JOURNAL OF COMPUTATIONAL PHYSICS 95, 387–399 (1991)

Finite-Difference Operators in Anisotropic Inhomogeneous Dielectrics: General Case

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Received November 18, 1988; revised March 23, 1990

This work is aimed at the obtention of finite-difference equations for inhomogeneous anisotropic media for the general case of free orientation of eigen-vectors. Equations corresponding to boundary points are established.

INTRODUCTION

The finite difference method is a tool for solving partial differential equations. It is based on an approximate discretization of the differential equations in a finite set of grid points. This method has been widely used for solving Laplace's equation [1] and for solving elliptic partial differential equations with mixed partial derivatives in regular grids [2].

This paper deals with the solution of electrostatic potential in inhomogeneous anisotropic media by means of finite difference equations (f.d.e.). It lies on the discretization of an elliptic partial differential equation using a rectangular non-regular grid. Our analysis is restricted to the bidimensional case.

Different methods can be applied in deriving finite difference approximations for differential equations, especially when the equation can be expressed as the divergence of a vector field [3]. It is well known that the most usual method is based on finite Taylor's series expansions of the solution. In this paper two alternative f.d.e.s derived from this are presented for continuous media in a non-regular grid. The validity of these results does not depend on the orientation of the tensor permittivity eigendirections. This accounts for a more general approach than that of former results [4]. For this f.d.e. the local truncated error is calculated. The main purpose is to provide useful results without carrying out a rigorous error analysis.

0021-9991/91 $3.00

Besides, the discontinuous media are also considered by means of the boundary between two homogeneous anisotropic media as the limit of an inhomogeneity, providing the f.d.e. for both regular and singular boundary points. Finally, some examples showing the results of the proposed method are commented upon.

DIFFERENCE EQUATIONS

It is well known that the electrostatic potential in a space region without free charges obeys the equation

$$\operatorname{div}(\mathbf{K}\ \text{grad}\ V) = 0, \tag{1}$$

where $\mathbf{K}$ is the medium dielectrical tensor permittivity. For bidimensional and linear media, it can be represented in a matrix form as

$$\mathbf{K}(\mathbf{r}) = \begin{pmatrix} K_{11}(\mathbf{r}) & K_{12}(\mathbf{r}) \\ K_{12}(\mathbf{r}) & K_{22}(\mathbf{r}) \end{pmatrix}. \tag{2}$$

This matrix is symmetric in cases of physical importance and the eigen-values are real and greater than one [5]; thus Eq. (1) becomes an elliptic partial differential equation.

A square grid, with grid size h, is widely used to discretize the partial differential equations. Unfortunately, the boundary geometry of some problems does not fit with such a grid and a non-uniform rectangular grid has to be considered [6].

Let us denote "star" for the subset of points of the grid related in a f.d.e., as indicated in Fig. 1; "0" is an internal grid point and e, n, w, s are parameters that stand for the asymmetry of the star in geographic nemothecnia, accomplishing the relation $0 < e, n, w, s < 1$.

In order to obtain a relation among potentials in 0, 1, ..., 8 points, the derivatives

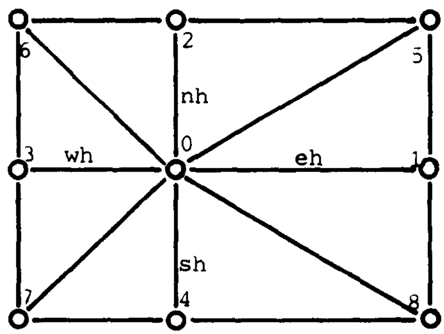

FIG. 1. A "star" or set of points related in a f.d.e.

which appear in Eq. (1) can be obtained from Taylor's series expansions and introduced in Eq. (1) that also can be written as

$$K_{11} V_{xx} + K_{12} V_{xy} + K_{22} V_{yy} + K_x V_x + K_y V_y = 0, \tag{3}$$

where

$$V_{xx} = \frac{h^2}{2} \frac{\partial^2 V}{\partial x^2}, \qquad V_{xy} = h^2 \frac{\partial^2 V}{\partial x\, \partial y}, \qquad V_{yy} = \frac{h^2}{2} \frac{\partial^2 V}{\partial y^2}, \qquad V_x = h \frac{\partial V}{\partial x},$$

$$V_y = h \frac{\partial V}{\partial y}, \qquad K_x = \frac{h}{2}\left(\frac{\partial K_{11}}{\partial x} + \frac{\partial K_{12}}{\partial y}\right), \qquad K_y = \frac{h}{2}\left(\frac{\partial K_{12}}{\partial x} + \frac{\partial K_{22}}{\partial y}\right).$$

The potential of the points 1, ..., 8 expressed as Taylor's expansions are

$$\begin{aligned}
V_1 &= V_0 + eV_x + e^2 V_{xx} + \cdots \\
V_2 &= V_0 + nV_y + n^2 V_{yy} + \cdots \\
V_3 &= V_0 - wV_x + w^2 V_{xx} + \cdots \\
V_4 &= V_0 - sV_y + s^2 V_{yy} + \cdots \\
V_5 &= V_0 + eV_x + nV_y + e^2 V_{xx} + neV_{xy} + n^2 V_{yy} + \cdots \\
V_6 &= V_0 - wV_x + nV_y + w^2 V_{xx} - nwV_{xy} + n^2 V_{yy} + \cdots \\
V_7 &= V_0 - wV_x - sV_y + w^2 V_{xx} + swV_{xy} + s^2 V_{yy} + \cdots \\
V_8 &= V_0 + eV_x - sV_y + e^2 V_{xx} - seV_{xy} + s^2 V_{yy} + \cdots,
\end{aligned} \tag{4}$$

where the potential derivatives are evaluated at the 0-point.

A combination of the expansions of $V_1, ..., V_4$ allow us to obtain the expressions of V_x, V_y, V_{xx}, and V_{yy} as linear functions of the potentials of the points 0, 1, ..., 4 and terms containing powers of h greater than 2.

The expression V_{xy} can be obtained from the combination of $V_1, ..., V_8$ expansions. Among all the possibilities giving V_{xy} as linear functions of the potentials of the points 0, 1, ..., 8 and terms containing powers of h greater than 2, the form indicated in expression (5) is considered [2]

$$V_5 - V_6 + V_7 - V_8. \tag{5}$$

Taking into account these derivative expressions Eq. (3), particularly at the 0-point, can be written in a compact form as

$$\sum_{i=1}^{8} A_i V_i - \left(\sum_{i=1}^{8} A_i\right) V_0 = \Theta(h^3), \tag{6}$$

where

$$\Theta(h^3) = \left[(e-w)\left(\frac{K_{11}}{6}\frac{\partial^3 V}{\partial x^3} + \frac{K_{12}}{2}\frac{\partial^3 V}{\partial x^2\,\partial y}\right) \right.$$
$$\left. + (n-s)\left(\frac{K_{22}}{6}\frac{\partial^3 V}{\partial y^3} + \frac{K_{12}}{2}\frac{\partial^3 V}{\partial x\,\partial y^2}\right)\right] h^3 + \cdots. \tag{7}$$

Neglecting the truncation error, $\Theta(h^3)$, Eq. (6) shows V_0 as a potential weighted mean of the star points. When the star is symmetric ($e=w$ and $n=s$), the truncation error of this f.d.e., (7), contains only terms with powers of h greater than 3.

The A_i coefficients are given by

$$A_1 = \frac{1}{e(e+w)}(K_{11}+wK_x), \qquad A_2 = \frac{1}{n(n+s)}(K_{22}+sK_y)$$
$$A_3 = \frac{1}{w(e+w)}(K_{11}-eK_x), \qquad A_4 = \frac{1}{s(n+s)}(K_{22}-nK_y) \tag{8}$$
$$A_5 = -A_6 = A_7 = -A_8 = \frac{K_{12}}{(n+s)(e+w)}.$$

Although some of these coefficients are negative, this fact does not imply a contradiction with the Theorem of Medium Value [7]. By imposing the adequate conditions in each case, the coefficients (8) lead to the f.d.e. obtained in the particular cases previously mentioned. Thus, if the eigenvector directions of tensor permittivity coincide with the coordinate axes $K_{12}=0$, resulting in $A_5=A_6=A_7=A_8=0$, and consequently four points are sufficient to discretize Eq. (3) for this approximation [4].

From Green's second identity a Theorem of Medium Value form can be obtained for isotropic inhomogeneous media [8],

$$K(\mathbf{r})\,V(\mathbf{r}) = \langle K(\mathbf{r}')\,V(\mathbf{r}')\rangle_s + \frac{1}{4\pi}\int_v \frac{V(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3}(\mathbf{r}-\mathbf{r}')\cdot\nabla K\,dv,$$

which suggests an alternative way of obtaining the f.d.e.

Thus, one can obtain other different coefficients if, instead of using the serie expansions (4), also expansions of values (9) are considered,

$$\begin{matrix} K_{11(1)}V_1; & K_{22(2)}V_2; & K_{11(3)}V_3; & K_{22(4)}V_4; \\ K_{12(5)}V_5; & K_{12(6)}V_6; & K_{12(7)}V_7; & K_{12(8)}V_8, \end{matrix} \tag{9}$$

where each subindex between brackets indicates the point at which K_{ij} is evaluated.

As in the previous case, the expansions of the first four values of (9) provide the expressions of V_x, V_y, V_{xx}, and V_{yy}, while V_{xy} is expressed in terms of the linear combination

$$K_{12(5)}V_5 - K_{12(6)}V_6 + K_{12(7)}V_7 - K_{12(8)}V_8. \tag{10}$$

With these expressions, Eq. (3) becomes one of the same type as Eq. (6), where the A_i coefficients are

$$\begin{aligned}
&A_1 = \frac{K_{11(1)}}{e(e+w)}\left(1 - w\frac{K_x}{K_{11}}\right); && A_2 = \frac{K_{22(2)}}{n(n+s)}\left(1 - s\frac{K_y}{K_{22}}\right);\\
&A_3 = \frac{K_{11(3)}}{w(e+w)}\left(1 + e\frac{K_x}{K_{11}}\right); && A_4 = \frac{K_{22(4)}}{s(n+s)}\left(1 + n\frac{K_y}{K_{22}}\right);\\
&A_5 = \frac{K_{12(5)}}{(n+s)(e+w)}; && A_6 = -\frac{K_{12(6)}}{(n+s)(e+w)};\\
&A_7 = \frac{K_{12(7)}}{(n+s)(e+w)}; && A_8 = -\frac{K_{12(8)}}{(n+s)(e+w)}.
\end{aligned} \tag{11}$$

Note that in (8) the implied elements of the tensor permittivity are refered to the 0-point (the absence of the indicative position must be interpreted in this manner). However, the tensor permittivity elements refered to each point of the star including the 0-point are present at (11). This is due to the expansions used.

Equation (6) with (11) represents an alternative f.d.e. when $\Theta(h^3)$ is neglected. Now the truncation term is

$$\begin{aligned}
\Theta(h^3) = \Bigg[&(e-w)\left(\frac{K_{11}}{6}\frac{\partial^3 V}{\partial x^3} + \frac{1}{2}\frac{\partial K_{11}}{\partial x}\frac{\partial^2 V}{\partial x^2} + \frac{1}{2}\frac{\partial^2 K_{11}}{\partial x^2}\frac{\partial V}{\partial x} + \frac{K_{12}}{2}\frac{\partial^3 V}{\partial x^2\,\partial y}\right.\\
&\left. + \frac{\partial K_{12}}{\partial x}\frac{\partial^2 V}{\partial x\,\partial y} + \frac{1}{2}\frac{\partial K_{12}}{\partial y}\frac{\partial^2 V}{\partial x^2} + \frac{1}{2}\frac{\partial^2 K_{12}}{\partial x^2}\frac{\partial V}{\partial y} + \frac{\partial^2 K_{12}}{\partial x\,\partial y}\frac{\partial V}{\partial x}\right)\\
&+ (n-s)\left(\frac{K_{22}}{6}\frac{\partial^3 V}{\partial y^3} + \frac{1}{2}\frac{\partial K_{22}}{\partial y}\frac{\partial^2 V}{\partial y^2} + \frac{1}{2}\frac{\partial^2 K_{22}}{\partial y^2}\frac{\partial V}{\partial y} + \frac{K_{12}}{2}\frac{\partial^3 V}{\partial x\,\partial y^2}\right.\\
&\left. + \frac{\partial K_{12}}{\partial y}\frac{\partial^2 V}{\partial x\,\partial y} + \frac{1}{2}\frac{\partial K_{12}}{\partial x}\frac{\partial^2 V}{\partial y^2} + \frac{1}{2}\frac{\partial^2 K_{12}}{\partial y^2}\frac{\partial V}{\partial x} + \frac{\partial^2 K_{12}}{\partial x\,\partial y}\frac{\partial V}{\partial y}\right)\Bigg] h^3 + \cdots.
\end{aligned} \tag{12}$$

Taking into account the truncation error a priori, the two f.d.e. forms lead to similar results, and, in consequence, the use of one or the other will depend on the specific application. Thus, in order to calculate the potential of a region with only one continuous dielectrical medium, it is more convenient to use the coefficients (8) due to their greater simplicity, while the use of (11) is necessary to find the f.d.e. at points belonging to boundaries between two homogeneous anisotropic dielectric media.

Boundaries between Homogeneous Anisotropic Dielectrics

The points belonging to the boundary between two different media present singularities in the permittivity derivatives. For geometries in which the normal directions to the boundary surfaces are well determined, the application of the boundary conditions on the field vectors provides the valid f.d.e. for these points. Nevertheless, when these surfaces do not have such a direction defined, as in the case of edges or apexes, other procedures are necessary. For the sake of simplycity the "inhomogeneous layer" method has been chosen. This method has already been used in isotropic media as well as in anisotropic media [4] when the eigen-directions of tensor permittivity coincide with the grid direction.

Let us first consider the case of a plane boundary between two homogeneous anisotropic media and let us use stars with equal arms centered on this boundary as shown in Fig. 2. The relative permittivity of both media are represented by the **W** and **E** tensors. The principal directions of the tensors do not coincide, in general, either with themselves or with the boundary directions. We will let the latter coincide with one of the coordinate axes (i.e., the Y-axis).

The development of the method implies the consideration of an inhomogeneous layer interposed between both media. The value $\mathbf{K}(x)$ and its derivatives coincide with the original media at common points and are continuous in the whole layer width. Figure 3 shows the state of the stars derived from the introduction of this layer.

Using the coefficients obtained in (11) to establish the corresponding relations of the stars centered at $0E$ and $0W$, we obtain

$$A_{0E}V_{0E} = \frac{E_{11}}{2+t}V_1 + \frac{W_{11}}{(1+t)(2+t)}V_3 + E_{22}(V_{2E}+V_{4E}) + \frac{E_{12}}{2(2+t)}(V_5 - V_8) + \frac{W_{12}}{2(2+t)}(V_7 - V_6) \tag{13}$$

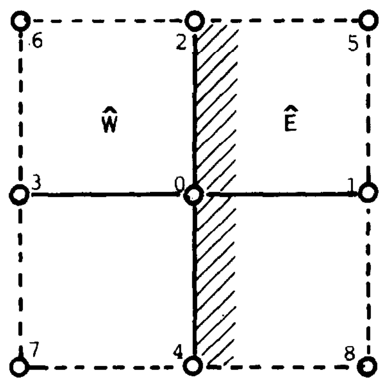

FIG. 2. Star centered in a regular boundary point.

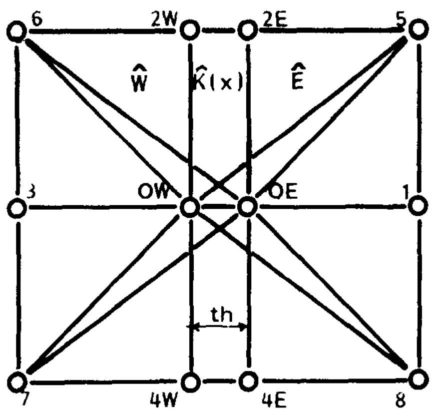

FIG. 3. Composed star including an inhomogeneous layer between **E** and **W** media.

and

$$A_{0W}V_{0W}=\frac{W_{11}}{2+t}V_3+\frac{E_{11}}{(1+t)(2+t)}V_1+W_{22}(V_{2W}+V_{4W})$$
$$+\frac{E_{12}}{2(2+t)}(V_5-V_8)+\frac{W_{12}}{2(2+t)}(V_7-V_6). \tag{14}$$

When making $t\to 0$ the points $0E$ and $0W$ tend to become confused at the 0-point in the same way as their potentials. In a similar way the $2E$ and $2W$ points and the $4E$ and $4W$ points become confused at 2 and 4 points, respectively, so that, at the limit, the sum of Eq. (13) and (14) turns out to be

$$2(E_{11}+W_{11}+E_{22}+W_{22})V_0=2E_{11}V_1+2W_{11}V_3+(E_{22}+W_{22})(V_2+V_4)$$
$$+E_{12}(V_5-V_8)+W_{12}(V_7-V_6), \tag{15}$$

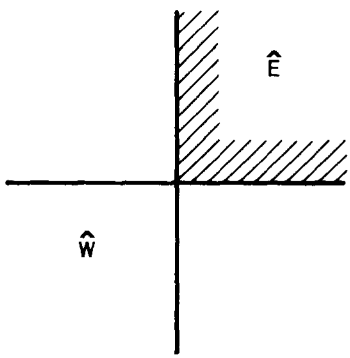

FIG. 4. Boundary between **E** and **W** media with a non-regular boundary point.

which is the f.d.e. expression corresponding to the case presented. The result for a horizontal boundary case can be straightforwardly obtained.

In a similar way the method is applicable to points where it is not possible to use the boundary conditions, where the normal direction is not defined. Figure 4 illustrates the distribution of the media which will be considered below. As in the previous case, an inhomogeneous layer is interposed between both media with the continuity conditions previously fixed. Figure 5 shows the star state derived from this model. In this case, it produces four stars centered on NE, NW, SE, and SW, and applying expression (11) to each star in the same way as in the previous case, the equations obtained are

$$\begin{aligned}
A_{NE}V_{NE} &= \frac{E_{11}}{2+t}V_{1N} + \frac{W_{11}}{(1+t)(2+t)}V_{3N} + \frac{E_{22}}{2+t}V_{2E} + \frac{W_{22}}{(1+t)(2+t)}V_{4E} \\
&\quad + \frac{E_{12}V_5 - W_{12}V_6 + W_{12}V_7 - W_{12}V_8}{(2+t)^2} \\
A_{NW}V_{NW} &= \frac{W_{11}}{2+t}V_{3N} + \frac{E_{11}}{(1+t)(2+t)}V_{1N} + \frac{E_{22}}{2+t}V_{2W} + \frac{W_{22}}{(1+t)(2+t)}V_{4W} \\
&\quad + \frac{E_{12}V_5 - W_{12}V_6 + W_{12}V_7 - W_{12}V_8}{(2+t)^2} \\
A_{SE}V_{SE} &= \frac{W_{11}}{2+t}V_{1S} + \frac{W_{11}}{(1+t)(2+t)}V_{3S} + \frac{W_{22}}{2+t}V_{4E} + \frac{E_{22}}{(1+t)(2+t)}V_{2E} \\
&\quad + \frac{E_{12}V_5 - W_{12}V_6 + W_{12}V_7 - W_{12}V_8}{(2+t)^2} \\
A_{SW}V_{SW} &= \frac{W_{11}}{2+t}V_{3S} + \frac{W_{11}}{(1+t)(2+t)}V_{1S} + \frac{W_{22}}{2+t}V_{4W} + \frac{W_{22}}{(1+t)(2+t)}V_{2W} \\
&\quad + \frac{E_{12}V_5 - W_{12}V_6 + W_{12}V_7 - W_{12}V_8}{(2+t)^2},
\end{aligned} \tag{16}$$

where the coefficients of the first member are always the sum of those corresponding to the second. The direct sum of these equations gives us a relation between 16 points of the composite star of Fig. 5. Considering the coincidence of points and their potentials, the limit for $t \to 0$ finally results in

$$\begin{aligned}
&(E_{11} + E_{22} + E_{12} + 3W_{11} + 3W_{22} - W_{12})V_0 \\
&\quad = (E_{11} + W_{11})V_1 + (E_{22} + W_{22})V_2 \\
&\qquad + 2W_{11}V_3 + 2W_{22}V_4 + E_{12}V_5 + W_{12}(V_7 - V_6 - V_8)
\end{aligned} \tag{17}$$

which is the f.d.e. expression corresponding to the case presented. A single rotation of the subindex provides the f.d.e. corresponding to similar geometries.

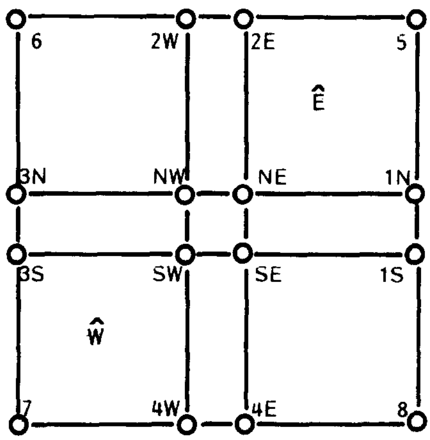

FIG. 5. Composed star including an inhomogeneous layer between **E** and **W** media including an edge.

EXAMPLES OF APPLICATION: DIRICHLET PROBLEMS INVOLVING ANISOTROPIC MEDIA

As an example of the application of the method we present a solution for a Dirichlet problem outlined in Fig. 6. The idea is to find the potential distribution inside a square region. This region is partially occupied by an anisotropic medium limited by the $y = \pm 0.7$, $x = \pm 0.3$ lines. The tensor permittivity eigenvalues are 12 and 3.

The symmetry allows us to predict an antisymmetry with respect to the centre and to reduce the problem to one-half of the region. We will take this semi-region as $y \leqslant 0$.

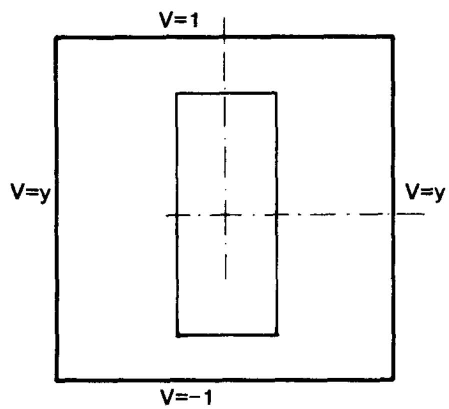

FIG. 6. Contour and boundary in the first example.

TABLE I

		Known potential		29
		Unknown potential:		
		Anisotropic medium	30	
Antisymmetrical contour:		Isotropic medium	122	
Isotropic medium	12	Regular boundary	17	
Anisotropic med.	5	Singular boundary	2	
Regular boundary	2		19	190

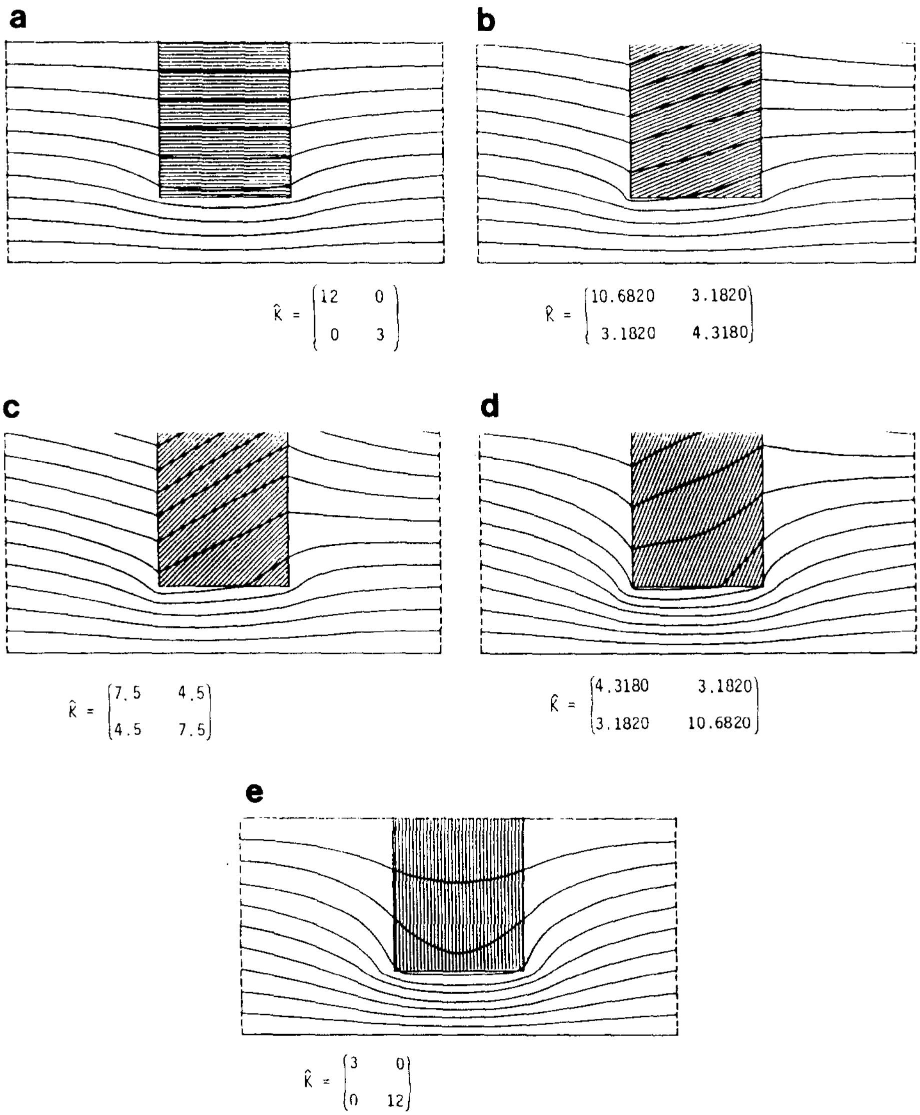

FIG. 7. Equipotential solution lines for different shapes of anisotropic material. The angles between the X-axis and fibre are 0, $\pi/8$, $\pi/4$, $3\pi/8$, and $\pi/2$.

The grid of points is established by means of 10 equidistant lines parallel to the X-axis and 19 equidistant lines parallel to the Y-axis. In this way we have 219 points distributed as shown in Table I.

To solve this problem an iterative over-relaxation method (Frankel and Young method) has been used, with a convergence factor ω estimated as 1.35 [9]. The iteration was carried out until all the residuals were less than 0.001. On this structure, the result for the five trials carried out are presented; for the same material all these were separated into different eigenvector orientations of the tensor permittivity directions. The first and the last correspond to a previous study [8].

In Figs. 7a—e the families of equipotential lines separated by 0.1 units of potential are presented. The shaded region in the dielectric medium in each case indicates the eigen-vector direction which corresponds to the greatest permittivity eigen-value.

Finally, the potential distribution of the problem outlined in Fig. 8 is found. An anisotropic material having empty cylindrical holes, with diameter 0.7 and an axis parallel to the Z-axis, is placed between two parallel electrodes (i.e., $x = 0$, $x = 1$).

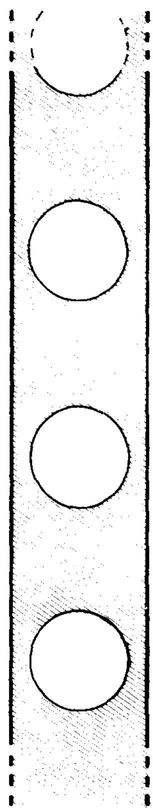

FIG. 8. Pierced dielectric between plane electrodes.

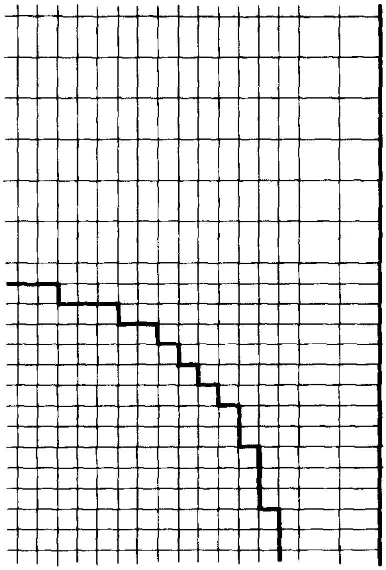

FIG. 9. Pattern grid in the second example.

Tensor permittivity is defined by $K_{11}=9$, $K_{22}=6$, and $K_{12}=4$. The shaded region in the dielectric medium indicates the eigen-vector direction which corresponds to the greatest permittivity eigen-value.

The periodic distribution allows us to reduce this problem to a region with a single hole, considering a suitable expression in this boundary, without taking into account the foreseable antisymmetry.

The grid points are established by two sets of lines, 41 parallel to the X-axis and 30 parallel to the Y-axis (Fig. 9). The polygonal line is the boundary of a hole with a diameter between 0.6994 and 0.7082. (See Table II.)

In this case we have taken 1.80 as the convergence factor and 0.0003 as the maximum residual in a complete iteration. Figure 10 shows families of equipotential lines separated by 0.1 from the potential of the electrodes.

TABLE II

		Known potential		82
		Unknown potential:		
Isotropic medium:		Anisotropic medium	449	
Sym. star $e=w=n=s$	196	Regular boundary	36	
Sym. star $e=w\neq n=s$	324	Singular boundary	68	
Asym. s. $e\neq w$ or $n\neq s$	132	Periodic boundary	62	
Asym. s. $e\neq w$ and $n\neq s$	4		656	1271

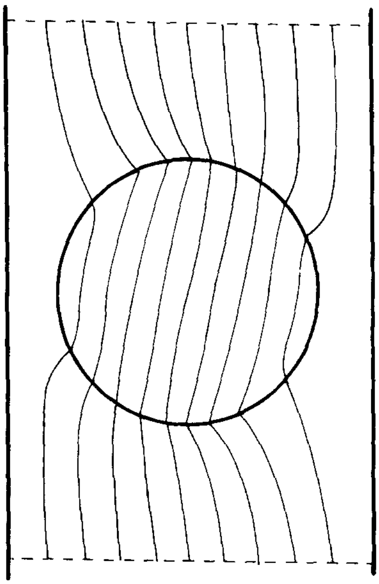

FIG. 10. Equipotential solution lines in the second example.

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