Textures and Microstructures, 1996, Vol. 25, pp. 183–195
Reprints available directly from the publisher.
Photocopying permitted by license only

DETERMINATION OF DOMAINS OF DEPENDENCE THROUGH THE SOLUTION OF AN ULTRAHYPERBOLIC DIFFERENTIAL EQUATION

T. I. SAVYOLOVA

MIFI (Moscow Engineering Physical Institute), Kashirskoe Shosse 31, 115409, Russia

(Received 10 October 1995)

Pole figures are represented as the sum of solutions of two ultrahyperbolic differential equations. We derive the domains of dependence for pole figures and apply the method of continuation to solve the ultrahyperbolic equations.

KEY WORDS: Ultrahyperbolic differential equation, Domain of dependence, Orientation distribution function.

INTRODUCTION

An orientation distribution function (ODF) f(g), $g \in SO(3)$, is the solution of the equations (Matthies, 1979)

$$P_{\bar{h}_i}(\bar{y}) = (4\pi)^{-1}\int_0^{2\pi}\{f(\{\phi, \theta, \varphi\}^{-1}\{\eta, \chi, 0\}) + f(\{\phi+\pi, \pi-\theta, \varphi\}^{-1}\{\eta, \chi, 0\})\}d\varphi, \tag{1}$$

where $\bar{h}_i = \{\theta, \phi\}$, $\bar{y} = \{\chi, \eta\}$, $0 \le \theta, \chi \le \pi$, $0 \le \phi, \eta < 2\pi$, are the spherical coordinates of unit vectors $\bar{h}_i$, $\bar{y}$, $i = 1, 2, \ldots$. Pole figures (PF) $P_{\bar{h}_i}(\bar{y})$ can be determined from x-ray or neutron measurements.

Let SO(3) denote the rotation group, SU(2) the group of unitary unimodular matrices of second order, RP^3 the three dimensional projective space and SU(2) / {±1} the factor-group for subgroup {±1}, 1 being the unit of group SU(2).

Using the isomorphisms

$$SO(3) \sim SU(2)\ /\ \{\pm 1\} \sim RP^3, \tag{2}$$

we find (Savyolova, 1982), that the paths of integration in eq.(1)

$$\pm\bar{h}_i = g\bar{y} \tag{3}$$

can be written as

$$\bar{x}^{\pm} = \bar{a}^{\pm}t + \bar{b}^{\pm} \tag{4}$$

with

$$\bar{a}^{\pm} = \{\bar{a}_1^{\pm}, \bar{a}_2^{\pm}, 1\},$$

$$\bar{b}^{\pm} = \{\bar{b}_1^{\pm}, \bar{b}_2^{\pm}, 0\}.$$

If $\bar{h}_i = \{h_1, h_2, h_3\}$, $\bar{y} = \{y_1, y_2, y_3\}$, are the coordinates of the unit vectors $\bar{h}_i$, $\bar{y}$ respectively, $h_3 \neq \pm y_3$, $\bar{x} = \{x_1, x_2, x_3\}$ is a point in space RP^3, $|t| < +\infty$ is a parameter, then we have

$$a_1^{\pm} = -\frac{y_1 \pm h_1}{y_3 \mp h_3}, \qquad a_2^{\pm} = -\frac{y_2 \mp h_2}{y_3 \mp h_3},$$
$$b_1^{\pm} = \frac{y_2 \pm h_2}{y_3 \mp h_3}, \qquad b_2^{\pm} = -\frac{y_1 \mp h_1}{y_3 \mp h_3}. \tag{5}$$

Using (2) we can rewrite the equation (1) (Ivanova, Savyolova, 1993)

$$P_{\bar{h}_i}(y) = \frac{1}{|y_3 - h_3|} F^{+}(\bar{a}^{+}, \bar{b}^{+}) + \frac{1}{|y_3 + h_3|} F^{-}(\bar{a}^{-}, \bar{b}^{-}) \tag{6}$$

with

$$F^{\pm}(\bar{a}^{\pm}, \bar{b}^{\pm}) = \int_{-\infty}^{+\infty} \frac{8f(\bar{a}^{\pm}t + \bar{b}^{\pm})dt}{A^{\pm}t^2 + 2B^{\pm}t + C^{\pm}} \tag{7}$$

where $A^{\pm}$, $B^{\pm}$, $C^{\pm}$ are given by

$$A^{\pm} = (a_1^{\pm})^2 + (a_2^{\pm})^2 + 1, \qquad C^{\pm} = (b_1^{\pm})^2 + (b_2^{\pm})^2 + 1, \tag{8}$$
$$B^{\pm} = a_1^{\pm}b_1^{\pm} + a_2^{\pm}b_2^{\pm}.$$

From equations (6) we derive the ultrahyperbolic equation for pole figures (Savyolova, 1982)

$$\frac{\partial^2 F^{\pm}}{\partial a_1^{\pm}\partial b_2^{\pm}} = \frac{\partial^2 F^{\pm}}{\partial a_2^{\pm}\partial b_1^{\pm}}. \tag{9}$$

Now setting

$$r = 2\frac{\sqrt{y_1^2 + y_2^2}}{|y_3 \mp h_3|}, \quad \tan\varphi = \frac{y_2}{y_1}, \tag{10}$$
$$\rho = 2\frac{\sqrt{h_1^2 + h_2^2}}{|y_3 \mp h_3|}, \quad \tan\psi = \frac{h_1}{h_2},$$

then we get equation (9) in polar coordinates

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial F}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 F}{\partial \varphi^2} = \frac{1}{\rho}\frac{\partial}{\partial \rho}\left(r\frac{\partial F}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 F}{\partial \psi^2}. \tag{11}$$

In any bounded domain the solution of equation (11) is given by the series

$$F(r, \varphi, \rho, \psi) = \sum_{m,n=-\infty}^{+\infty} \sum_{k=0}^{+\infty} A_{mnk}\, J_n(\lambda_{nk}\frac{r}{a})\, J_m(\lambda_{nk}\frac{\rho}{a}) \times \exp\{i(n\varphi + m\psi)\}, \tag{12}$$

where $J_n(\lambda_{nk}) = 0$ (or $J'n(\lambda_{nk}) = 0$), if $F|_{r=a} = 0$ (or $\left.\frac{\partial F}{\partial r}\right|_{r=a} = 0$). (13)

The coefficients A_{mnk} are calculated from the boundary conditions. If the domain is not bounded then the solution of equation (11) is represented as

$$F(r, \varphi, \rho, \psi) = \sum_{m,n=-\infty}^{+\infty} \{\int_0^{+\infty} A_{mnk}\ (\lambda) J_n(\lambda r) J_m(\lambda\rho)\lambda d\lambda\} \times \exp\{i(n\varphi + m\psi)\}, \tag{14}$$

where the function $A_{mn}(\lambda)$ can be calculated from the additional conditions for the function F.

CALCULATION OF DOMAINS OF DEPENDENCE FOR POLE FIGURES FROM ONE POLE FIGURE

From formula (6) we get

$$P_{\bar{h}_i}(\bar{y})\, 2\sin\chi = r^+F^+ + r^-F^-, \tag{15}$$

where in accordance with (5)

$$r^{\pm} = \frac{2\sin\chi}{|\cos\chi \mp \cos\theta|}, \qquad p^{\pm} = \frac{2\sin\theta}{|\cos\chi \mp \cos\theta|}, \tag{16}$$

$$F^{\pm} = F(r^{\pm}, \varphi^{\pm}, \rho^{\pm}, \psi).$$

Suppose that from the diffraction experiment the pole figure $P_{\bar{h}_1}(\bar{y})$ is known with $\bar{h}_1 = \{\theta_1, \phi_1\}$, where $0 < \theta_1 \le \frac{\pi}{2}$. For every PF the variables $r^{\pm}$ and $\rho^{\pm}$ are dependent and have two branches

$$\rho_{1,2}(r) = \sqrt{\frac{4\alpha}{1-\alpha} + r^2 + 4} \mp 2\sqrt{\frac{\alpha}{1-\alpha}}, \tag{17}$$

where

$$\alpha = \cos^2\theta_1 = \frac{(r^2 - \rho^2 + 4)^2}{(r^2 - \rho^2)^2 + 16 + 8(r^2 + \rho^2)}, \quad \alpha \ne 1. \tag{18}$$

When $\theta_1 = \frac{\pi}{2}$ $(\alpha = 0)$, we get from formulas (15), (17)

$$\rho_{1,2}^{\pm} = \sqrt{r^2 + 4},\ r^+ = r^- = 2|tg\chi|,\ \rho^+ = \rho^- = \frac{2}{|\cos\chi|},\ F^+ = F^-. \tag{19}$$

For any other PF we have

$$r^+ \ne r^-,\ \rho^+ \ne \rho^-,\ F^+ \ne F^-. \tag{20}$$

If is easy to see that

$$\text{(i) if } \chi = 0, \text{ then } r^{\pm} = 0,\ \rho^{\pm} = \frac{2\sin\theta_1}{1 \mp \cos\theta_1} = \begin{cases} 2ctg\,\frac{\theta_1}{2} = k_2, \\ \\ 2tg\,\frac{\theta_1}{2} = k_1, \end{cases} \tag{21}$$

$$\text{(ii) if } \chi = \pi, \text{ then } \rho^{\pm} = 0,\ r^{\pm} = \frac{2\sin\theta_1}{1 \pm \cos\theta_1} = \begin{cases} 2tg\,\frac{\theta_1}{2} = k_1, \\ \\ 2ctg\,\frac{\theta_1}{2} = k_2. \end{cases} \tag{22}$$

When $0 < \theta_1 \le \frac{\pi}{2}$, we have $k_1 < k_2$.

The graphs of the functions $r^{\pm}(\chi), \rho^{\pm}(\chi)$ are shown in figures 1a, 1b, for $0 < \theta_1 \le \frac{\pi}{2}$. We have $r^+(\chi) = r^-(\pi - \chi)$, $\rho^+(\chi) = \rho^-(\pi - \chi)$, $0 \le \chi \le \pi$. If $0 \le \chi \le \theta_1$ then $0 \le r^+ \le +\infty$, $k_2 \le \rho^+ < +\infty$. If $\theta_1 \le \chi \le \pi$ then $0 \le r^+ < +\infty$, $k_1 \le \rho^+ < +\infty$. If $0 \le \chi \le \pi - \theta_1$ then $0 \le r^- < +\infty$, $k_1 \le \rho^- < +\infty$, and if $\pi - \theta_1 \le \chi \le \pi$ then $0 \le r^- < +\infty$, $k_2 \le \rho^- < +\infty$.

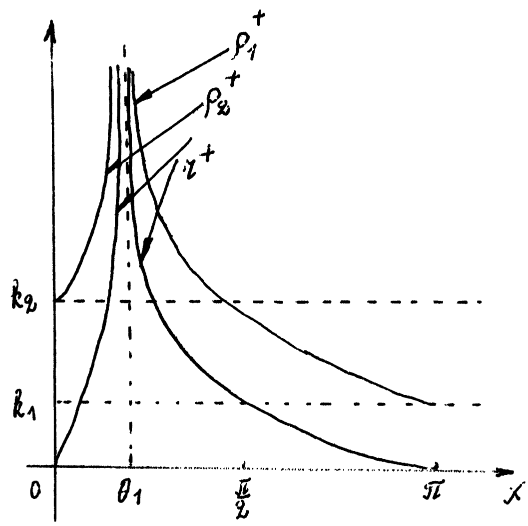


Figure 1a The functions $r^+(\chi)$, $\rho^+(\chi)$.

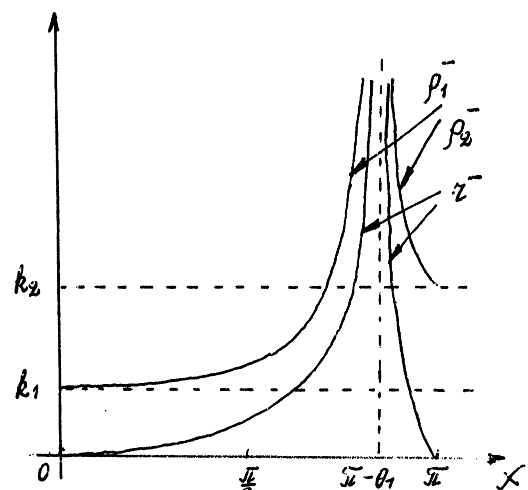


Figure 1b The functions $r^-(\chi)$, $\rho^-(\chi)$.

Two curves $\rho^{\pm}_{1,2}$ (17) are shown in figures 2a, 2b. We can see that $\rho_1^{\pm} < \rho = \sqrt{r^2+4}$, $\rho_2^{\pm} > \rho = \sqrt{r^2+4}$. When $\alpha \to 0$ then the two curves merge into one $\rho = \sqrt{r^2+4}$. When $\alpha \to 0$ then $k_1 = 2tg\frac{\theta_1}{2} \to 0$, $k_2 = 2ctg\frac{\theta_1}{2} \to +\infty$.

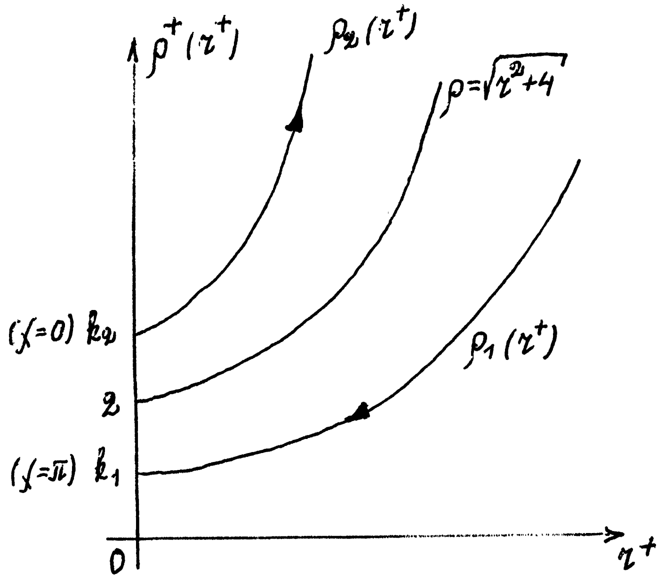


Figure 2a The functions $\rho_1^+(r)$, $\rho_2^+(r)$.

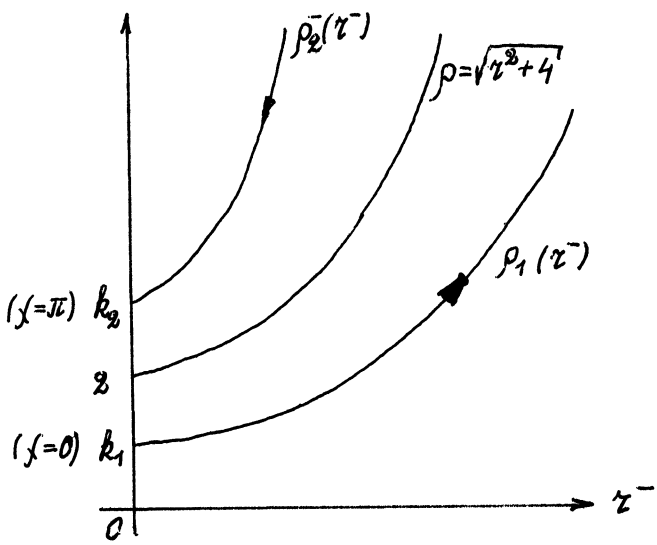


Figure 2b The functions $\rho_1^-(r)$, $\rho_2^-(r)$.

Let

$$G_1^{\pm} = \{r^{\pm} + \rho^{\pm} \geq k_1\}, \qquad G_1 = G_1^{+} \cap G_1^{-}, \tag{23}$$

$$G_2^{\pm} = \{r^{\pm} + \rho^{\pm} \geq k_2\}, \qquad G_2 = G_2^{+} \cap G_2^{-}.$$

It is obvious that $G_2 \subseteq G_1$ since $k_2 \geq k_1$.

We get

$$G_1^{+} = \{|\chi - \theta| \leq \pi - \theta_1\}, \tag{24}$$

$$G_1^{-} = \begin{cases} 0 < \theta < \theta_1, & \theta_1 - \theta < \chi < \pi - (\theta_1 - \theta), \\ \theta_1 < \theta < \frac{\pi}{2}, & 0 < \chi < \pi; \end{cases}$$

analagously,

$$G_2^{+} = \{|\chi - \theta| \leq \theta_1\}, \tag{25}$$

$$G_1^{-} = \{\pi - \theta_1 - \theta < \chi < \pi + \theta_1 - \theta\}.$$

These domains $G_1^{\pm}$, $G_2^{\pm}$ are shown in figures 3, 3a-3d displaying their constituents $0 \leq \chi, \theta \leq \pi$. The domains G_1^{+} and G_1^{-} are shown in figures 3a, 3b, the domains G_2^{+} and G_2^{-} are represented in figures 3c, 3d respectively. Finally, their intersections $G_1 = G_1^{+} \cap G_1^{-}$ and $G_2 = G_2^{+} \cap G_2^{-}$ are shown in figures 3.

Let us consider now the method to calculate the function F in the indicated domains.

Let us consider the set of pole figures with $\bar{h}_i = \{\theta_i, \phi_0\}$ when $\phi_0 = \text{const}$. In this case the function F does not depend on the variable ψ. Using the representation (14), let

$$F^{1,2}(r, \varphi, \rho, \phi_0) = \sum_{n=-\infty}^{+\infty} \exp\{in\varphi\}\left(\int_0^{+\infty} A_n^{1,2}(\lambda) J_n(\lambda r) J_0(\lambda\rho)\lambda d\lambda\right) \tag{26}$$

denote the function F in the domains G_1 and G_2 respectively.

If we know the PF with $\bar{h}_1 = \{\theta_1, \phi_0\}$, we can calculate the integral

$$F_n(\chi, \theta_1) = \int_0^{2\pi} P_{\bar{h}_1}(\bar{y}) \exp\{-in\varphi\} 2 \sin\chi \, d\varphi, \quad n = 0, \pm 1, \ldots. \tag{27}$$

Using the formulas (15), (26), we get

$$F_n(\chi, \theta_1) = \int_0^{+\infty} \exp\{-in\varphi\}(r^{+}F^{+} + r^{-}F^{-})d\varphi = (2\pi)$$

$$\begin{cases} 0 \leq \chi \leq \theta_1, & r^{+}\left(\int_0^{+\infty} A_n^2(\lambda) J_n(\lambda r^{+}) J_0(\lambda\rho_2(r^{+}))\lambda\right) d\lambda + \\ & \quad + r^{-}\left(\int_0^{+\infty} A_n^1(\lambda) J_n(\lambda r^{-}) J_0(\lambda\rho_1(r^{-}))\right) \lambda \, d\lambda; \\ \theta_1 \leq \chi \leq \frac{\pi}{2}, & \int_0^{+\infty} A_n^1(\lambda)\{r^{+} J_n(\lambda r^{+}) J_0(\lambda\rho_1(r^{+})) + \\ & \quad + r^{-} J_n(\lambda r^{-}) J_0(\lambda\rho_1(r^{-}))\}\lambda d\lambda. \end{cases} \tag{28}$$

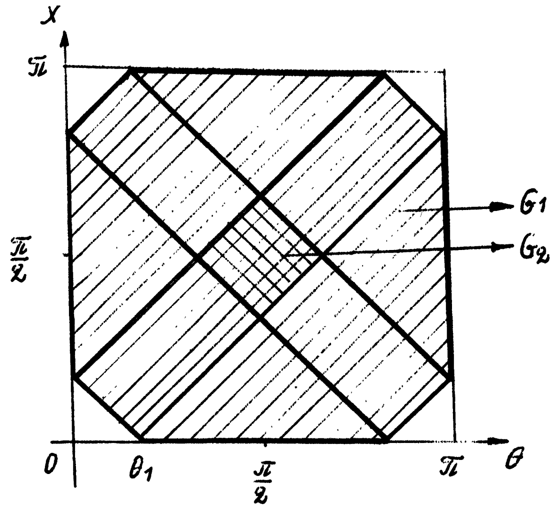


Figure 3 The domains $G_1 = G_1^+ \cup G_1^-$, $G_2 = G_2^+ \cup G_2^-$.

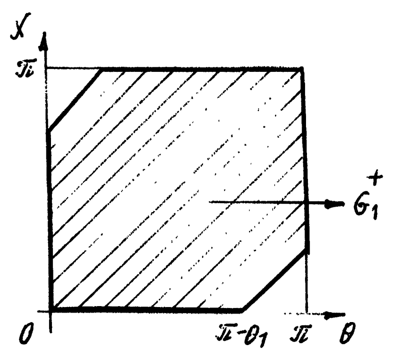


Figure 3a The domain G_1^+

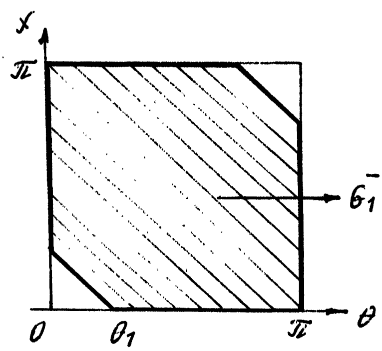


Figure 3b The domain G_1^-

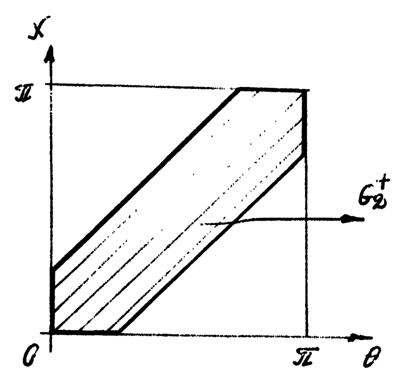


Figure 3c The domain G_2^+

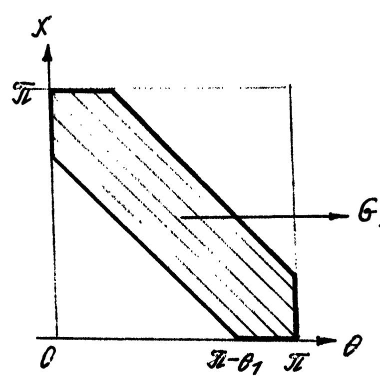


Figure 3d The domain G_2^-

Thus, we have set up the system of integral equations (28) with the unknown functions $A_n^{1,2}(\lambda)$ for the representation (26) of the functions $F^{1,2}$. If $\theta_1 = \frac{\pi}{2}$, then $r^+ = r^- = r$, $A_n^1(\lambda) = A_n^2(\lambda) = A_n(\lambda)(F^1 = F^2)$. In that case we get from equation (28)

$$F_n(\chi, \frac{\pi}{2}) = 2r \int_0^{+\infty} A_n(\lambda) J_n(\lambda r) J_0(\lambda \rho(r)) \lambda \, d\lambda, \tag{29}$$

where $r = 2|tg\chi|$, $\rho(r) = \sqrt{r^2 + 4}$. In accordance with equation (29) the problem to calculate the function F is easier if $\bar{h}_1 = \{\frac{\pi}{2}, \phi_0\}$.

For example the pole figures which can be calculated in the domains of dependence by solving the system of equations (29): $\{10\bar{1}0\}$, $\{10\bar{1}1\}$, $\{10\bar{1}2\}$ or $\{11\bar{2}0\}$, $\{11\bar{2}1\}$, $\{11\bar{2}2\}$ etc for hexagonal or trigonal lattice symmetry; $\{110\}$. $\{111\}$, $\{112\}$ and others for cubic lattice symmetry.

In figures 4, 4a-4c and 5, 5a-5c the domains G_1 and G_2 are shown for different PFs with $\bar{h}_i = \{\theta_i, \phi_0\}$, $0 < \theta_1 < \theta_2 < \theta_3 = \frac{\pi}{2}$. The domain G_1 increases when the parameter θ_i decreases. If $\theta_1 \to 0$ we get almost all pole figures. Conversely the domain G_2 decreases and puts in domain, determined from PF with $\bar{h}_i = \{\frac{\pi}{2}, \phi_0\}$ if θ_i decreases. The pole figure with $\bar{h}_i = \{0, \phi_0\}$ is the only PF that cannot be determined from other PFs since for this PF we have $\rho = 0$.

The problem to determine the domains of dependence for PFs when we know the bounded domain of PFs with $\bar{h}_i = \{\theta_1, \phi_0\}$, $0 \le \theta_1 = \frac{\pi}{2}$, can be solved analagously. We must find the domains

$$\begin{aligned} G_1^{\pm} &= \{k_1 \le r^{\pm} + \rho^{\pm} \le a_1\}, \\ G_2^{\pm} &= \{k_2 \le r^{\pm} + \rho^{\pm} \le a_2\}. \end{aligned} \tag{30}$$

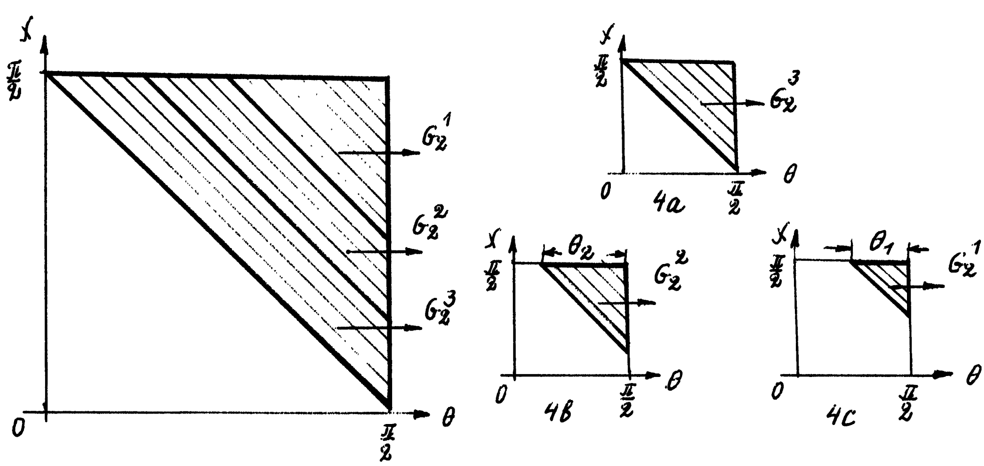


Figure 4 The domains $G_2^1 \subset G_2^2 \subset G_2^3$ for $0 < \vartheta_1 < \vartheta_2 < \vartheta_3 = \pi/2$

Figure 4a The domain G_2^3 for $\vartheta_3 = \pi/2$.

Figure 4b The domain G_2^2 for $\vartheta_2 < \vartheta_3 = \pi/2$.

Figure 4c The domain G_2^1 for $0 < \vartheta_1 < \vartheta_2$.

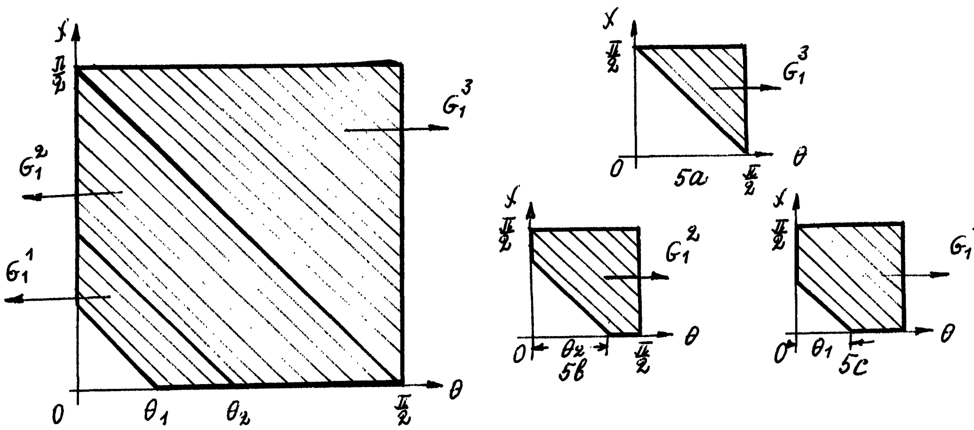


Figure 5 The domains $G_1^1 \supset G_1^2 \supset G_1^3$ for $0 < \vartheta_1 < \vartheta_2 < \vartheta_3 = \pi/2$.

Figure 5a The domain G_1^3 for $\vartheta_3 = \pi/2$.

Figure 5b The domain G_1^2 for $\vartheta_2 < \vartheta_3 = \pi/2$.

Figure 5c The domain G_1^1 for $0 < \vartheta_1 < \vartheta_2$.

where $k_1 < a_1$, $k_2 < a_2$. It is necessary to solve the system of algebraic equations analagous to (28) to determine the functions F_1 and F_2 as represented by the series expansion (12) in the domains G_1 and G_2.

In figures 6a–6d the domains G_1 and G_2 are shown for four cases: 6a, $0 < \theta_1 \leq \frac{\pi}{4}$; 6b, $\theta_1 = \frac{\pi}{4}$; 6c, $\frac{\pi}{4} < \theta_1 < \frac{\pi}{2}$; 6d, $\theta_1 = \frac{\pi}{2}$. When the parameter θ_1 increases then

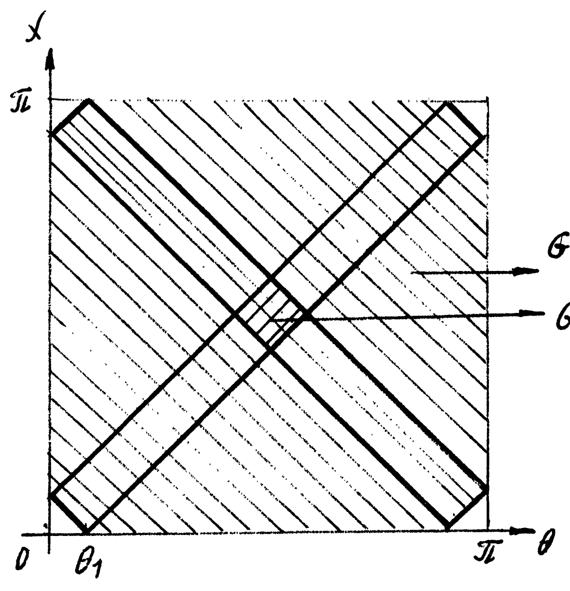


Figure 6a The domains G_1 and G_2 for $0 < \vartheta_1 < \pi/4$.

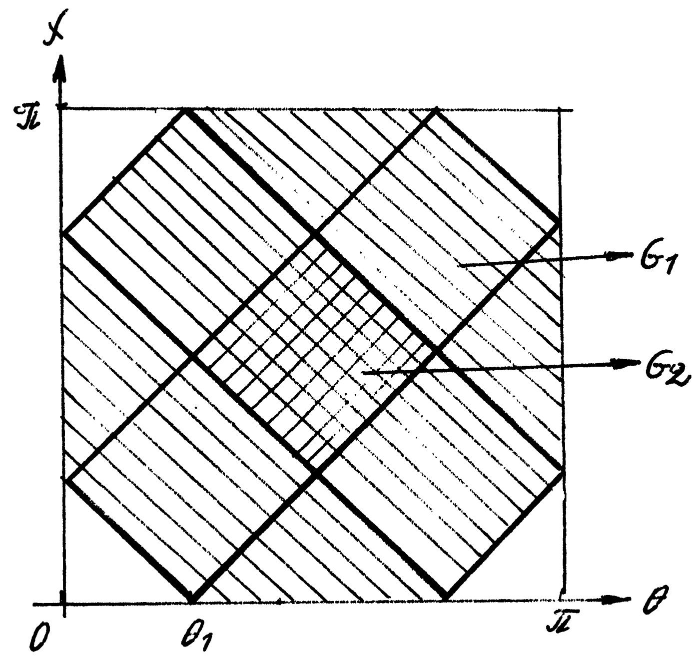


Figure 6b The domains G_1 and G_2 for $\vartheta_1 = \pi/4$.

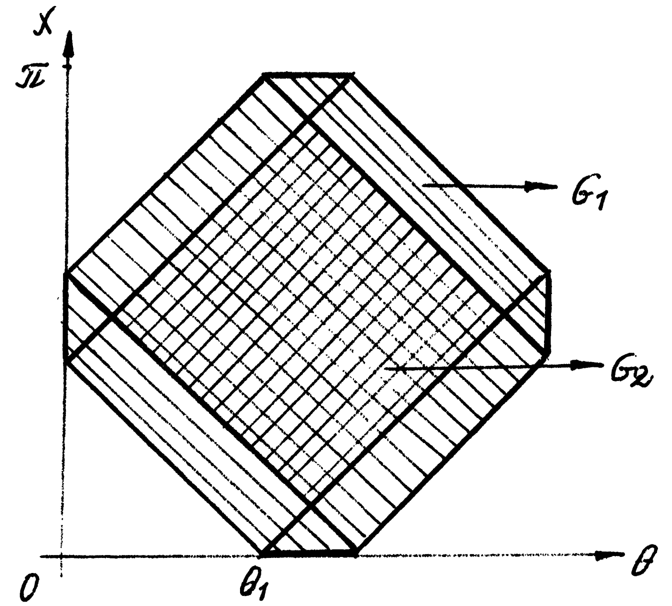


Figure 6c The domains G_1 and G_2 for $\pi/4 < \vartheta_1 < \pi/2$.

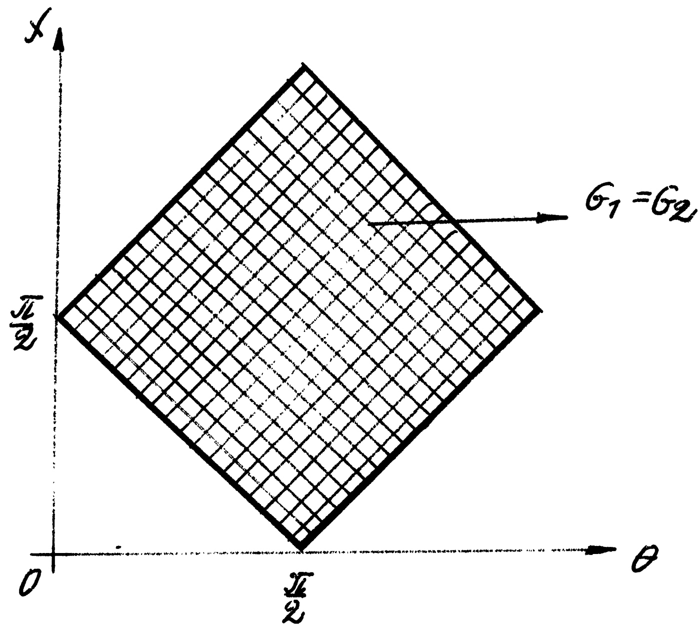


Figure 6d The domain $G_1 = G_2$ for $\vartheta_1 = \pi/2$.

the domain G_1 decreases and the domain G_2 increases. When $\theta_1 = \frac{\pi}{2}$ the domains G_1 and G_2 coincide (see figure 6d).

In figures 7, 7a–7d the domains of dependence are shown that can be calculated from PF with $\bar{h}_1 = \{\frac{\pi}{2}, \phi_0\}$. The PF with $\bar{h}_1 = \{\frac{\pi}{2}, \phi_0\}$ is divided into parts: $0 < \chi < \frac{\pi}{4}$ (double dashed line) and $\frac{\pi}{4} < \chi < \frac{\pi}{2}$ (dashed line) (see figure 7a). The domains of dependence are shown for other PFs with $\bar{h}_i = \{\theta_i, \phi_0\}$: $\frac{3\pi}{8} < \theta_i < \frac{\pi}{2}$ (figure 7b), $\frac{\pi}{4} < \theta_i < \frac{3\pi}{8}$ (figure 7c), $0 < \theta_i < \frac{\pi}{4}$ (figure 7d).

CONCLUSION

In this paper we apply the continuation method to solve the ultrahyperbolic differential equation which determines the domains of dependence for pole figures. Solving this problem basically consists in the numerical solution of the integral equation (28).

Acknowledgement

The author would like to thank her students Shurigin A. S. for calculating several examples of the solution by continuation of the ultrahyperbolic equation for model functions, and Nagaev I.R. for preparing this manuscript on computer. The author is grateful to Dr. Schaeben H. for the interest to these results.

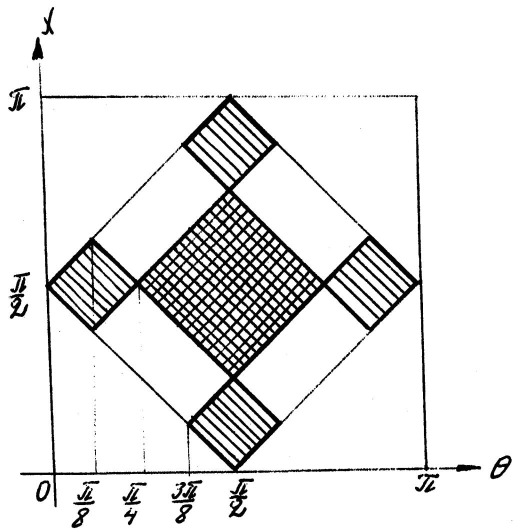
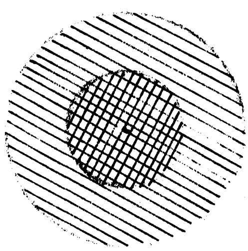
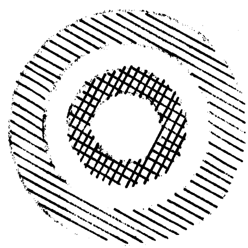


Figure 7 The domains of dependence for PF with $\vec{h}_1 = \{\pi/2, \Phi_0\}$.

(a)  (b) 

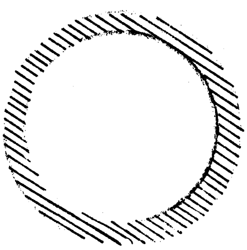
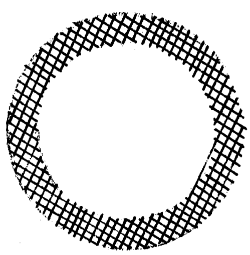
(c)  (d) 

Figure 7a The domains on PF with $\vec{h}_1 = \{\pi/2, \Phi_0\}$ $0 < \chi < \pi/4$ (double dashed line), $\pi/4 < \chi < \pi/2$ (dashed line).

Figure 7b The domains of dependence on PF with $\vec{h}_i = \{\vartheta_i, \Phi_0\}$, $3\pi/8 < \vartheta_i < \pi/2$.

Figure 7c The domains of dependence on PF with $\vec{h}_i = \{\vartheta_i, \Phi_0\}$, $\pi/4 < \vartheta_i < 3\pi/8$.

Figure 7d The domains of dependence on PF with $\vec{h}_i = \{\vartheta_i, \Phi_0\}$, $0 < \vartheta_i < \pi/4$.

References

Ivanova, T. M. and Savyolova, T. I. (1993). Programming and mathematical techniques in physics. International conference in Dubna, Russia, June 14–19, 224–225.

Matthies, S. (1979). On the Reproducibility of Orientation Distribution Function of Texture Samples from Pole Figures (Ghost Phenomena). *Phys. stat. sol.*, (b), **92**, 9, K135–K137.

Savyolova, T. I. (1982). On solution of the inverse problem of diffraction. Reports of Academy of Sciences USSR, **266**, 3, 590–593, (in Russian).