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Note

A Collocation Method for Solving Laplace's Equation

In previous papers (Refs. [1, 2, 3]) a least squares collocation method has been developed for solving Laplace's equation for cylindrically symmetric systems, and the method has been used to give the potential distributions, focal lengths, and spherical aberration coefficients of electrostatic lenses of two and three apertures. The usual relaxation methods were found to be unsatisfactory for giving the potential distributions for these lenses, due to the singular behaviour of the fields at the aperture edges. In the present paper the collocation method is used to calculate the potential distribution for a single aperture, the analytic form of which is known. This enables the accuracy and convergence of the method to be assessed.

1. The Least Squares Collocation Method

Figure 1 represents an aperture of unit radius in an infinite thin flat conducting diaphragm of zero potential, with asymptotic fields to the left and right equal to 0 and -1, respectively. The potential distribution along the axis is known to be [4]

$$\phi(0, z) = \frac{1}{\pi} + z\left(\frac{1}{2} + \frac{1}{\pi}\arctan z\right), \tag{1}$$

where z is measured from the plane of the diaphragm, and the potential inside the aperture (in the plane of the diaphragm) is

$$\phi(r, 0) = \frac{1}{\pi}(1 - r^2)^{1/2}. \tag{2}$$

For the purposes of the following calculations, a cylinder of radius R (>1), coaxial with the axis of symmetry of the aperture, and having zero potential, has been added to the left of the aperture, and a similar cylinder has been added to the right of the aperture, but with a potential equal to z, as shown in the figure. The presence of these cylinders does not affect the potential distribution at large values of $|z|$.

The functions

$$V_{\mathrm{I}} = \sum_{n=1}^{N} A_n \exp(+k_n z)\, J_0(k_n r) \tag{3}$$

and

$$V_{\mathrm{II}} = z + \sum_{n=1}^{N} B_n \exp(-k_n z)\, J_0(k_n r) \tag{4}$$

satisfy Laplace's equation to the left and right, respectively, of the aperture [5], and have the correct asymptotic values at $z = \pm\infty$. They also satisfy the boundary conditions at $r = R$ if the values of k_n are chosen to be the successive solutions of the equation

$$J_0(k_n R) = 0 \tag{5}$$

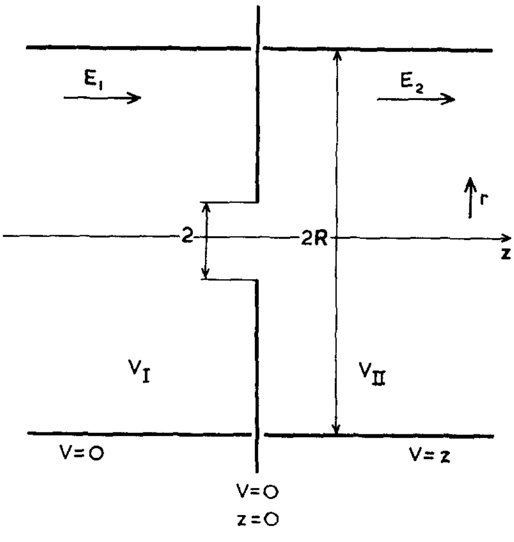

FIG. 1.

If the coefficients A_n and B_n can be chosen so that the boundary conditions at the plane of the diaphragm are reasonably well satisfied, then the potentials V_{I} and V_{II} should be reasonably good solutions for this problem.

The condition that V_{I} and V_{II} should be equal at $z = 0$ is easily satisfied, since the orthogonality relationship for the Bessel functions gives $A_n = B_n$, thus reducing the number of unknown coefficients to N. Because the potential of the diaphragm is zero, one also has that

$$\sum_{n=1}^{N} A_n J_0(k_n r) = s_V(r) = 0 \tag{6}$$

for values of r from 1 to R.

A further condition is that the field in the z direction should be continuous across the aperture, which gives

$$\sum_{n=1}^{N} A_n k_n J_0(k_n r) - 0.5 = s_E(r) = 0 \tag{7}$$

for values of r from 0 to 1. Equations (6) and (7) are therefore the conditions which must be used to give the coefficients A_n.

The method of collocation consists of satisfying Eqs. (6) and (7) exactly at N different values of r between 0 and R, to give the N coefficients A_n. This procedure did not result in convergence as the number N was increased, but instead gave rise to violently oscillating values for the coefficients A_n. For values of r between those chosen, Eqs. (6) and (7) were poorly satisfied. In order to overcome this difficulty a "least squares" method was developed. This consisted in forming the quantity

$$S = \sum_{r=0}^{1} s_E(r)^2 + \sum_{r=1}^{R} s_V(r)^2 \tag{8}$$

and then obtaining N equations from the conditions

$$\frac{\partial S}{\partial A_n} = 0. \tag{9}$$

The total number, M, of collocation points must be greater than N.

The set of linear equations (9) are of the form

$$bA = c \tag{10}$$

where b is a symmetric positive definite $N \times N$ matrix, and A is the column vector of coefficients A_n. This equation was solved either by Gaussian elimination or by Choleski's method [6]. No difficulties were experienced in solving these equations, even when the matrices were of order 210 [2], provided that the elements of b and c were all reduced to the order of unity by multiplying A, b, and c by suitably chosen matrices. All the computational work was done on the Atlas computer at Manchester University. The total computing time required to find the potential distributions, when $N = 70$ and $M = 280$, was 126 secs.

2. Results for the Single Aperture

In all cases the coefficients A_n were calculated, and then these were used to calculate the potential distribution along the axis and the potential distribution in the plane of the aperture, which were then compared with the correct values given by Eqs. (1) and (2), respectively. These results can be further condensed to three numbers, viz., (i) e_0, the error in $\phi(0, 0)$; (ii) e_{axial}, the root-mean-square error in $\phi(0, z)$ (between $z = \pm 2$); (iii) e_{aperture}, the root-mean-square error in $\phi(r, 0)$ (from $r = 0$ to 1).

The electric field is discontinuous and singular at the edge of the aperture. Because of this the most accurate results were obtained by concentrating the collocation points near the edge. In practice, $M/2$ points were equidistantly spaced between 3/4 and 5/4, $M/4$ were equidistantly spaced between 0 and 3/4, and the remaining $M/4$ were equidistantly spaced between 5/4 and R.

To investigate the effect of varying R, the potential distributions were calculated for various values of R, with N and M fixed at 70 and 280 respectively. The results are summarized in Fig. 2. For values of R smaller than those shown, e_0 becomes large and negative. In all the following calculations, R was given the value three.

Figure 3 shows the effect of varying the number of coefficients in the potential expansions. The number of collocation points is taken to be either 280 or $4N$,

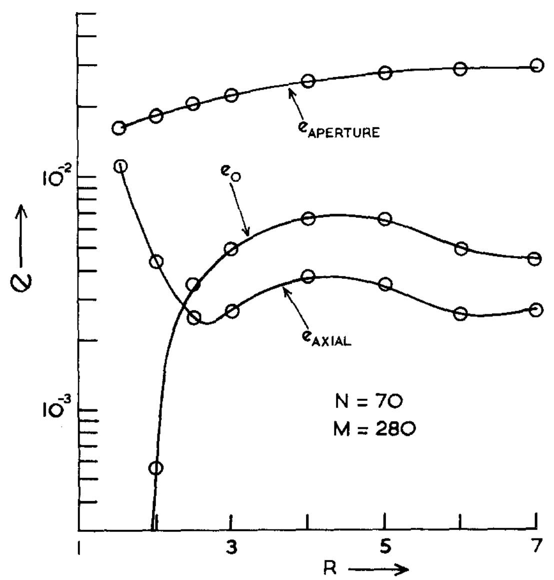

Fig. 2.

as shown. For both e_0 and e_{axial} the variation with N is approximately of the form

$$e \propto N^{-x}, \tag{11}$$

where $x = 1$ for the root-mean-square axial potential error, and $x = 0.75$ for the error in the potential of the midpoint. The lines on the figure show these dependences.

The accuracy of the potential distributions depends, of course, on the accuracy with which the boundary conditions are satisfied. Conversely, one might hope that the accuracy with which the boundary conditions are satisfied may be used to estimate the accuracy of the potential distributions. This was the approach used in the earlier calculations of two and three-aperture lenses [1, 2]. In the present case the boundary conditions are given by Eqs. (6) and (7). Let d_V and d_E be the root-mean-square values of s_V and s_E, respectively (these values being

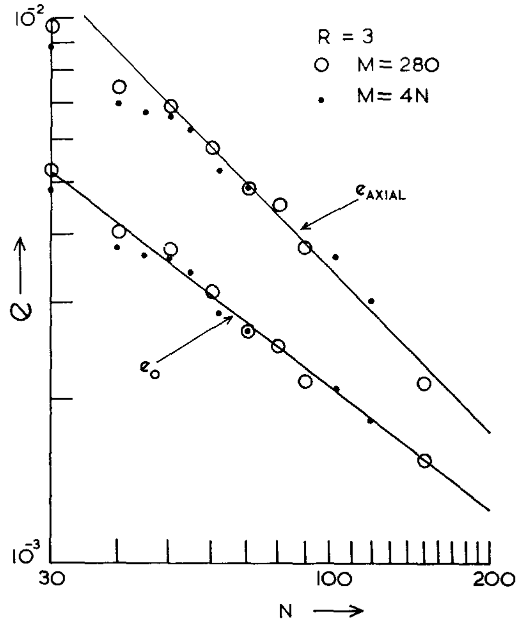

FIG. 3.

computed by taking a large number of values of r which are in general different from these of the collocation points). In general d_V was found to be approximately equal to $4e_{\text{axial}}$. As found in Ref. [1] and [2], the major contribution to d_V comes from values of r near to one.

In general d_E is larger than d_V (the opposite was the case in two and three-aperture lenses), and d_E decreases more slowly than does d_V with increasing N. It seems that d_E is a less reliable guide than d_V to the accuracy of the potential distributions. For the case in which $N = 70$, $M = 280$, and $R = 3$, the actual values of d_V, d_E, e_0, and e_{axial} are 0.011, 0.015, 0.005, and 0.003 respectively.

The above remarks about the boundary conditions do not apply when the number of collocation points is less than about twice the number of coefficients A_n.

Perhaps most attention should be paid to the accuracy of the axial potential distribution, e_{axial}, since it is this which determines the accuracy of calculated lens parameters. In the calculation of the axial potential distributions of lenses of more complicated geometry, it would seem to be a reasonable extrapolation from the results of the present work that the number of collocation points should be larger than twice the number of parameters, that the root-mean-square error in the axial potential should be of the same order as the root-mean-square error in fitting the potential boundary conditions, and that this error is approximately inversely proportional to the number of parameters.

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References

1. F. H. Read, *J. Sci. Instrum. (Proc. Phys. Soc., London, Sect. E)* **2** (1969), 165–169.
2. F. H. Read, *J. Sci. Instrum. (Proc. Phys. Soc., London, Sect. E)* **2** (1969), 679–684.
3. F. H. Read, *J. Sci. Instrum. (Proc. Phys. Soc., London, Sect. E)* **3** (1970), 127–131.
4. P. Grivet, "Electron Optics," Pergamon, London, 1965.
5. E. Weber, "Electromagnetic Fields," John Wiley and Sons, New York, 1950.
6. J. H. Wilkinson, "The Algebraic Eigenvalue Problem," Oxford University Press, 1965.

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