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To cite this version:
Claude Esling, Jacques Muller, Hans-Joachim Bunge. An integral formula for the even part of the texture function or ” the apparition of the $f\pi$ and $f\omega$ ghost distributions ”. Journal de Physique, 1982, 43 (2), pp.189-195. <10.1051/jphys:01982004302018900>. <jpa-00209388>

HAL Id: jpa-00209388
https://hal.archives-ouvertes.fr/jpa-00209388
Submitted on 1 Jan 1982

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An integral formula for the even part of the texture function

or

« The apparition of the \( f_{II} \) and \( f_{I} \) ghost distributions »

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Résumé. — Dans un récent travail [1], l'utilisation de méthodes efficaces de la théorie des groupes a permis d'établir une formule d'inversion des figures de pôles que S. Matthies avait proposée, sans justification, dans une note brève [2]. Comme les figures de pôles expérimentales sont centrosymétriques soit par la centrosymétrie des cristaux, soit par effet de la loi de Friedel, l'application de cette formule d'inversion ne détermine que la partie paire \( f(g) \) de la fonction de texture.

L'utilisation des mêmes méthodes de centralisation a permis d'établir, au prix d'un minimum de calculs, une formule intégrale exprimant \( f(g) \) en fonction de \( f(g) \). Ainsi, il est rigoureusement démontré que \( f(g) \) ne restitue que la moitié de \( f(g) \), flanquée de deux distributions fantômes \( f_0 \) et \( f_9 \). Dans sa note brève [2], S. Matthies avait proposé une formule similaire, avec toutefois un ordre différent pour les intégrales multiples du terme \( f_9 \). Notre travail montre que l'ordre d'intégration donné par S. Matthies, respecté littéralement, peut conduire à la divergence du terme \( f_9 \).

Enfin, le présent travail montre que l'interprétation des fantômes \( f_{II} \) et \( f_I \) devient particulièrement manifeste en termes de fonctions généralisées.

Abstract. — A recent work [1], using efficient group theory methods, has established an inversion formula for pole figures which had been proposed, but not justified, by S. Matthies [2]. Since the experimental pole figures are centrosymmetrical either by the centrosymmetry of the crystals or by virtue of Friedel's law, the application of this inversion formula determines only the even part \( f(g) \) of the texture function.

The use of the same centralization methods has established, with minimal calculation, an integral formula expressing \( f(g) \) in terms of \( f(g) \). So, it is rigorously proved that \( f(g) \) makes restitution only of the half of \( f(g) \), flanked by two ghost distributions \( f_{II} \) and \( f_{I} \). In his short note [2], S. Matthies had suggested a similar formula, but for a different order of the multiple integrals in the term \( f_{I} \). Our work shows that the integration sequence as given by S. Matthies, if formally obeyed, can lead to the divergence of the term \( f_{I} \).

The present work also shows that the interpretation of the ghosts \( f_{II} \) and \( f_{I} \) becomes obvious in terms of generalized functions.

1. Introduction. — It is at present well established that pole figures allow a straightforward determination of the even part \( f(g) \) of the texture function [1-3]. As these experimental pole figures are centrosymmetrical either by the centrosymmetry of the crystals or by virtue of Friedel's law, they do not contain, from the strictly mathematical point of view, any information on the odd part \( f(g) \). However,
pole figures which present large null domains supply indirectly information on the odd part \( \tilde{f} \), since the positivity condition:

\[
\tilde{f}(g) + \tilde{f}(g) > 0
\]

(1)
turns into an equality for the null domains in the orientation space [4]. Considering this difficulty in principle, it is worthwhile expressing \( \tilde{f}(g) \) in terms of \( f(g) \) by means of an integral relation.

This integral relationship will allow one to study the location and the intensity of the « ghost » components [5, 6] which exist in \( \tilde{f} \) but disappear from the full function \( f \).

2. Notations. — The notations introduced in the previous work on the inversion formula are continued [1]. So \( G \) denotes the SO(3) group of rotation matrices \( g \); the angle \( \omega \) of this rotation is denoted:

\[
\omega = |g|.
\]

(2)
If otherwise \( \sigma \), unitary vector on the sphere \( S_2 \) in the \( \mathbb{R}^3 \)-space, denotes the axis of the rotation \( g \), this latter will be written:

\[
g = e^{i\sigma}.
\]

(3)
A function \( f \) is central when the conjugation relation holds:

\[
f(g') = f(gg'g^{-1}) \quad \forall g \in G.
\]

(4)
It then only depends on \( \cos |g| \), which can be written, for the sake of brevity:

\[
f(g) = f(\cos |g|) = f(|g|) = f(\omega).
\]

(5)
Such a central function can be expanded in a series of characters [3]

\[
f = \sum_{l=0}^{\infty} c_l \chi_l.
\]

(6)
The characters of \( G \):

\[
\chi_l(g) = \sum_{m=-l}^{l} T_l^{(m)}(g) = \frac{\sin(2l+1)\frac{\omega}{2}}{\sin \frac{\omega}{2}} = \chi_l(\omega)
\]

(7)
form a complete system of orthonormal functions in the space of central functions. Taking into account the integration formula on SO(3):

\[
\int_G f(g) \, dg = \frac{2}{\pi} \int_0^{\pi} \, d\omega \sin \frac{\omega}{2} \int_{S_2} d\sigma f(e^{i\sigma})
\]

\[
\int_G \, dg = 1; \quad \int_{S_2} d\sigma = 1
\]

(8)
and the orthonormalization of the characters, the coefficients \( c_l \) of the expansion equation (6) are obtained by:

\[
c_l = \int_G df(g) \chi_l(g) = \frac{2}{\pi} \int_0^{\pi} \, d\omega \sin \frac{\omega}{2} f(\omega) \chi_l(\omega).
\]

(9)

3. Integral expression of the even part \( \hat{f} \) in terms of \( f \). — As for the establishment of the inversion formula [1], the computation of the integral expression for \( f(g) \) can be reduced to the calculation of the value at \( g = 1 \) (identity) for a centralized function [1, 8].

3.1 Reduction to the calculation of the value at the identity for a function \( \tilde{f}^c \). — Let \( \tilde{f}^c \) be the texture function

\[
\tilde{f}^c(g') = f(gg')
\]

(10)
obtained by a rotation \( g \) of the sample fixed coordinate system.

By consideration of the uniqueness of the expansion in generalized spherical harmonics and the addition theorem, it follows that

\[
(\tilde{f}^c) = (\hat{f})^c
\]

(11)
which yields for the identity \( g' = 1 \)

\[
f(g) = \hat{f}(1).
\]

(12)

3.2 Reduction to the calculation of a centralized function. — The centralized function of \( f \) will be defined by

\[
f^c(g') = \int_G df(gg'g^{-1}).
\]

(13)
Taking into account equation (3) and equation (5), the centralized function of \( f \) can be written

\[
f^c(\omega) = f^c(e^{i\omega}) = \int_G df(e^{i\omega})
\]

\[
= \int_G df(e^{i\omega}) = \int_{S_2} d\sigma f(e^{i\sigma})
\]

(14)
where \( \sigma = gN \) defines the point on \( S_2 \), transformed of the north pole \( N \) by \( g \). According to equation (4), \( f^c \) is a central function which fulfills

\[
(\tilde{f}^c) = (\hat{f})^c
\]

(15)
for the same reasons as those referred to in the previous section 3.1. Moreover

\[
f^c(1) = \hat{f}(1).
\]

(16)

3.3 Computation of \( \hat{f}(1) \) for a centralized function. — From

\[
f = \sum_{l \geq 0} c_l \chi_l
\]

(17)
it follows that
\[ \tilde{f}(t) = \tilde{f}(1, l) = \tilde{f}(\omega = 0) = \sum_{l=0}^{\infty} c_{2l} \chi_{2l}(0) = \sum_{l=0}^{\infty} c_{2l}(4l + 1). \quad (18) \]

From equation (9) and equation (7) one obtains
\[ c_l = \frac{2}{\pi} \int_0^{\pi} \sin^2 \frac{\omega}{2} d\omega \cos \omega \sin^2 \frac{\omega}{2} = a_l - a_{l+1} \quad (19) \]

by setting
\[ a_l = \frac{1}{\pi} \int_0^{\pi} d\omega f(\omega) \cos \omega. \quad (20) \]

Taking into account equation (19), series equation (18) can be written
\[ \sum_{l=0}^{\infty} 2a_l(-1)^l l = \frac{1}{\pi} \int_{-\pi}^{\pi} \frac{g(\omega) \cos \frac{\omega}{2}}{\sin \frac{\omega}{2}} d\omega = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(\omega) \cos \frac{\omega}{2} d\omega = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(\omega) \cos \frac{\omega}{2} d\omega = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(\omega) \cos \frac{\omega}{2} d\omega. \quad (24) \]

The last term in equation (28) can be transformed by an integration by parts
\[ \int_0^{\pi} d\omega \cos \frac{\omega}{2} \frac{df}{d\omega} = \int_0^{\pi} d\omega \cos \frac{\omega}{2} \frac{d}{d\omega} (f(\omega) - f(\pi)) = \left[ \cos \frac{\omega}{2} (f(\omega) - f(\pi)) \right]_0^{\pi} + \frac{1}{2} \int_0^{\pi} d\omega \cos^2 \frac{\omega}{2}. \quad (29) \]

In spite of appearances, there is no singularity at \( \omega = \pi \). Indeed, from the parity of the function \( f(\omega) \), equation (26), it follows that the function \( f(\omega + \pi) \) has the property of parity too:
\[ f(\pi - \omega) = f(-\pi + \omega) = f(2\pi - \pi + \omega) = f(\pi + \omega). \quad (30a) \]

Consequently, the Taylor series of \( f(\pi + \omega) - f(\pi) \) in the neighbourhood of \( \omega = 0 \) starts with the quadratic term \( \omega^2 \):
\[ f(\pi + \omega) - f(\pi) \propto \omega^2. \quad (30) \]
which ensures the vanishing of the first term and the integrability of the second term of equation (29). Thus, equation (28) can be written

\[ f(0) = \frac{f(0)}{2} + \frac{f(\pi)}{2} + \frac{1}{2\pi} \int_0^{\infty} d\omega \tan^2 \frac{\omega}{2} (f(\pi) - f(\omega)). \]

(31)

3.4 Return to the initial texture function. — Replacing in equation (31) \( f \) by \((f^{\eta})^{\omega}\), according to equations (10) and (14)

\[ (f^{\eta})^{\omega}(\omega) = \int_{S_2} d\sigma f (g e^{\omega}) \]

one finally obtains

\[ f(\omega) = \frac{1}{2} f(g) + \frac{1}{2} \int_{S_2} d\sigma f (g e^{\omega}) + \frac{1}{2\pi} \int_0^{\infty} d\omega \tan^2 \frac{\omega}{2} \int_{S_2} d\sigma (f (g e^{\omega}) - f (g e^{\omega})) \]

\[ = \frac{1}{2} f(g) + f_s(\omega) + f_d(\omega). \]

(33)

A similar formula has been given, without proof, by S. Matthies [2], for which however the order of integration \( \int_0^{\infty} d\omega ... \int_{S_2} d\sigma \) has been interchanged in the last term \( f_{\Omega} \). Such an integration sequence, if formally followed, may lead to divergent integrals, as can be proved with some straightforward examples.

3.5 Obligation for the right integration sequence in the term \( f_{\Omega} \). — The detailed analysis of the proof in paragraph 3.3 for the case of a central function shows the importance of the parity and differentiability of the function, in order that the mentioned integral converges. Indeed, in the term \( f_{\Omega} \) of equation (33), it is the centralization integral \( \int_{S_2} d\sigma ... \) which, performed at first, ensures the parity in the variable \( \omega \) and eliminates the eventual problems of divergence.

As an example, consider the function

\[ f(g) = \langle N | g | N \rangle = g_{33} = \cos \Phi \]

(34)

where the tilt angle \( \Phi \) denotes the second of the Euler angles:

\[ g = \{ \varphi_1, \Phi, \varphi_2 \}. \]

(35)

Using the well-known formula which gives the transform of the vector \( x \) through the rotation \( e^{\omega} \)

\[ e^{\omega} x = \cos \omega (x - (x, \sigma) \sigma) + \sin \omega \sigma \times x + (x, \sigma) \sigma \]

(36)

it is possible to write successively

\[ f(g e^{\omega}) = \langle g^{-1} N | e^{\omega} N \rangle = \cos \omega (\sigma N | u) - \langle \sigma | N \rangle (\sigma | u) + \sin \omega (\sigma \times N | u) + \langle N | \sigma \rangle (\sigma | u) \]

(37)

with \( u = g^{-1} N \), and then

\[ f(g e^{\omega}) - f(g e^{\omega}) = -(1 + \cos \omega) (\sigma N | u) - \langle \sigma | N \rangle (\sigma | u) - \sin \omega (\sigma \times N | u). \]

(38)

Indeed, the integral

\[ \int_0^{\infty} d\omega \tan^2 \frac{\omega}{2} (f(g e^{\omega}) - f(g e^{\omega})) \]

diverges if \( \sigma \times N | u \neq 0 \), which is the case when \( \sigma \) is outside the great circle cut out by the equatorial plane defined by \( N \) and \( u \). On the other hand, if the centralization integral is performed first, it ensures the convergence of the following integral in \( \omega \).

4. Expansion of the terms \( f_{\Omega} \) and \( f_{\Omega} \) into series of generalized spherical harmonics. — Let

\[ f(g) = T^{\nu m}_{\nu}(g). \]

(40)

Then, according to equations (10) and (14), one obtains

\[ f(g)^{\eta}(\omega) = \int_{S_2} d\sigma f(g) e^{\omega} = \frac{\chi(\omega)}{2l + 1} f(g) \]

(41)

by using the addition and orthogonality relations of the generalized spherical harmonics.

Hence

\[ f_{\Omega}(g) = \frac{1}{2} (f^{\eta})^{\nu} (II) = \frac{1}{2} \chi_1 (II) f(g) = \frac{1}{2} (\nu - 1)^l f(g) \]

(42)

and

\[ f_{\Omega}(g) = \frac{1}{2} \int_0^\infty d\omega \tan^2 \frac{\omega}{2} (f^{\eta})^{\nu} (II) - (f^{\eta})^{\nu} (\omega)) \]

\[ = \frac{1}{2} \chi_1 (II) - \chi_1 (\omega) \]

(43)

the integral in \( \omega \) being obtained by recurrence on \( l \).

From these calculations performed for a generalized spherical harmonic, one immediately gets the serial expansions:

\[ f_{\Omega}(g) = \frac{1}{2} \sum_{l \geq 0} (\nu - 1)^l C^{\nu m}_{\nu} T^{\nu m}(g) \]

(44)
and
\[ f_{d}(g) = \frac{1}{2} \sum_{n=0}^{\infty} \left( -1 \right)^{n} \frac{2 \omega T_{n}^{\text{mm}}}{2 n + 1} \text{T}_{n}^{\text{mm}}(g). \tag{45} \]

This form presents essentially an interest for the numerical computation of the terms \( f_{n} \) and \( f_{d} \). Similar formulas have been recently given, without proof, by S. Matthies and J. Pospiech [6], and applied to a numerical illustration.

5. Extension to generalized functions. — In the case of an ideal orientation, symbolized by the Dirac-function \( \delta(g) \) centred at the origin 1, it is possible to get explicit formulas for the decomposition equation (33), without proceeding to the series expansions in spherical harmonics, equations (44) and (45). However, since formula (33) has only been proved for smooth functions, it has to be extended to generalized functions [7].

Let us recall that a generalized function \( D \) is characterized by the integration rule by which it operates on smooth functions \( f \)
\[ \langle D, f \rangle = \int_{G} D(g) f(g) \, dg. \tag{46} \]

Thus, in the case of the Dirac function \( D = \delta \), one obtains
\[ \langle \delta, f \rangle = \int_{G} \delta(g) f(g) \, dg = f(1). \tag{47} \]

It is natural to extend to generalized functions the formula
\[ \langle \delta, f \rangle = \langle D, \hat{f} \rangle \tag{48} \]

which is obvious if \( D \) is a differentiable function, because of the orthogonality relations. In particular, the generalized function \( \delta \) is thus defined by the integration rule
\[ \langle \delta, f \rangle = \langle \delta, \hat{f} \rangle = \hat{f}(1) \tag{49} \]

which corresponds to set \( g = 1 \) in equation (33). Thus, one has the following decomposition of \( \delta \) :
\[ \delta = \frac{1}{2} \delta + \delta_{II} + \delta_{a} \tag{50} \]
with
\[ \langle \delta_{II}, f \rangle = f_{II}(1) = \frac{1}{2} \int_{S^{2}} \text{d}\sigma f(e^{j\sigma}) \tag{51} \]
and
\[ \langle \delta_{a}, f \rangle = f_{a}(1) = \frac{1}{2} \int_{0}^{\pi} \text{d}\omega \sin\frac{\omega}{2} \frac{1}{2} \int_{S^{2}} \text{d}\sigma f(e^{j\sigma}) \times \tag{52} \]
\[ \int_{S^{2}} \text{d}\sigma f(e^{j\sigma}) - f(e^{j\sigma}) \]

6. Study of the decomposition of \( \delta \) or the appearance of ghosts. — The first term in the decomposition equation (50) shows that \( \delta \) gives restitution, through \( 1/2 \delta \), of the half of the true distribution. The ghost component \( \delta_{II} \) is a distribution equally concentrated on a surface defined by \( |g| = II \), which we shall call \( \Pi \)-surface, with S. Matthies [9]. Since this distribution is positive, it can be interpreted as texture function of a crystallite distribution, deduced from the true orientation \( \delta \), by rotations of angle \( \Pi \) around axes \( \sigma \) distributed at random on the sphere \( S^{2} \).

Finally, the ghost distribution:
\[ \delta_{a}(g) = -\frac{1}{4} Pp \frac{1}{\cos^{2} \frac{|g|}{2}} \tag{53} \]
is the principal part of the function \( -1/4 \cos^{2} \frac{|g|}{2} \), the resort to the principal part being necessary because of non integrable singularities of this last function in the neighbourhood of the \( \Pi \)-surface, where the denominator vanishes. Indeed, if \( f \) is a function which vanishes in the neighbourhood of the \( \Pi \)-surface, equation (52) reads:
\[ \langle \delta_{II}, f \rangle = -\frac{1}{2\Pi} \int_{0}^{\pi} \text{d}x \sin^{2} \frac{\omega}{2} \frac{1}{\cos^{2} \frac{\omega}{2}} \int_{S^{2}} \text{d}\sigma f(e^{j\sigma}) \]
\[ = -\frac{1}{4} \int_{0}^{\pi} \frac{1}{\cos^{2} \frac{|g|}{2}} f(g) \, dg \tag{54} \]

according to the integration formula on \( G \), equation (8). This equation (54) shows that, outside of the \( \Pi \)-surface, the generalized function \( \delta_{II}(g) \) coincide with the smooth function \( -1/4 \cos^{2} \frac{|g|}{2} \).

It is a very useful illustration to plot the terms of this decomposition; this is shown figures 1 and 2.

![Fig. 1. — Schematic representation of the decomposition of the even part of an ideal orientation centred at the origin, or cube texture; \( \alpha_{b} = 1/5 \) rad. in the figure fixes the half-width of the gaussian distribution. The total positive charge is only restituted for a half at the origin (1/2 \( \delta_{1} \)), flanked by a positive ghost charge distributed over the \( \Pi \)-surface.](image-url)
Figure 1 gives a representation of the orientation space $G$, in which the rotation $e^{\omega \sigma}$ is represented by the vector $\omega \sigma$ belonging to the closed ball of radius $\Pi$. On this boundary, sphere of radius $\Pi$, each couple of diametrically opposite points have to be identified.

In this representation, which respects the topological structure of $G$, the repartition of the different components $\delta_0(g)$, $\delta_1(g)$ and $\delta_2(g)$ appears in a much more comprehensible way than in the traditional cube parameterized by the Euler angles $\{\varphi_1, \Phi, \varphi_2\}$. So, the $\Pi$-surface, support of the positive generalized function $\delta_\omega$, is represented in figure 1 by the sphere of radius $\Pi$, whereas it shows the complicated shape of a double-saddle in the Euler parameters [9].

Though it is not possible to define, with the utmost rigour, the restriction to a straight line of a generalized function defined in a volume, the figure 2 plotted in the variable $\omega = |\varphi|$, angle of the rotation $\varphi$. The dashed curve represents the volume distribution $\delta_\omega(|\varphi|)$ in the limit case of a Dirac-function ($\omega_0 \rightarrow 0$).

This figure shows that the true distribution is only restored for a half at the origin, flanked by a ghost distribution with equal mass located at $\omega = \Pi$.

Furthermore, the ghost distribution $\delta_\omega(\omega)$, a smooth function outside the neighbourhood of $\Pi$, presents a discontinuity for $\omega \rightarrow \Pi$. In the neighbourhood of $\omega = \Pi$, $\delta_\omega$ (which can no longer be represented by a smooth function) and $\delta_\Pi$ compete against each other, the issue of which depends, in all generality, on the chosen regularization for the generalized functions $\delta_\omega$ and $\delta_\Pi$.

However, with the classical regularizations by gaussian functions, the curve $\delta_\omega$ after having followed the negative values of the ideal equation (53) (dotted curve in Fig. 2) over quite a long distance, rises suddenly in the vicinity of $\Pi$ and reaches a positive maximum at $\Pi$. Thus, for narrow gaussian curves (small half-width), the generalized function $\delta_\Pi$ is predominant, in the vicinity of $\Pi$, as compared to the generalized function $\delta_\Pi$ [10]. As a consequence, the curve figure 2, which is the sum of the two ghost functions, shows a negative minimum which is rather flat, immediately followed by a steep increase up to a positive maximum reached at $\omega = \Pi$.

7. Conclusion. — The even part $f$ of a texture function makes restitution only of the half $1/2 f$ of the true function, flanked by two ghosts $f_0$ and $f_0$ of which an integral expression can be given in terms of $f$. In the case of the Dirac distribution, these integral expressions are particularly striking. So, if the texture function is a $\delta$, Dirac distribution corresponding to $2N$ crystallites in orientation identity $g = 1$ (cube texture), the even part $\delta_\Pi$ gives only restitution of half of them, the $N$ other crystallites being turned by an angle $\Pi$ around randomly oriented axes $\sigma$ in order to build up the $\Pi$-ghost. Thus, each true peak of the even texture function $f$ drags along with it, in a strict geometrical relation, its $\Pi$-ghost. (Leaving aside the $\Omega$-ghost which has for effect to weaken certain orientations, figure 2, but the geometrical interpretation of which is less obvious). The determination of such a close correlation between the geometrical locations (and also the respective intensities) of the peaks and their associated $\Pi$-ghosts constitute an important step in the difficult problem of ghost correction procedures development.

Acknowledgments. — The authors express their gratitude to Pr. J. Faraut, University of Strasbourg, for having suggested to use the centralization method, in order to establish an inversion formula. One of the authors (C.E.) would like to thank Dr S. Matthies for very informative discussions he had with him when participating in and contributing to the Spring School organized by the Zentralinstitut für Kernforschung at Wehlen near Dresden, G.D.R. Thanks to these discussions the last paragraph in section 6 (Study of the decomposition of $\delta$ or the apparition of ghosts) could be put in more proper terms and it was possible to determine the asymptotic behaviour as $\omega_0^2$ of the ghost functions on the $\Pi$-surface (Figs. 1 and 2).

Note added in proof. — Since this paper was returned for correction (Feb. 2, 1981), several studies on ghost functions have appeared. Some papers published by S. Matthies [11, 12, 13] provide more detailed information as compared to his earliest short note [2] on his approach. However, these papers do not always give a full mathematical demonstration either of the inversion formula or the integral relation for $\tilde{f}(g)$. This demonstration has been announced among the titles given in his own bibliography, in the form of a more extensive publication internal to the Z.F.K. [14]. A systematic investigation of Gaussian texture ghost...
functions in relation to symmetries and half-widths has been published by Jura et al. [15]. Unfortunately this work does not derive any benefit from the centralness of Gaussian functions and is developed on cumbersome series of generalized spherical harmonics whereas we simply consider developing them into series of characters (see equation (7) in the present paper).

References