Performance Testing of the STAFF Spectrum Analyser

using

A Simulated Wave Field with known Stokes' Parameters

C.C. Harvey,

M. Belkacemi & B. Pairault

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1 Introduction

The Stokes' parameters Q, U, and V describe fully the polarisation state of a plane electromagnetic wave (*Lecacheux et al.* (1979)). These three parameters are entirely equivalent to the following three parameters: degree of polarisation, degree of ellipticity, and orientation of the principle axis of the polarisation ellipse.

Stokes' parameters are traditionally used for describing electromagnetic waves propagating in free-space, and they are normally defined with respect to the electric field. In free space, the two characteristic modes of wave propagation are degenerate (they satisfy the same dispersion relation), and therefore the wave polarisation is arbitrary. In an anisotropic medium this is not the case: the wave polarisation is imposed by the characteristics of the ambient medium, and Stokes' parameters are not generally used.

In this document we describe tests performed upon the STAFF Spectrum Analyser. This instrument measures the 5×5 correlation matrix formed using three components of the magnetic field and two components of the waves electric field. We simulate data using simple waves with the characteristics of an electromagnetic wave propagating in free space, and then analyse this data with the instrument. But this instrument is designed for, and will be used in, the more general anisotropic plasma environment. Therefore we need to change slightly the definition of Stokes' parameters, for the following reason.

In free space, the wave electric field is perpendicular to the direction of propagation; in an anisotropic medium, this is not generally the case. However, the magnetic field always satisfies Maxwell's equation

$$\frac{\partial \mathbf{B}}{\partial t} = -\text{curl } \mathbf{E}$$

which, for a plane wave, gives

$$\mathbf{B} = -\mathbf{k} \times \mathbf{E}/\omega \ . \tag{1}$$

Clearly the magnetic field $\mathbf{B}$ is perpendicular to the wave vector $\mathbf{k}$ even in an anisotropic medium, except near a resonance, where the electric field becomes longitudinal (parallel to $\mathbf{k}$), and $\mathbf{B}$ falls to zero.

Therefore we define the Stokes' parameters Q, U, and V in terms of the magnetic field. This suggestion is not original: the magnetic field is also generally used for describing the wave polarisation state in magneto-ionic theory (*Ratcliffe* (1962)). Note that there is no reason why this definition can not be used for during data analysis, it is perfectly possible to determine the (magnetic) Stokes' parameters of a magnetohydrodynamic wave. Indeed, the magnetic Stokes' parameters are a convenient quantitative representation of the "hodograms" frequently drawn by space plasma physicists; they contain useful information which can be compared, for example, with the values of the same parameters derived from plasma models or numerical simulations.

Use of the magnetic Stokes' parameters has another great advantage for the STAFF Spectrum Analyser: the instrument does measure all three components of the magnetic field.

1.1 Coordinate System

There is considerable confusion concerning coordinate systems. Traditionally in space plasma physics the z-axis is used to denote a direction close to the spacecraft spin axis, such as the spin axis itself when using spacecraft coordinates, or the direction of the north Ecliptic pole when using GSE coordinates. But Cluster has defined this as the x-direction. To limit the resulting confusion, we use here an O123 set of othogonal axes, with the spacecraft spin parallel to the O3-axis. The correspondance between Cluster coordinates and the present coordinate system is

$$B_x = B_3, \quad B_y = B_1, \quad \text{and} \quad B_z = B_2 \ .$$

The STAFF sensors measure B_1, B_2, B_3, E_1 and E_2.

2 Generation of the Wave

We generate a wave propagating at latitude θ with respect to the O12-plane and longitude ϕ measured from the O1-axis. The wave is polarised with Stokes' parameters Q, U, and V. We start by generating the fully polarised wave ($Q^2 + U^2 + V^2 = 1$), then we add noise.

2.1 The fully polarised wave

If the wave were propagating along the $O1$-axis, *i.e.*, the direction $\theta = 0, \phi = 0$, it would have the magnetic and electyric fields given by

$$\left.\begin{array}{rcl} B_k &=& B_k^{(u)}\cos(\omega t) + B_k^{(v)}\sin(\omega t) \\ E_k &=& E_k^{(u)}\cos(\omega t) + E_k^{(v)}\sin(\omega t) \end{array}\right\} \tag{2}$$

where $E_k^{(u)}$ and $E_k^{(v)}$ are given by equation 8 below, and the vectors $B_k^{(u)}$ and $B_k^{(v)}$ are given in terms of the unit vectors

$$e_k^1 = \begin{pmatrix} e_1^1 \\ e_2^1 \\ e_3^1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \text{and} \quad e_k^2 = \begin{pmatrix} e_1^2 \\ e_2^2 \\ e_3^2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{3}$$

by

$$\left.\begin{array}{rcl} B_k^{(u)} &=& \cos\alpha\ (\ \ \cos\xi\ e_k^1 + \sin\xi\ e_k^2) \\ B_k^{(v)} &=& \sin\alpha\ (-\sin\xi\ e_k^1 + \cos\xi\ e_k^2) \end{array}\right\} \tag{4}$$

where (*Lecacheux et al.* (1979))

$$\alpha = \frac{1}{2}\tan^{-1}\left(\frac{V}{\sqrt{Q^2+U^2}}\right) , \tag{5}$$

$$\xi = \frac{1}{2}\tan^{-1}(U,Q) , \tag{6}$$

where $\tan^{-1}(U,Q)$ is the function (well-known to FORTRAN programmers) with the value $\tan^{-1}(U/Q)$ when $Q \geq 0$ and $\pi + \tan^{-1}(U/Q)$ when $Q \leq 0$). For a fully polarised waved,

$$Q^2 + U^2 + V^2 = 1 .$$

At this point it is helpful to note some simple cases. The table below shows the polarisation of a wave propagating in the $\theta = 0, \phi = 0$ direction with particular values of the Stokes' parameters.

$Q = +1$,	$U = 0$,	$V = 0$	linear polarisation in the equatorial plane
$Q = -1$,	$U = 0$,	$V = 0$	linear polarisation in the meridian plane
$Q = 0$,	$U = +1$,	$V = 0$	linear polarisation in the 45° plane
$Q = 0$,	$U = -1$,	$V = 0$	linear polarisation in the −45° plane
$Q = 0$,	$U = 0$,	$V = +1$	right circular polarisation
$Q = 0$,	$U = 0$,	$V = -1$	left circular polarisation

The electric field is given by Maxwell's equation

$$\epsilon_0\epsilon\frac{\partial \mathbf{E}}{\partial t} = \text{curl } \mathbf{H}$$

which Fourier transforms to

$$\epsilon_0\epsilon\mathbf{E} = \mathbf{k}\times\mathbf{B}/\mu_0\omega .$$

Note that if ϵ is anisotropic, then $\mathbf{E}$ will not be perpendicular to $\mathbf{k}$. In an isotropic medium, taking

$$c^2 = \frac{1}{\mu_0\epsilon_0} = 1 , \tag{7}$$

we obtain

$$E_i^{(u)} = \epsilon_{ijk}k_jB_k^{(u)} \quad \text{and} \quad E_i^{(v)} = \epsilon_{ijk}k_jB_k^{(v)} \tag{8}$$

where ϵ_{ijk} is the permutation operator. Written explicitly, this is

$$\left.\begin{array}{llll} E_1^{(u)} = & 0 & E_1^{(v)} = & 0 \\ E_2^{(u)} = & -B_3^{(u)} & E_2^{(v)} = & -B_3^{(v)} \\ E_3^{(u)} = & B_2^{(u)} & E_3^{(v)} = & B_2^{(v)} . \end{array}\right\} \tag{9}$$

To rotate to a coordinate system with the wave propagation direction at latitude θ, we rotate about the O2-axis by contracting $E_k^{(u)}$, $E_k^{(v)}$, $B_k^{(u)}$, and $B_k^{(v)}$ with

$$S_{jk} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix} = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix} . \tag{10}$$

To rotate the wave propagation direction to longitude ϕ, we rotate about the O3-axis by contracting with

$$T_{ij} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{11}$$

Thus, eq. 2 becomes

$$\left.\begin{aligned} \mathcal{E}_i(t) &= \mathcal{E}_i^{(u)}\cos(\omega t) + \mathcal{E}_i^{(v)}\sin(\omega t) \\ \mathcal{B}_i(t) &= \mathcal{B}_i^{(u)}\cos(\omega t) + \mathcal{B}_i^{(v)}\sin(\omega t) \end{aligned}\right\} \tag{12}$$

with

$$\left.\begin{aligned} \mathcal{E}_i^{(u)} &= T_{ij}S_{jk}E_k^{(u)} \\ \mathcal{E}_i^{(v)} &= T_{ij}S_{jk}E_k^{(v)} \\ \mathcal{B}_i^{(u)} &= T_{ij}S_{jk}B_k^{(u)} \\ \mathcal{B}_i^{(v)} &= T_{ij}S_{jk}B_k^{(v)} \end{aligned}\right\} \tag{13}$$

These four vectors need be computed only once; then the wave fields $\mathcal{E}_k(t)$ and $\mathcal{E}_k(t)$ can be computed at successive times t from eq. 12.

It is important to note that after these two successive rotations of axes, the Stokes' parameters Q and U are defined with respect to the intersection of the plane of the wave front and the equatorial plane.

2.2 The addition of noise

The total power in the electric and magnetic components of the fully coherent wave of eq. 12 are respectively

$$\Sigma_{i=1}^3 \mathcal{E}_i^2 = \frac{1}{2}W^2 \quad \text{and} \quad \Sigma_{i=1}^3 \mathcal{B}_i^2 = \frac{1}{2}W^2 \tag{14}$$

where

$$W^2 = Q^2 + U^2 + V^2 . \tag{15}$$

The electric and magnetic field powers are the same simply because the electric field is measured in units of cB (nanoTesla $\times$ velocity of light), so as to obtain eq. 7.

Noise may be included by adding random signals to each of the field components given by eq. 12. The degree of polarisation is the fraction m of the total wave power in that mode (*Lecacheux et al.* (1979)). If each of the random signals added to the five inputs has the same variance $W/3$, the signal/noise ratio will be unity and the degree of polarisation $m = \frac{1}{2}$; other signal/noise ratios may be produced by changing this variance. If the noise signals added to the different sensors do not all have the same variance, the definition (and calculation) of the signal/noise ratio is more complicated; but its effect upon the measurements is very interesting, it will perturb the determination of both the direction θ, ϕ, and the Stokes' parameters Q, U and V.

3 Interpretation of the Results

The output from the spectrum analyser should be analysed using the methods proposed respectively by McPherron, Means, and Samson, and also by examination of the wave distribution function. All these methods fail, like any other, when the Stokes' V parameter is zero.

3.1 The minimum variance method

McPherron et al. (1972) have proposed that the real part of the cross-spectral matrix S_{ij} be diagonalised and that the eigenvector assocaited with the smallest eigenvalue be used as an approximation to the direction of propagation of the principal component of the wave spectrum.

3.2 Means' method

Means (1972) method of determining the direction of propagation in effect diagonalises the imaginary part of the S_{ij}. Writing this as $\begin{pmatrix} 0 & ix_3 & -ix_2 \\ -ix_3 & 0 & ix_1 \\ ix_2 & -ix_1 & 0 \end{pmatrix}$, the eigenvector (x_1, x_2, x_3), the only one with eigenvalue 0, is taken to be the direction of wave propagation.

3.3 The maximum variance method

Samson (*Samson*, 1973; *Samson and Olsen*, 1980) has suggested a method which uses both the real and the imaginary parts of S_{ij}. This method yields an estimate of the wave normal direction, an estimates of both the size and the orientation the corresponding error ellipse, and an evaluation of the possibility that the given S_{ij} can actually represent a monochromatic plane wave superimposed on isotropic noise. Details of the method are in the Appendix.

The plan of calculation is as follows:

1. Diagonalize the Hermitian matrix S_{ij} to obtain the eigenvectors and eigenvalues arranged in ascending order, $\lambda^{(1)} \leq \lambda^{(2)} \leq \lambda^{(3)}$.

2. The polarisation is
$$P = \frac{\lambda^{(3)} - \lambda^{(2)}}{\lambda^{(1)} + \lambda^{(2)} + \lambda^{(3)}} . \tag{16}$$

3. The quality of the representation is
$$R = 1 - \frac{2(\lambda^{(2)} - \lambda^{(1)})}{\lambda^{1} + \lambda^{2} + \lambda^{3}} . \tag{17}$$

4. The next step is to renormalise the eigenvector $u_i^{(3)}$ corresponding to the largest eigenvalue, and separate it into its real and imaginary parts $r_i^{(a)}$ and $r_i^{(b)}$, as follows:
$$r_i^{(a)} + i r_i^{(b)} = u_i^{(3)} \left[\frac{\left(u_i^{(3)} u_i^{(3)}\right)^2}{\left|u_i^{(3)} u_i^{(3)}\right|^2} \right]^{-\frac{1}{4}} . \tag{18}$$
There are four possible values for the root; one (of the two) which yield $|r_i^{(a)}| \geq |r_i^{(b)}|$ should be chosen.

5. Provided that $r_i^{(b)} r_i^{(b)} \neq 0$, the direction of propagation is
$$\hat{k}_i = k_i \;/\; |k| \qquad \text{where} \qquad k_i = \epsilon_{ijk} r_j^{(a)} r_k^{(b)} . \tag{19}$$
Note that the sense of $\hat{k}_i$ is indeterminate, it depends upon which one (of the two) possible solutions has been chosen at step 4.

6. The axes of the standard error ellipse have semi-lengths (in radians) of
$$\frac{\lambda^{(1)} + 2\lambda^{(2)}}{\lambda^{(3)} - \lambda^{(2)}} \frac{1}{|r^{(a)}|} \qquad \text{and} \qquad \frac{\lambda^{(1)} + 2\lambda^{(2)}}{\lambda^{(3)} - \lambda^{(2)}} \frac{1}{|r^{(b)}|} \tag{20}$$
(N.B., these expressions need better justification.) and the major axis is oriented towards the direction $r_i^{(a)}$.

7. Stokes' parameters are given by
$$\left.\begin{array}{rcl} Q & = & P \cos 2\alpha \cos 2\xi \\ U & = & P \cos 2\alpha \sin 2\xi \\ V & = & P \sin 2\alpha \end{array}\right\} \tag{21}$$

where P is given by equation 16 and

$$\tan\alpha = \frac{\left|k, r^{(a)}, r^{(b)}\right|}{|k|\ \left|r^{(a)}\right|^2} \qquad \text{and} \qquad \tan\xi = \frac{\left(k_1^2 + k_2^2\right) r_3^{(a)} - k_3\left(k_1 r_1^{(a)} + k_2 r_2^{(a)}\right)}{|k|\left(k_1 r_2^{(a)} - k_2 r_1^{(a)}\right)}\,. \tag{22}$$

It was noted (at step 5) that the direction of $\hat{k}_i$ is indeterminate; we assumed that $\hat{k}_i$, $r_j^{(a)}$, and $r_k^{(b)}$ form (eq. 19) a right orthogonal triad. They could form a left orthogonal triad, or we could have chosen the alternative solution at step 4. If there is some physical reason to inverse the sense of $\hat{k}_i$, then V must be replaced by $-V$ and U replaced by $-U$, while Q remains unchanged.

4 Test Plan

Complete testing of the spectrum analyser requires simulation of waves in different directions, for several values of Q, U and V. Five values (*e.g.*, -1, $-\frac{1}{2}$, 0, $+\frac{1}{2}$, $+1$) of each of Q, U and V would alone require $5^3 = 125$ simulations *for each direction* θ, ϕ. Clearly it is impossible to perform a systematic and complete simulation; a rather sparce simulation must be conducted, with the intention exploring which is not understood or which seems in any way anomalous on a case-by-case basis.
The following test plan is therefore proposed:

- perform simulations for the two values 0 and $+\frac{1}{2}$ of each of Q, U and V (yielding $2^3 = 8$ simulations for each direction θ, ϕ);
- perform simulations at four latitudes θ, with corresponding longitudes ϕ as shown in the table. It is assumed that there is symmetry in the four quadrants of ϕ; and in the first quadrant, there should be symmetry about the direction $\phi = 45°$, so that the simulations of values of ϕ in *italics* are of lower priority.

θ	Corresponding values of ϕ
0	0, 15, 30, 45, *60, 75, 90*
30	0, 18, 36, *54, 72, 90*
60	0, 30, *60, 90*
90	0

The angular separation in the θ direction is approximately twice the angular separation in the ϕ direction.

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5 Appendix

Any Hermitian matrix can be expressed in terms of its eigenvalues and eigenvectors, thus:

$$S_{ij} = \sum_{\lambda=1}^{3} \lambda^{(\lambda)} u_i^{(\lambda)} u_j^{*(\lambda)}$$

where $u_i^{(\lambda)}$ is the eigenvector corresponding to the eigenvalue $\lambda^{(\lambda)}$. Thus the information content of the eigenvalues and eigenvectors is identical to that of S_{ij}. In the reference frame defined by its eigenvectors, S_{ij} is diagonal,

$$S_{ij} = \begin{pmatrix} \lambda^{(1)} & 0 & 0 \\ 0 & \lambda^{(2)} & 0 \\ 0 & 0 & \lambda^{(3)} \end{pmatrix} .$$

For a pure monochromatic wave, S_{ij} has only one non-zero eigenvalue. In the general case, let the eigenvalues be ordered $\lambda^{(1)} \leq \lambda^{(2)} \leq \lambda^{(3)}$. Then S_{ij} may be expressed

$$S_{ij} = \lambda^{(1)} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (\lambda^{(2)} - \lambda^{(1)}) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (\lambda^{(3)} - \lambda^{(2)}) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The first term is the contribution from fully isotropic uncorrelated (unpolarised) noise, and the last term is the contribution from a fully polarised wave. The proportion of the power in the fully polarised wave is

$$P = \frac{\lambda^{(3)} - \lambda^{(2)}}{\lambda^{(1)} + \lambda^{(2)} + \lambda^{(3)}} . \tag{23}$$

The middle term can be used as an indicator of the feasibility of interpreting S_{ij} as a fully polarised wave in the presence of isotropic noise, for example, by the parameter

$$R = 1 - \frac{2(\lambda^{(2)} - \lambda^{(1)})}{\lambda^{1} + \lambda^{2} + \lambda^{3}} . \tag{24}$$

Both P and R lie in the range $0 \leq P, R \leq 1$. $P = 1$ corresponds to 100% polarisation of the signal (implying no noise). R indicates whether S_{ij} can represent a monochromatic plane wave superimposed on isotropic noise; the closer R is to unity the better. A high value of R is a necessary but not a sufficient condition to be able to determine that the wave normal direction: in particular, $r_i^{(b)}$ (see below) may be zero.

If $u_i^{(3)}$ is an eigenvector corresponding to the largest eigenvalue of S_{ij}, then so is $e^{i\phi} u_i^{(3)}$. Let us write

$$e^{i\phi} u_i^{(3)} = r_i^{(a)} + i r_i^{(b)} \tag{25}$$

where $r_i^{(a)}$ and $r_i^{(b)}$ are two vectors in real space. The phase factor $e^{i\phi}$ may be chosen so that $r_i^{(a)}$ and $r_i^{(b)}$ are mutually orthogonal:

$$\begin{aligned} 0 = r_i^{(a)} r_i^{(b)} &= \mathcal{R}e\{e^{i\phi} u_i^{(3)}\} \mathcal{I}m\{e^{i\phi} u_i^{(3)}\} \\ &= \left(e^{i\phi} u_i^{(3)} + e^{-i\phi} u_i^{*(3)}\right) \left(e^{i\phi} u_i^{(3)} - e^{-i\phi} u_i^{*(3)}\right) \\ &= e^{2i\phi} u_i^{(3)} u_i^{(3)} - e^{-2i\phi} \left(u_i^{(3)} u_i^{(3)}\right)^* \quad , \end{aligned}$$

which is satisfied if

$$e^{-4i\phi} = \frac{u_i^{(3)} u_i^{(3)}}{\left(u_i^{(3)} u_i^{(3)}\right)^*} = \frac{\left(u_i^{(3)} u_i^{(3)}\right)^2}{\left|u_i^{(3)} u_i^{(3)}\right|^2} . \tag{26}$$

This equation for ϕ has four solutions; they correspond to a pair of vectors $r_i^{(a)}$ and $r_i^{(b)}$, another pair anti-parallel to the first pair, and the same pairs with $r_i^{(a)}$ and $r_i^{(b)}$ interchanged. These changes are not important, there are effectively only two real vectors $r_i^{(a)}$ and $r_i^{(b)}$; and we may conveniently choose the solution with $|r_i^{(a)}| \geq |r_i^{(b)}|$. Then, for a sinusoidal wave, $r_i^{(a)}$ and $r_i^{(b)}$ define the plane of the magnetic field, $r_i^{(a)}$ is in the direction of the major axis, $r_i^{(b)}$ is in the direction of the minor axis, and the ratio of the axes is $|r^{(b)}|/|r^{(a)}|$. The direction of propagation

$$\hat{k}_i = k_i \;/\; |k| \qquad \text{where} \qquad k_i = \epsilon_{ijk} r_j^{(a)} r_k^{(b)} \,. \tag{27}$$

may be determined, provided that $r_k^{(b)}$ is not too small.

Finally, we determine the Stokes' parameters Q, U and V via the angles α and ξ. $\tan\alpha$ is the ratio of the minor to the major axis of the polarisation ellipse, taking into account the sense of the polarisation with respect to the direction $\hat{k}$ as determined by the argument of eq. (25). The sense of $r_i^{(b)}$ is arbitrary depending upon which root of eq. (26) has been chosen, but once a root has been selected, the sense of $\hat{k}$ is determined with respect to $r_i^{(a)}$ and the (arbitrarily) chosen $r_i^{(b)}$. The vectors $\epsilon_{ijk}\hat{k}_j r_k^{(a)}$, $r^{(a)}$ and $\hat{k}$ form a right-handed orthogonal triad; therefore $\epsilon_{ijk}\hat{k}_j r_k^{(a)}$ is either parallel or antiparallel to $r^{(b)}$. Consequently, α may is determined in both magnitude and sign by

$$\tan\alpha = \frac{\left|\hat{k}, r^{(a)}, r^{(b)}\right|}{\left|r^{(a)}\right|^2} \,.$$

ξ is the angle between $r_i^{(a)}$ and the intersection of the plane of the wave with the equatorial plane. This intersection lies in the direction

$$\hat{e}_i = \frac{1}{\sqrt{(k_1^2 + k_2^2)}}\,(-k_2, k_1, 0)$$

where the sense of $\hat{e}_i$ has been chosen so that $\hat{e}_i$, the O3 axis, and $\hat{k}_i$ form a right-handed (although not orthogonal) triad. Then ξ is the angle of rotation from $\hat{e}_i$ to $r_i^{(a)}$ about the $\hat{k}_i$ direction. To determine this angle completely (*i.e.*, $-\pi < \xi \le \pi$) we need both $\cos\xi$ and $\sin\xi$; these are given by

$$\cos\xi = \frac{\hat{e}_i r_i^{(a)}}{\left|r^{(a)}\right|} \qquad \text{and} \qquad \sin\xi = \frac{\left|\hat{e}, r^{(a)}, k\right|}{\left|r^{(a)}\right| |k|} = \begin{vmatrix} \hat{e}_1 & r_1^{(a)} & k_1 \\ \hat{e}_2 & r_2^{(a)} & k_2 \\ \hat{e}_3 & r_3^{(a)} & k_3 \end{vmatrix} \Bigg/ \left|r^{(a)}\right| |k| \,.$$

We require the principle value of ξ (in the range $-\pi/2 < \xi \le \pi/2$), given by

$$\tan\xi = \frac{\left(k_1^2 + k_2^2\right) r_3^{(a)} - k_3\left(k_1 r_1^{(a)} + k_2 r_2^{(a)}\right)}{|k|\left(k_1 r_2^{(a)} - k_2 r_1^{(a)}\right)}$$