2C_{11} & \frac{1}{2}(\rho^2C_{13}-3C_{23}) \\ \dots & \dots & \frac{1}{4}(3\rho^4C_{11}-2\rho^2C_{12}+3C_{22}) \end{pmatrix}. \tag{11}$$

3. Hill's polarization tensor expressed as a simple integral for three-dimensional bodies

Consider in this section a three-dimensional elastic body. Let Ω be the ellipsoidal region specified by:

$$\left(\frac{x_1}{a_1}\right)^2+\left(\frac{x_2}{a_2}\right)^2+\left(\frac{x_3}{a_3}\right)^2=1.$$

The components of the Hill polarisation $\boldsymbol{P}$-tensor in the principal axis of the ellipsoidal are (see, for instance, Suvorov and Dvorak, 2002):

$$P_{ijkl}=\frac{1}{4\pi}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}M_{ijkl}(\theta,\phi)\sin(\theta)\,\mathrm{d}\theta\,\mathrm{d}\phi. \tag{12}$$

As previously:

$$M_{ijkl}=\frac{1}{4}\left(A^{-1}_{jk}x_ix_l+A^{-1}_{ik}x_jx_l+A^{-1}_{jl}x_ix_k+A^{-1}_{il}x_jx_k\right),$$

with

$$x_1=\frac{\sin(\theta)\cos(\phi)}{a_1},\quad x_2=\frac{\sin(\theta)\sin(\phi)}{a_2},\quad x_3=\frac{\cos(\theta)}{a_3},$$

and $\boldsymbol{A}^{-1}$ the inverse of:

$$A_{ik}=C_{ijkl}x_jx_l,$$

which reduces to the acoustic tensor for a spherical inclusion ($a_1=a_2=a_3=1$). As for the two-dimensional body, the determinant of $\boldsymbol{A}$ exhibits pairs of complex conjugate roots which are the Stroh eigenvalues for the three-dimensional body.

3.1. Stroh eigenvalues for three-dimensional anisotropic bodies

As in Ting and Lee (1997), the vector $\boldsymbol{x}$ is denoted by:

$$\boldsymbol{x}=\boldsymbol{n}\cos(\theta)+\boldsymbol{m}\sin(\theta), \tag{13}$$

($\boldsymbol{n}$ and $\boldsymbol{m}$ are defined by $\left(0,0,\frac{1}{a_3}\right)$ and $\left(\frac{\cos(\phi)}{a_1},\frac{\sin(\phi)}{a_2},0\right)$, respectively). Denoting by:

$$Q_{ik}=C_{ijkl}n_jn_l=C_{i3k3}n_3^2,$$
$$R_{ik}=C_{ijkl}n_jm_l=C_{i3k1}m_1n_3+C_{i3k2}m_2n_3,$$
$$T_{ik}=C_{ijkl}m_jm_l=C_{i1k1}m_1^2+(C_{i1k2}+C_{i2k1})m_1m_2+C_{i2k2}m_2^2$$

(the Euler angle ϕ is omitted hereafter to shorten notations) we have:

$$\boldsymbol{A}=\boldsymbol{Q}\cos^2(\theta)+\underbrace{(\boldsymbol{R}+\boldsymbol{R}^{\mathrm{T}})}_{\boldsymbol{S}}\cos(\theta)\sin(\theta)+\boldsymbol{T}\sin^2(\theta).$$

Given that:

$$\det(\boldsymbol{A})=\varepsilon_{mnl}A_{m1}A_{n2}A_{l3}$$

(ε_{mnl} the permutation tensor), we obtain ($\theta \neq 0$):

$$[\det(\boldsymbol{A})](\theta) = \sin^6(\theta) q\left(\frac{1}{tg(\theta)}\right),$$

q being the polynomial function of degree six:

$$q(z) = \sum_{i=0}^{i=6} q_i z^i$$

with

$$\begin{aligned}
&q_6 = \varepsilon_{mnl} Q_{m1} Q_{n2} Q_{l3}, \quad q_5 = \varepsilon_{mnl}(Q_{m1}(S_{n2}Q_{l3} + Q_{n2}S_{l3}) + S_{m1}Q_{n2}Q_{l3}),\\
&q_4 = \varepsilon_{mnl}(Q_{m1}(S_{n2}S_{l3} + Q_{n2}T_{l3} + T_{n2}Q_{l3}) + S_{m1}(Q_{n2}S_{l3} + S_{n2}Q_{l3}) + T_{m1}Q_{n2}Q_{l3}),\\
&q_3 = \varepsilon_{mnl}(Q_{m1}(S_{n2}T_{l3} + T_{n2}S_{l3}) + S_{m1}(S_{n2}S_{l3} + Q_{n2}T_{l3} + T_{n2}Q_{l3}) + T_{m1}(Q_{n2}S_{l3} + S_{n2}Q_{l3})),\\
&q_2 = \varepsilon_{mnl}(Q_{m1}T_{n2}T_{l3} + S_{m1}(S_{n2}T_{l3} + T_{n2}S_{l3}) + T_{m1}(Q_{n2}T_{l3} + T_{n2}Q_{l3} + S_{n2}S_{l3})),\\
&q_1 = \varepsilon_{mnl}(S_{m1}T_{n2}T_{l3} + T_{m1}(S_{n2}T_{l3} + T_{n2}S_{l3})), \quad q_0 = \varepsilon_{mnl}T_{m1}T_{n2}T_{l3}.
\end{aligned} \tag{14}$$

Hereafter, the three complex numbers (z_1, z_2, z_3) denote the roots with a positive imaginary part of the sextic equation $q(z) = 0$. When the moduli tensor exhibits an orthotropic symmetry, this sextic equation reduces to a cubic equation in z^2 (see Appendix B).

3.2. Hill's polarization $\boldsymbol{P}$-tensor expressed as a simple integral

Consider now the following integral:

$$P_{(\phi)ijkl} = \frac{1}{2\pi}\int_0^{\pi} M_{ijkl}(\theta)\sin(\theta)\,\mathrm{d}\theta. \tag{15}$$

The components $P_{(\phi)ijkl}$ of the fourth-order tensor $\boldsymbol{P}_\phi$ are functions of the Euler angle ϕ (obviously M_{ijkl} depends also on ϕ but the Euler angle ϕ is omitted in next expressions to shorten notations). Substituting relation (13) in the definition of M_{ijkl} yields:

$$\begin{aligned}
M_{ijkl}(\theta) = \frac{1}{4}\Big(&\cos^2(\theta)(A^{-1}_{jk}n_in_l + A^{-1}_{ik}n_jn_l + A^{-1}_{jl}n_in_k + A^{-1}_{il}n_jn_k) + \cos(\theta)\sin(\theta)(A^{-1}_{jk}(n_im_l + n_lm_i)\\
&+A^{-1}_{ik}(n_jm_l + n_lm_j) + A^{-1}_{jl}(n_im_k + n_km_i) + A^{-1}_{il}(n_jm_k + n_km_j))\\
&+\sin^2(\theta)(A^{-1}_{jk}m_im_l + A^{-1}_{ik}m_jm_l + A^{-1}_{jl}m_im_k + A^{-1}_{il}m_jm_k)\Big).
\end{aligned}$$

Furthermore, the inverse of the matrix $\boldsymbol{A}$ reads:

$$\begin{aligned}
A^{-1}_{ij} &= \frac{1}{2\det(\boldsymbol{A})}\varepsilon_{ikl}\varepsilon_{jmn}A_{km}A_{ln}\\
&= \frac{1}{\det(\boldsymbol{A})}\left(\hat{A}^0_{ij}\cos^4(\theta) + \hat{A}^1_{ij}\cos^3(\theta)\sin(\theta) + \hat{A}^2_{ij}\cos^2(\theta)\sin^2(\theta) + \hat{A}^3_{ij}\cos(\theta)\sin^3(\theta) + \hat{A}^4_{ij}\sin^4(\theta)\right)
\end{aligned}$$

with

$$\begin{aligned}
&\hat{A}^0_{ij} = \frac{1}{2}\varepsilon_{ikl}\varepsilon_{jmn}Q_{km}Q_{ln}, \quad \hat{A}^1_{ij} = \frac{1}{2}\varepsilon_{ikl}\varepsilon_{jmn}(Q_{km}S_{ln} + S_{km}Q_{ln}),\\
&\hat{A}^2_{ij} = \frac{1}{2}\varepsilon_{ikl}\varepsilon_{jmn}(Q_{km}T_{ln} + S_{km}S_{ln} + T_{km}Q_{ln}), \quad \hat{A}^3_{ij} = \frac{1}{2}\varepsilon_{ikl}\varepsilon_{jmn}(S_{km}T_{ln} + T_{km}S_{ln}),\\
&\hat{A}^4_{ij} = \frac{1}{2}\varepsilon_{ikl}\varepsilon_{jmn}T_{km}T_{ln}.
\end{aligned} \tag{16}$$

As a result, the integrand $M_{ijkl}(\theta)$ of the simple integral (15) is a rational function whose denominator is the determinant of the matrix $\boldsymbol{A}$ while its numerator reads:

$$\frac{1}{4}\quad\sum_{u=0}^{u=4}(\hat{A}^u_{jk}n_in_l+\hat{A}^u_{ik}n_jn_l+\hat{A}^u_{jl}n_in_k+\hat{A}^u_{il}n_jn_k)\cos^{6-u}(\theta)\sin^u(\theta)$$
$$+\sum_{u=0}^{u=4}(\hat{A}^u_{jk}(n_im_l+n_lm_i)+\hat{A}^u_{ik}(n_jm_l+n_lm_j)+\hat{A}^u_{jl}(n_im_k+n_km_i)+\hat{A}^u_{il}(n_jm_k+n_km_j))\cos^{5-u}(\theta)\sin^{1+u}(\theta)$$
$$\left.+\sum_{u=0}^{u=4}(\hat{A}^u_{jk}m_im_l+\hat{A}^u_{ik}m_jm_l+\hat{A}^u_{jl}m_im_k+\hat{A}^u_{il}m_jm_k)\cos^{4-u}(\theta)\sin^{u+2}(\theta)\right).$$

When the inclusion is cylindrical ($a_3\to\infty$), the former expression of $M_{ijkl}(\theta)$ does not depend on Euler angle θ. In that particular case, the simple integral $P_{(\phi)ijkl}$ reduces to:

$$P_{(\phi)ijkl}=\frac{1}{4\pi}\frac{\hat{A}^4_{jk}m_im_l+\hat{A}^4_{ik}m_jm_l+\hat{A}^4_{jl}m_im_k+\hat{A}^4_{il}m_jm_k}{\varepsilon_{mnl}T_{m1}T_{n2}T_{l3}}.$$

Suvorov and Dvorak (2002) provided general expressions of the Hill polarization $\boldsymbol{P}$-tensor in that situation (orthotropic symmetry). More recently, Gruescu et al. (2005) developed explicit expressions for a crack (infinite cylinder with low aspect ratio) in an orthotropic solid.

In general, the integrand $M_{ijkl}(\theta)$ is a rational function. Its numerator and denominator are polynomial functions of the variables $(\cos(\theta),\sin(\theta))$. By the substitution $t=1/tg(\frac{\theta}{2})$, the former integral P_ϕ reduces to:[1]

$$P_{(\phi)ijkl}=\frac{1}{2\pi}\int_0^{+\infty}\frac{t\ p_{ijkl}(\frac{t^2-1}{2t})}{(1+t^2)^2q(\frac{t^2-1}{2t})}\,\mathrm{d}t,$$

where p_{ijkl} is a polynomial function of degree six, namely:

$$p_{ijkl}(t)=\sum_{u=0}^{u=4}\underbrace{(\hat{A}^u_{jk}n_in_l+\hat{A}^u_{ik}n_jn_l+\hat{A}^u_{jl}n_in_k+\hat{A}^u_{il}n_jn_k)}_{p^u_{(1)ijkl}}t^{6-u}$$
$$+\sum_{u=0}^{u=4}\underbrace{(\hat{A}^u_{jk}(n_im_l+n_lm_i)+\hat{A}^u_{ik}(n_jm_l+n_lm_j)+\hat{A}^u_{jl}(n_im_k+n_km_i)+\hat{A}^u_{il}(n_jm_k+n_km_j))}_{p^u_{(2)ijkl}}t^{5-u}$$
$$+\sum_{u=0}^{u=4}\underbrace{(\hat{A}^u_{jk}m_im_l+\hat{A}^u_{ik}m_jm_l+\hat{A}^u_{jl}m_im_k+\hat{A}^u_{il}m_jm_k)}_{p^u_{(3)ijkl}}t^{4-u}$$
$$=p^0_{(1)ijkl}t^6+(p^1_{(1)ijkl}+p^0_{(2)ijkl})t^5+(p^2_{(1)ijkl}+p^1_{(2)ijkl}+p^0_{(3)ijkl})t^4+(p^3_{(1)ijkl}+p^2_{(2)ijkl}+p^1_{(3)ijkl})t^3$$
$$+(p^4_{(1)ijkl}+p^3_{(2)ijkl}+p^2_{(3)ijkl})t^2+(p^4_{(2)ijkl}+p^3_{(3)ijkl})t+p^4_{(3)ijkl}.\tag{17}$$

To calculate this last integral, we consider the closed path C_2 of the complex plane (see Fig. 2) and the line integral:

$$\int_{C_2}\ln(z)\frac{z\ p_{ijkl}(\xi(z))}{(1+z^2)^2q(\xi(z))}\,\mathrm{d}z$$

where $\ln(z)$ denotes the principal value of the natural logarithm and $\xi(z)=\frac{z^2-1}{2z}$. In the limit as the radius of the path R approaches infinity, the integral over the outer circle vanishes (Jordan's lemma) while:

$$\lim_{r\to0}\int_{C_2^I\cup C_2^{II}}\ln(z)\frac{z\ p_{ijkl}(\xi(z))}{(1+z^2)^2q(\xi(z))}\,\mathrm{d}z=-2\imath\pi\int_0^{+\infty}\frac{t\ p_{ijkl}(\xi(t))}{(1+t^2)^2q(\xi(t))}\,\mathrm{d}t.$$

[1] Notice that the degree of the polynomial function $q(t)$ is at the least equal to the one of the numerator polynomial function $p_{ijkl}(t)$. Then, the integrand tends to zero for the lower $t=0$ and upper limit $t\to+\infty$. Hence, the improper integral is (as expected) convergent.

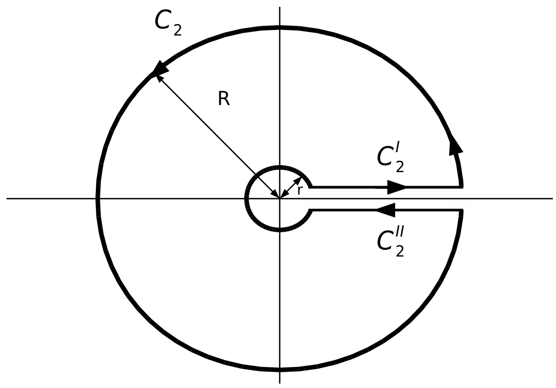

Fig. 2. Contour integral of Eq. (18).

As a result:

$$P_{(\phi)ijkl} = -\frac{1}{4\imath\pi^2}\int_{C_2} \ln(z)\frac{z\, p_{ijkl}(\xi(z))}{(1+z^2)^2 q(\xi(z))}\,\mathrm{d}z. \tag{18}$$

Let $\mathrm{Img}(z)$ and $\mathrm{Re}(z)$ denote, respectively, the imaginary and real parts of any complex number z. Using Cauchy's theory of residues (see Appendix C), this last integral reads:

$$P_{(\phi)ijkl} = \frac{1}{4\pi}\left(\mathrm{Img}\left(\frac{\imath\, p_{ijkl}(\imath)}{q(\imath)}\right) - \sum_{u=1}^{u=3}\mathrm{Re}\left[\left(2\ln\left(z_u+\sqrt{1+z_u^2}\right)-\imath\pi\right)\frac{p_{ijkl}(z_u)}{(1+z_u^2)^{\frac{3}{2}}q'(z_u)}\right]\right). \tag{19}$$

Finally, the evaluation of Hill's polarization $\boldsymbol{P}$-tensor reduces to the calculation of the following simple integrals:

$$P_{ijkl} = \frac{1}{8\pi}\int_0^{2\pi}\left(\mathrm{Img}\left(\frac{\imath p_{ijkl}(\imath)}{q(\imath)}\right) - \sum_{u=1}^{u=3}\mathrm{Re}\left[\left(2\ln\left(z_u+\sqrt{1+z_u^2}\right)-\imath\pi\right)\frac{p_{ijkl}(z_u)}{(1+z_u^2)^{\frac{3}{2}}q'(z_u)}\right]\right)\mathrm{d}\phi, \tag{20}$$

where:

- $q(z)$ and $p_{ijkl}(z)$ are polynomial functions of degree six whose coefficients are defined by relations (14) and (17) as a function of the shape of the ellipsoid, the angle ϕ and the moduli tensor ($q'(z)$ denotes the derivative of $q(z)$),
- the three complex numbers (z_1, z_2, z_3) are the complex roots with a positive imaginary part of the sextic equation $q(z) = 0$.

3.3. Additional relations (degenerate cases) for three-dimensional body

General expression (19) is no longer valid for the following degenerate cases. If $\imath$ is one of the root of the sextic equation ($z_3 = \imath$), we define the polynomial function of degree four $\hat{q}$ as $q(z) = (1+z^2)\hat{q}(z)$. The residues theorem gives:

$$\begin{aligned} P_{(\phi)ijkl} = \frac{1}{4\pi}\Bigg(&\mathrm{Img}\left[\frac{3p'_{ijkl}(\imath)\hat{q}(\imath)+p_{ijkl}(\imath)(4\imath\hat{q}(\imath)-3\hat{q}'(\imath))}{6\hat{q}^2(\imath)}\right] \\ &-\sum_{u=1}^{u=2}\mathrm{Re}\left[\left(2\ln\left(z_u+\sqrt{1+z_u^2}\right)-\imath\pi\right)\frac{p_{ijkl}(z_u)}{(1+z_u^2)^{\frac{3}{2}}q'(z_u)}\right]\Bigg). \end{aligned} \tag{21}$$

If $z_1 = z_2 \neq \imath$, the polynomial function of degree four $\hat{q}$ is now defined by $q(z) = (z-z_1)^2(z-\bar{z}_1)^2\hat{q}(z)$ and the valid expression is:

$$P_{(\phi)ijkl} = \frac{1}{4\pi} \quad -\mathrm{Re}\left[\frac{1}{\sqrt{1+z_1^2}}\left(f'_{ijkl}(z_1) - \frac{z_1}{1+z_1^2} f_{ijkl}(z_1)\right)(2\ln(Z_1) - \imath\pi)\right.$$
$$\left. + \frac{2f_{ijkl}(z_1)}{1+z_1^2} + \left(2\ln\left(z_3 + \sqrt{1+z_3^2}\right) - \imath\pi\right)\frac{p_{ijkl}(z_3)}{(1+z_3^2)^{\frac{3}{2}} q'(z_3)}\right] + \mathrm{Img}\left(\frac{\imath p_{ijkl}(\imath)}{q(\imath)}\right)\Bigg), \tag{22}$$

with $f_{ijkl}(z) = \frac{p_{ijkl}(z)}{(1+z^2)(z-\bar{z}_1)^2 \hat{q}(z)}$ and $Z_1 = z_1 + \sqrt{1+z_1^2}$. The degenerate case $z_1 = z_2$ and $z_3 = i$ may easily be deduced from the previous relations (21) and (22). However the case $z_1 = z_2 = i$ has not been investigated. If $z_1 = z_2 = z_3 \neq \imath$, the residues theorem yields:

$$P_{(\phi)ijkl} = \frac{1}{4\pi}\left(\mathrm{Re}\left[Z_2 g'_{(1)ijkl}(Z_1) + Z_1 g'_{(2)ijkl}(Z_2) - \frac{1}{2} g''_{(1)ijkl}(Z_1)(2\ln(Z_1) - \imath\pi)\right] + \mathrm{Img}\left(\frac{\imath p_{ijkl}(\imath)}{q(\imath)}\right)\right) \tag{23}$$

($u = 1, 2 : g_{(u)ijkl} = \frac{\hat{g}_{ijkl}(z)}{(z - Z_{(3-u)})^3}$, $\hat{g}_{ijkl}(z) = \frac{8z^2 p_{ijkl}(\xi(z))}{q_6(1+\xi^2(z))(\xi(z)-\bar{z}_1)^3}$ and $Z_2 = Z_1 - 2\sqrt{1+z_1^2}$) while if $z_1 = z_2 = z_3 = \imath$, the valid expression is:

$$P_{(\phi)ijkl} = \frac{1}{4\pi}\left(\frac{1}{7} p^0_{(1)ijkl} + \frac{2}{35}(p^2_{(1)ijkl} + p^1_{(2)ijkl} + p^0_{(3)ijkl}) + \frac{8}{105}(p^4_{(1)ijkl} + p^3_{(2)ijkl} + p^2_{(3)ijkl} + 6p^4_{(3)ijkl})\right). \tag{24}$$

3.4. Application

Here, we consider a spheroidal inclusion ($a_2 = a_3 = 1$) embedded in an infinite elastic body. This elastic body exhibits a cubic symmetry $\left(\frac{C_{1122}}{C_{1111}} = 0.57, \frac{C_{1212}}{C_{1111}} = 0.49\right)$. In that case, Hill's polarization ***P***-tensor is computed by the two following methods:

- the former (classical) method: the double integrals defined by the relations (12) are computed numerically. In the sequel, N_ϕ and N_θ denote, respectively, the numbers of integration steps over the two Euler angles ϕ and θ.
- the new method proposed in this work: for a given ϕ Euler angle, the integrals $P_{\phi(ijkl)}$ are computed algebraically to reduce the previous double integrals to simple ones over Euler angle ϕ (see the new expression (20)).

Both methods make use of the same numerical method of integration (the trapezoidal rule) with the same required accuracy.

For different aspect ratios a_1/a_3 of the inclusion, the numbers of integrations steps (N_ϕ, N_θ) have been determined to achieve the required accuracy (see Table 1). As expected, the numbers of integration steps increase with the degree of anisotropy. For each value of a_1/a_3, we have also reported on Table 1 the ratio of computation times defined as follows $\zeta = t_2/t_1$ where t_2 and t_1 denote, respectively, the times needed to compute Hill's polarization ***P***-tensor according to the new method and the former one. The following observations can be made:

- The computation time of the double integrals (12) increases as $N_\phi \star N_\theta$ while the simple integrals (20) depend linearly on N_ϕ. As a result, the ζ-ratio depends linearly on $1/N_\theta$ and this ratio decreases significantly when the aspect ratio a_1/a_3 ranges from 1 to 100.

Table 1
Numbers of integration steps (N_ϕ, N_θ) and computation times ratio (ζ) as a function of a_1/a_3

a_1/a_3	1	10	100
N_ϕ	64	256	1024
N_θ	32	128	512
ζ	0.16	0.04	0.011

- When $a_1/a_3 = 1$, the ζ-ratio is upper than $1/N_\theta = 1/32 \approx 0.03$. This result is related to the fact that the algebraic computation of $\boldsymbol{P}_\phi$-tensor requires significantly more operations (approximately 5 times more) than the computation of the integrand of expression (12).

In conclusion, the new proposed expressions turned to be efficient, especially for high degree of anisotropy. In this application, the degree of anisotropy was driven by the shape of the ellipsoidal inclusion. However, high degree of anisotropy should also be encountered for many other applications like homogenization of nonlinear heterogeneous media (see, for instance, Ghahremani, 1977). In all cases, the new expression (20) should improve significantly the computation of Hill's polarization $\boldsymbol{P}$-tensor.

4. Conclusions

In this work, the Cauchy theory of residues was used to derive new expressions of the Hill polarization tensor for general anisotropic bodies. When the body is two-dimensional, the final expression is explicitly given as a function of the roots with a positive imaginary part of a quartic equation (Eq. (9), Section 2). When the body is three-dimensional the double integral (Mura, 1982) is reduced to a simple one, the integrand being a function of the three roots (with a positive imaginary part) of a sextic equation (Eq. (20), Section 3). As expected, this reduction have been shown to improve significantly the computation time needed to evaluate Hill's polarization $\boldsymbol{P}$-tensor, especially when the degree of anisotropy is high (Section 3.4). Exact expressions have also been derived for degenerate cases (see Eqs. (10), (11), (21)–(24)).

Acknowledgments

The author expresses his gratitude to Prof. Andre Zaoui for his encouragement during the course of this work. Dr. Y. Monerie and Dr. M. Bornert are also gratefully acknowledged for their helpful comments.

Appendix A. Additional results for particular bi-dimensional media

If $\boldsymbol{C}$ is a definite positive fourth-order tensor, explicit expressions of the complex conjugate roots of the quartic equations are derived hereafter for particular material symmetry (the "material" axis coincide with the prinicipal axis of the elliptical inclusion). Contracted notations of fourth-order tensors $C_{IJ}(I,J=1,2,3)$ are adopted in this section.

A.1. Orthotropic $\boldsymbol{C}$ tensor

In that case, the non-zero components of the moduli tensor $\boldsymbol{C}$ are

$$C_{11},\ C_{22},\ C_{12}=C_{21},\ C_{33}.$$

Since $\boldsymbol{C}$ is positive definite:

$$C_{11}C_{22}-C_{12}^2>0 \quad C_{33}>0 \quad C_{11}C_{33}>0 \quad C_{22}C_{33}>0,$$

and the quartic equation reduces to a quadratic equation in $Z=z^2$:

$$C_{11}C_{33}+(-2C_{12}C_{33}+C_{11}C_{22}-C_{12}^2)Z+C_{22}C_{33}Z^2=0 \tag{A.1}$$

with positive coefficients. If

$$-2C_{12}C_{33}+C_{11}C_{22}-C_{12}^2-2\sqrt{C_{11}C_{33}}\sqrt{C_{22}C_{33}} \tag{A.2}$$

is negative, this quadratic equation displays complex conjugate roots. Denoting by Z_1 the root with positive imaginary part, the four roots of the quartic Eq. (6) are:

$$z_1=\sqrt{Z_1}, \quad z_2=-\bar{z}_1, \quad z_3=\bar{z}_1, \quad z_4=\bar{z}_2.$$

Alternatively, if expression (A.2) is positive, the four roots of the quartic equation are given by:

$$z_1 = \imath\sqrt{-Z_r}, \quad z_2 = \imath\sqrt{\frac{C_{11}}{-Z_r C_{22}}}, \quad z_3 = \bar{z}_1, \quad z_4 = \bar{z}_2,$$

where Z_r denotes one of the two real (negative) roots of the quadratic Eq. (A.1). If expression (A.2) is zero, the quartic display two roots (degenerate case) $z_1 = z_2 = \imath(\frac{C_{11}}{C_{22}})^{\frac{1}{4}}, z_3 = z_4 = \bar{z}_1$.

*A.2. Quadratic **C** tensor*

The additional relation $C_{11} = C_{22}$ holds in that case. If $Z = z + \frac{1}{z}$, the quartic equation reduces to

$$Z^2 + c = 0,$$

with:

$$c = \frac{C_{11}^2 - 2C_{12}C_{33} - C_{12}^2}{C_{11}C_{33}} - 2 = 2\frac{(\frac{1}{2}(C_{11} - C_{12}) - C_{33})(C_{11} + C_{12})}{C_{11}C_{33}}.$$

If $c > 0$, the fourth roots of the quartic equation are pure imaginary numbers, namely:

$$z_1 = \imath(\sqrt{4+c} - \sqrt{c}), \quad z_2 = \imath(\sqrt{4+c} + \sqrt{c}), \quad z_3 = -z_1 = \bar{z}_1, \quad z_4 = -z_2 = \bar{z}_2,$$

while the case $c < 0$ yields:

$$z_1 = \frac{1}{2}(\sqrt{-c} + \imath\sqrt{4+c}), \quad z_2 = \frac{1}{2}(-\sqrt{-c} + \imath\sqrt{4+c}), \quad z_3 = \bar{z}_1,\ z_4 = \bar{z}_2.$$

The case $\frac{1}{2}(C_{11} - C_{12}) - C_{33} = 0$ corresponds to a transversely isotropic $\boldsymbol{C}$ tensor (this is equivalent to the isotropic case for two-dimensional media). In this degenerate case the determinant of $\boldsymbol{A}_{2d}$ reduces to the constant $q_{0(2d)}$.

Appendix B. Additional results for orthotropic $\boldsymbol{C}$ tensor (three-dimensional media)

Contracted notations of fourth-order tensors are adopted in this section (for instance: $C_{23} = C_{2233}$, $C_{45} = C_{2313}$, $C_{16} = C_{1112}\ldots$). If the moduli tensor exhibits an orthotropic symmetry (with respect to the principal axis of the ellipsoidal inclusion), the following elastic stiffness vanish:

$$C_{14} = C_{24} = C_{34} = C_{15} = C_{25} = C_{35} = C_{45} = C_{16} = C_{26} = C_{36} = C_{46} = C_{56} = 0.$$

The matrices $\boldsymbol{Q}$, $\boldsymbol{S}$ and $\boldsymbol{T}$ are symmetric. Their remaining non zero components are:

$$\begin{aligned}
&Q_{11} = C_{55}n_3^2, \quad Q_{22} = C_{44}n_3^2, \quad Q_{33} = C_{33}n_3^2,\\
&S_{13} = (C_{55} + C_{31})m_1 n_3, \quad S_{23} = (C_{44} + C_{32})m_2 n_3,\\
&T_{11} = C_{11}m_1^2 + C_{66}m_2^2, \quad T_{22} = C_{66}m_1^2 + C_{22}m_2^2,\\
&T_{12} = (C_{12} + C_{66})m_1 m_2, \quad T_{33} = C_{55}m_1^2 + C_{44}m_2^2.
\end{aligned}$$

Further, the sextic equation reads: $q(z) = q_6 z^6 + q_4 z^4 + q_2 z^2 + q_0 = 0$, where

$$\begin{aligned}
&q_6 = Q_{11}Q_{22}Q_{33}, \quad q_4 = Q_{11}(Q_{22}T_{33} - S_{32}S_{23} + T_{22}Q_{33}) - S_{31}Q_{22}S_{13} + T_{11}Q_{22}Q_{33}\\
&q_2 = Q_{11}T_{22}T_{33} + S_{31}(T_{12}S_{23} - T_{22}S_{13}) + T_{11}(Q_{22}T_{33} + T_{22}Q_{33} - S_{32}S_{23})\\
&\qquad + T_{21}(S_{32}S_{13} - T_{12}Q_{33}), \quad q_0 = (T_{11}T_{22} - T_{12}^2)T_{33}.
\end{aligned}$$

This sextic equation can be easily reduced to a cubic equation in z^2 (algebraic resolution with the Cardan-Tartaglia method).

Appendix C. Derivation of relation (19)

Consider the rational function:

$$z \to \frac{z\, p_{ijkl}(\xi(z))}{(1+z^2)^2 q(\xi(z))}.$$

Obviously, $(\imath, -\imath)$ are poles of this rational function. Let $Z_1 = z_1 + \sqrt{1+z_1^2}, Z_2 = z_1 - \sqrt{1+z_1^2}, \ldots, Z_6 = z_3 - \sqrt{1+z_3^2}$ and since $q(\xi(Z_i)) = q(z_i) = 0 = q(\bar{Z}_i)$, the six complex numbers $(Z_1, \ldots, Z_6)$ and their complex conjugates are also poles of this function. As a result, the following development holds:

$$\frac{z\, p_{ijkl}(\xi(z))}{(1+z^2)^2 q(\xi(z))} = \sum_{i=1}^{i=6}\left(\frac{a(Z_i)}{z - Z_i} + \frac{a(\bar{Z}_i)}{z - \bar{Z}_i}\right) + \frac{a(\imath)}{z-\imath} + \frac{b(\imath)}{(z-\imath)^2} + \frac{a(-\imath)}{z+\imath} + \frac{b(-\imath)}{(z+\imath)^2}$$

with $(1 \leqslant i \leqslant 6)$:

$$\begin{aligned}
a(Z_i) &= \frac{Z_i p_{ijkl}(\xi(Z_i))}{(1+Z_i^2)^2 \lim_{z\to Z_i}\left(\frac{\mathrm{d}}{\mathrm{d}z}(q(\xi(z)))\right)} \\
&= \frac{1}{4}\left(\frac{2Z_i}{Z_i^2+1}\right)^3 \frac{p_{ijkl}(\xi(Z_i))}{q'(\xi(Z_i))}, \quad a(\bar{Z}_i) = \bar{a}(Z_i), \\
a(\imath) &= \lim_{z\to i}\left(\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{z p_{ijkl}(\xi(z))}{(z+\imath)^2 q(\xi(z))}\right)\right) \\
&= \lim_{z\to i}\quad \frac{\imath - z}{(z+\imath)^3}\frac{p_{ijkl}(\xi(z))}{q(\xi(z))} + \frac{z^2+1}{2z(z+\imath)^2}\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{p_{ijkl}(\xi(z))}{q(\xi(z))}\right)\Bigg) = 0 = a(-\imath) \\
b(\imath) &= \lim_{z\to i}\frac{z p_{ijkl}(\xi(z))}{(z+\imath)^2 q(\xi(z))} = -\frac{\imath p_{ijkl}(\imath)}{4q(\imath)}, \quad b(-\imath) = \bar{b}(\imath).
\end{aligned}$$

To proceed further, we consider the integrand $z \to \ln(z)\frac{z p_{ijkl}(\xi(z))}{(1+z^2)^2 q(\xi(z))}$ (the right term of (18)) to derive (Cauchy's theory of residues) the following algebraic result:

$$\boldsymbol{P}_{(\phi)ijkl} = \frac{1}{\pi}\quad \mathrm{Img}\left(\imath\frac{p_{ijkl}(\imath)}{4q(\imath)}\right) - \sum_{i=1}^{i=6}\mathrm{Re}(\ln(Z_i)a(Z_i))\Bigg). \tag{C.1}$$

Since $Z_{2i-1}Z_{2i} = -1$ $(1 \leqslant i \leqslant 3)$, the poles Z_i satisfy:

$$\frac{2Z_{2i}}{Z_{2i}^2+1} = -\frac{2Z_{2i-1}}{Z_{2i-1}^2+1} \Rightarrow a(Z_{2i}) = -\frac{1}{4}\left(\frac{2Z_{2i-1}}{Z_{2i-1}^2+1}\right)^3 \frac{p_{ijkl}(\xi(Z_{2i}))}{q'(\xi(Z_{2i}))}.$$

Since $\xi(Z_{2i-1}) = z_i = \xi(Z_{2i})$ and $\ln(Z_{2i-1}) + \ln(Z_{2i}) = \imath\pi$, the right term of (C.1) can be further simplified as follows:

$$\begin{aligned}
\sum_{i=1}^{i=6}\mathrm{Re}(\ln(Z_i)a(Z_i)) &= \sum_{i=1}^{i=3}\mathrm{Re}(\ln(Z_{2i-1})a(Z_{2i-1}) + \ln(Z_{2i})a(Z_{2i})) = \sum_{i=1}^{i=3}\mathrm{Re}((2\ln(Z_{2i-1}) - \imath\pi)a(Z_{2i-1})) \\
&= \sum_{i=1}^{i=3}\mathrm{Re}\quad (2\ln(Z_{2i-1}) - \imath\pi)\frac{1}{4}\left(\frac{2Z_{2i-1}}{Z_{2i-1}^2+1}\right)^3\frac{p_{ijkl}(z_i)}{q'(z_i)}\Bigg).
\end{aligned}$$

Substituting $z_i^2 + 1 = ((Z_{2i-1}^2+1)/(2Z_{2i-1}))^2$ in the latest relation yields the final expression (19).

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