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ABSTRACT

This paper presents some of the preliminary results of Project COEXIST at Dartmouth College, an NSF sponsored project to investigate ways to use computers in introductory physics and mathematics teaching. Students use the computer in a number of ways on homework, on individual projects, and in the laboratory. Students write their own programs, whenever possible. On occasion, it is more useful to have the student programs written and saved by the teacher. Five areas of work are described: (1) illustrations from a broad range of study areas are introduced to show the versatility of computer-connected graphic display devices such as X-Y plotters and cathode ray terminals; (2) a simple, intuitive approach to the propagation of waves in dispersive media is shown; (3) a program is described which can be used to calculate a large number of interference and diffractive patterns; (4) general methods are given to find a map field patterns for general distribution of charges and current loops; and (5) solutions are found to some simple Schrodinger equations using a computer program. (Author/TS)

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Waves in Dispersive Media: Another Use of Computers in
Introductory Physics

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ABSTRACT

This note presents a simple, intuitive approach to the propagation of waves in dispersive media. The method Fourier analyzes a wave pulse, propagates each component according to its wave-vector dependent phase velocity, and then resynthesizes the wave train. The method uses a computer to perform the algebra; a program which minimizes central processor time while maximizing the intuitive content of the calculation is given in the Appendix.

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I. Introduction

Wave propagation is usually limited to non-dispersive media in introductory physics. This limitation is primarily due to the complexity of the algebra of dispersive media. Similarly, Fourier analysis is usually just mentioned in most introductory physics courses. At most, Fourier analysis is applied to a few simple periodic functions. Again the limitation is essentially due to the complexity of the algebra involved -- not the sophistication of the concepts. Both dispersive wave theory and Fourier analysis are fairly simple in concept but algebraically complicated in practice.

This note demonstrates a simple, straight-forward way to introduce wave propagations through dispersive media by means of Fourier transforms. A simple computer program is introduced which Fourier analyzes the pulse, propagates each wave-vector component separately and then resynthesizes the wave. The student supplies the initial pulse shape and a formula for the wave-vector dependent phase velocity of the wave. The program has been used in second semester physics courses with students ranging from pre-medical majors through physics majors. Sophisticated students are able to understand the program and are able to write their own versions.

Use of this computer approach has deepened the student's understanding of non-dispersive wave theory as an approximation to real physical situations. The student's intuitive understanding of expansion processes such as Fourier analysis has also been strengthened.

II. Results

Figure I shows a triangular pulse propagated through a medium of lightly dispersive properties. The phase velocity of the wave is slightly wave-vector dependent in the form $V(k) = V_0 (1 + 0.01k)$. The top curve in Figure I (curve a) is a plot of the initial pulse shape at $t=0$. The origin of the spatial

coordinate ($X=0$) lies at the center of the figure and the right and left sides of the figure correspond to $\pm 4\pi$. All the figures are scaled this way and, within each figure, curves are offset vertically for clarity. Curve b of Figure I is the real part of the Fourier spectrum of the initial pulse; for the simple pulses shown as illustrations, there are no imaginary parts to the Fourier transforms. Curves c, d, e, f, and g in Figure I show the pulse after 2, 4, 6, 8 and 10 units of time has passed. The pulse moves to the right as expected, and, due to the dispersion of the propagation medium, the pulse distorts as time progresses. Components of the wave with wave-vectors greater than the average k vector ($k=0$ in this case) propagate faster than the average of the pulse; lower wave-vector components fall behind. The propagation accentuates the average wave-vector component and produces ripples preceding and following the pulse. This simple model of a lightly dispersive medium corresponds roughly to the edges of an optical absorption band. The present calculation does not include absorption itself, but the program is easily modified to include such effects.

Figure 2 shows the same triangular pulse undergoing ten times stronger dispersion. Now $V(k) = V_0(1+.1k)$ and the effects of dispersion are quite striking. Curves a and b are again the initial pulse and the real part of its Fourier transform. Curves c - f show the pulse after 2, 4, 6 and 8 units of time have passed. The distortion of the pulse follows the lines discussed in Figure I. Again the $k=0$ component is accentuated and higher and lower k components run ahead and fall behind respectively.

Figure 3 shows the effects of the stronger dispersion on a simple model of a wave packet. The original pulse (curve a) is two and one-half cycles of a cosine wave. The (real part of the) Fourier transform demonstrates the peaking near wave-vector components of the basic cosine wave. The Fourier transform also illustrates which wave vector components must be included in order to produce a simple pulse from a cosine wave train. Curves c, d and e (part B of Figure 3) show the real (or cosine) part of the pulse after propagation times of 2, 4 and

6 time units. Again the student observes the spreading of the pulse under the dispersion $V(k) = V_0(1 + ik)$. The spreading now accentuates the wave-vector components in the pulse near those of the basic cosine wave train. Figure 3C (curves f through h) shows the imaginary (or sine) part of the resynthesized pulse after 2, 4 and 6 time units. Figure 3 illustrates that dispersion not only effects the pulse envelope but also the phase relations within the pulse. The student can also examine $\sqrt{\text{Re}^2 + \text{Im}^2}$ or the relative phase as function of position for various times. He can demonstrate energy conservation by examining the total energy in the pulse as a function of propagation time.

Figure 4 shows the effect of propagating phonon wave packets with several basic wave-vectors k_0 through a one-dimensional lattice. The dispersion relation ω vs. k for lattice waves determining the wave-vector dependent phase velocity: $V(k) \propto \sin(ka/2)/k$. Figure 4A shows the initial pulse (curve a) and the Fourier transform (curve b) for a wave packet whose basic wavelength is considerably longer than the lattice spacing ($k_0 a = 1$ so that $\lambda = 2\pi a$). The Fourier transform is again peaked near $k = \pm k_0$, and all but a small fraction of the wave-vector components in the pulse have essentially the same phase velocity. The sharp changes in the initial pulse (i.e. the high wave-vector components) are influenced by dispersion, but the pulse shape remains approximately the same as time progresses. Curves c and d of Figure 4A show the pulse after 12 and 24 time units of propagation.

Figure 4B shows the same information as Figure 4A except that the basic wave length of the pulse is now somewhat closer to the lattice spacing ($k_0 a = 2$). Now a non-negligible fraction of the Fourier components are propagated with different velocities. The propagated pulse (curves g and h) is substantially distorted, and the motion of the center of the pulse (the group velocity) is noticeably less.

Figure 4C shows what happens when the basic wave-length is very near the lattice spacing ($k_0 a=3$). The Fourier transform (curve j) now has peaks near the Bragg reflection planes, and the propagated pulses (curves k, l and m having propagation times of 12, 24, 36 units) are highly distorted. The group velocity is close to zero (as suggested by $d\omega/dk$ at this point). The accentuation of the basic wave-vector is apparent.

Similar dispersive effects in other areas of physics can also be examined. The student can observe the distortions of quantum mechanical wave packets as time progresses or of electromagnetic waves in plasmas and the ionosphere. An interesting example is the propagation of a helicon or whistler wave pulse. The dispersion relation for that magneto-plasma wave has ω proportional to k^2 . The d. c. component of the wave packet sits still and the two dominant k values ($\pm k_0$) in the pulse propagate away.

Figure 5 is a simple test of the procedure which occurs to almost all students. The dispersion of the medium for Figure 5 is zero, that is $V(k) \equiv V_0$. The initial pulse keeps its shape when propagated either forward in time (curves c and d for +2 and +4 time units respectively) or backward in time (curve e for -6 time units). The imaginary or sine part of the resynthesized pulse is everywhere zero on the scale of this figure. Because the method of numerical integration is approximate, "ghost" (illegitimate replica) of the pulse occur for sufficiently large positive and negative wave-vectors. The infinite integral for the Fourier transform is approximated in the present program by a finite sum from -5π to $+5\pi$ in steps of $\pi/16$. This approximation is sufficient for most applications; a better approximation costs more central processor time to accomplish¹.

III. Method

A few comments on the computer method may be useful. The computer strategy is very simple; a form of the program in the Dartmouth form of the language BASIC is given in the Appendix. The program calculates the Fourier integral by the trapezoidal rule since the trapezoidal rule is more accurate than Simpson's rule for nearly periodic functions². The limits on the integral sum and the number of partitions are chosen to follow reasonable detail in the pulse structure and to keep "ghosts" away from the region of interest. To use the program, the student defines the original pulse shape as two functions FNR and FNI, the real and imaginary parts of the initial pulse. These functions are used to fill two vectors (R() and I()) whose elements are called repeatedly in the Fourier transform routine. The use of vectors is considerably faster in central processor time than repeated calls of the defined functions themselves. In programs which calculate Fourier integrals, every shortening of time is advantageous.

Fourier transforms need sines and cosines repeatedly. SIN and COS functions are quite slow on most machines and so vectors (S() and C()) are used. The sines and cosines obtained this way are only accurate to one degree, but this accuracy is usually sufficient. The INT function used to find the right sine or cosine element is usually a very fast function. Another fast form of sine and cosine, this one using the angle sum formulas, is used to fill the sine and cosine vectors initially.

After calculating and storing the real and imaginary parts of the Fourier transform, the transform is printed out as tables. Each Fourier component is then propagated the correct amount using the phase velocity $V(k)$ and the user supplied time. Finally, the resultant, resynthesized pulse is printed. The final result is the pulse as propagated the given time through a medium of supplied dispersion. On the Dartmouth GE635 system, each set of Fourier transforms (which produces a complete spectrum or curve) takes about five central

processor seconds so the student can examine several different propagation times during one RUN.

This computer method is fairly fast and introduces the student to programming methods which conserve computer time. The student is also introduced to real problems in numerical integration, to the practice of Fourier transform theory and to the effects of wave propagation in dispersive media.

IV. Conclusion

This note has presented a simple computer approach to the theory of waves propagated through dispersive media. The introductory student sees dispersive media as an extension of and a comparison to the non-dispersive wave propagation usually introduced in text books. The program given in the Appendix has been used by numbers of students ranging from pre-meds to physics majors at the introductory level. The response has been favorable. The program and illustrations of dispersive wave phenomena are useful from introductory physics courses through upper level solid state, plasma, and quantum mechanics courses.

FOOTNOTES

¹ Using the trapezoidal rule of integration, either larger limits on the integral sum or a finer mesh leads to more central processor time. Other integration schemes can be used. Gaussian-Hermite quadrature using order one-hundred gives about as good results as the trapezoidal rule; clever use of the Gaussian scheme seems to gain about a factor of two in CPU time. The author has not used Gaussian quadrature with classes since the integrations in the program are then complicated to describe. For discussions of more sophisticated integration schemes see A. H. Stroud and D. Secrest, Gaussian Quadrature Formulas, Prentice-Hall, Englewood Cliffs, New Jersey, 1966.

² For comments on this and other points having to do with numerical analysis see B. Carnahan, H.A. Luther, and J. O. Wilkes, Applied Numerical Methods, Wiley and Sons, Inc., New York, 1969.

CAPTIONS

Figure 1. Propagation of a triangular pulse through a lightly dispersive medium.

a) shows the original pulse; b) shows the real part of the Fourier transform of the initial pulse; c) through g) show the pulse after 2, 4, 6, 8, and 10 units of time have passed. The distortion of the pulse is due to the dispersive nature of the propagation medium. The zero of spatial and Fourier transform coordinates is at the center of the figure; the left and right sides of the figure correspond to -4π and $+4\pi$ respectively. All the figures are scaled this way. Curves are separated vertically for clarity.

Figure 2. Propagation of a triangular pulse through a strongly dispersive medium.

a) shows the original pulse; b) shows the real part of the Fourier transform; c) through f) show the pulse after propagating 2, 4, 6, and 8 units of time.

Figure 3. Propagation of a wave packet through a strongly dispersive medium.

A) shows the original pulse and the real part of its Fourier transform. The Fourier spectrum is peaked near plus and minus the wave-vector of the cosine part of the pulse shape. B) The real or cosine part of the pulse after propagating 2, 4, and 6 units of time. C) The imaginary or sine part of the pulse after propagating 2, 4, and 6 units of time.

Figure 4. Propagation of a phonon wave packet through a one-dimensional lattice.

A) Shows the initial pulse, its Fourier spectrum, and its propagation for 12 and 24 time units. This pulse has a wavelength substantially longer than the lattice spacing so the distortion is minimal. B) Shows the effects on a pulse whose basic wavelength is nearer the lattice spacing. The distortion is more noticeable and the group velocity is smaller. C) Shows the effects on a pulse whose basic wavelength is nearly the lattice spacing. The distortion is large, and the group velocity is nearly zero.

Figure 5. Propagation of a triangular pulse through a non-dispersive medium.

The original pulse and its Fourier transform are shown. The pulse after 2, 4 and -6 units of time are also shown. The similarity in pulse shapes gives the student confidence in the simulation method.

FIGURE 1

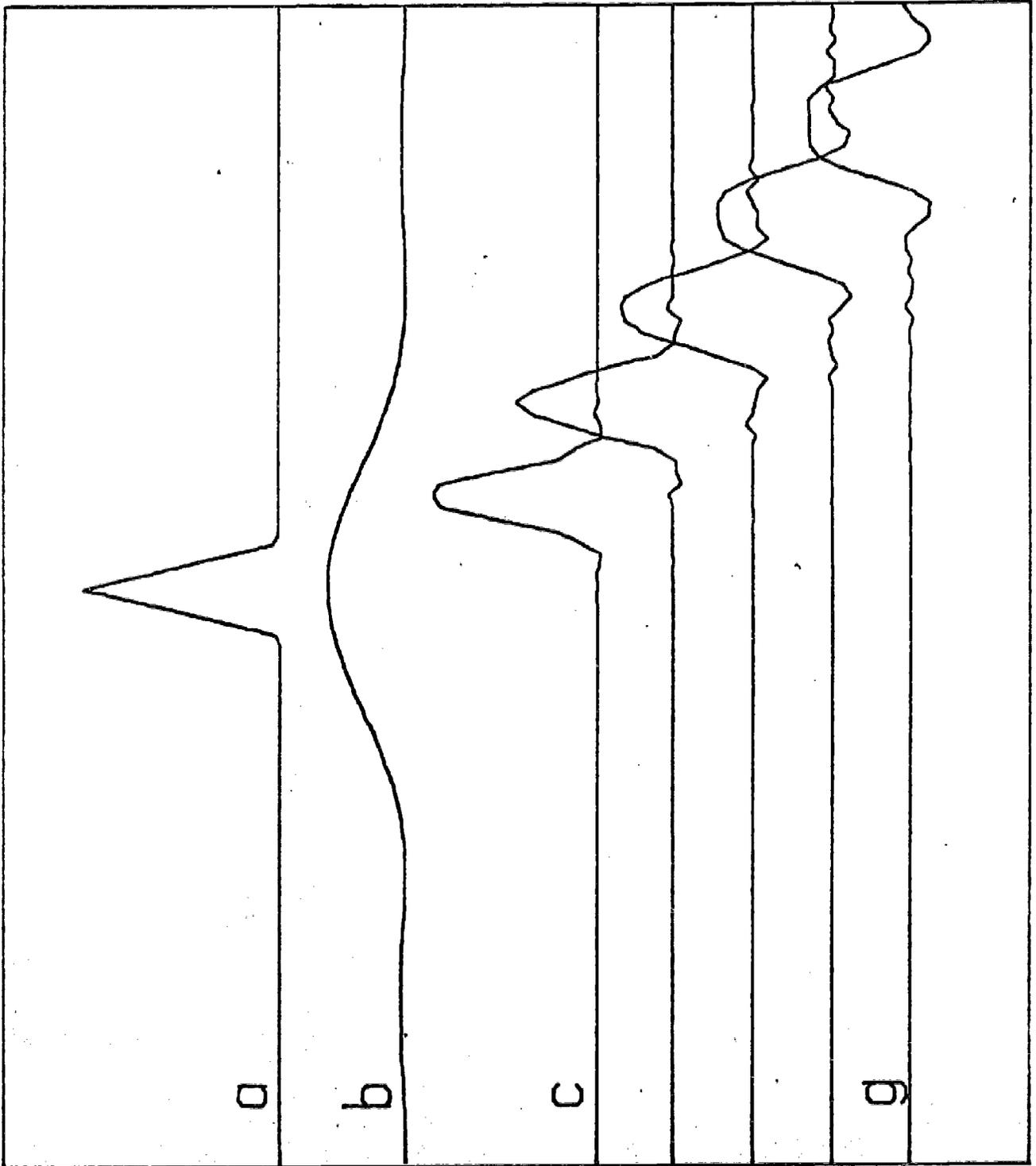


FIGURE 2

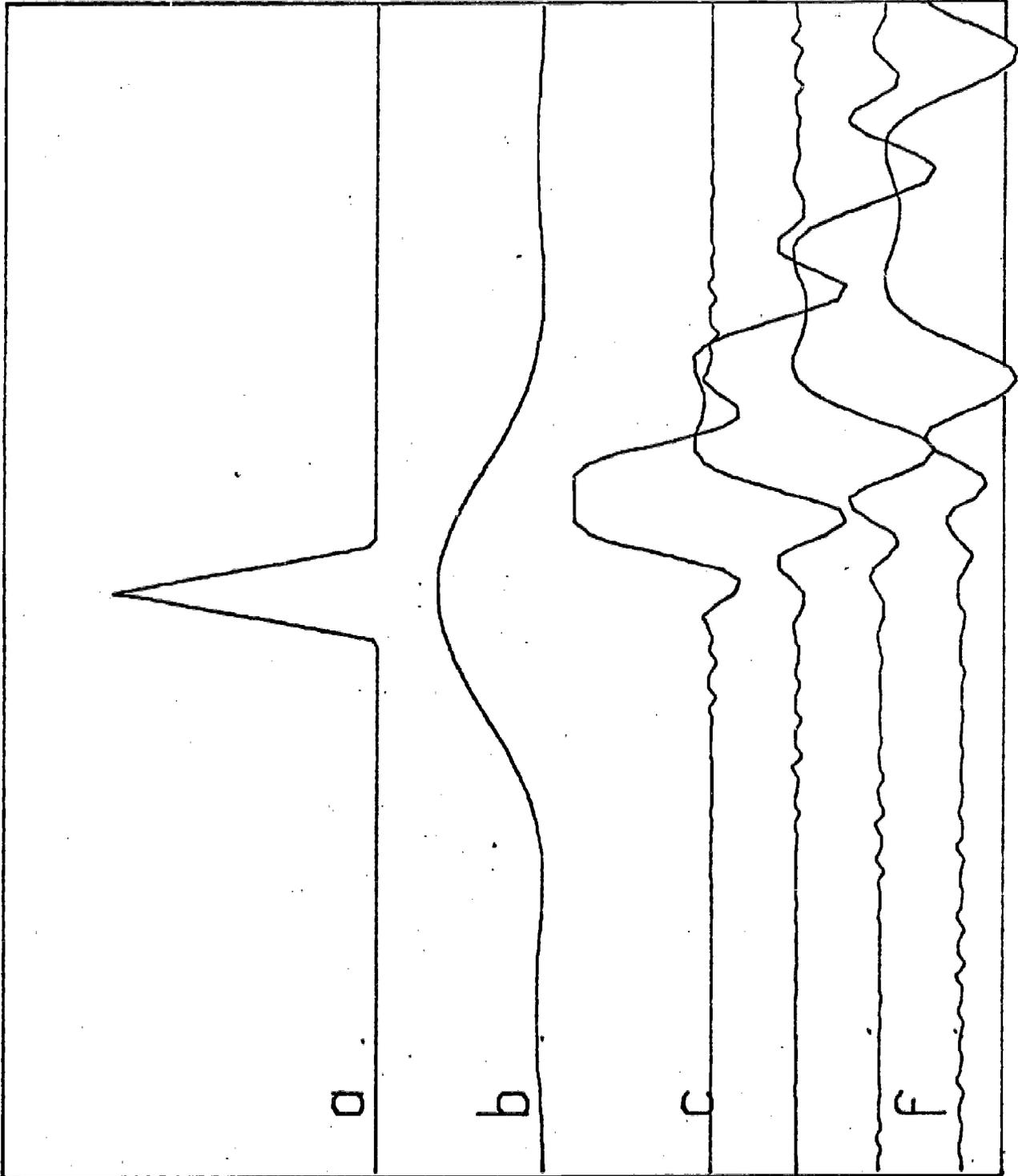


FIGURE 3A

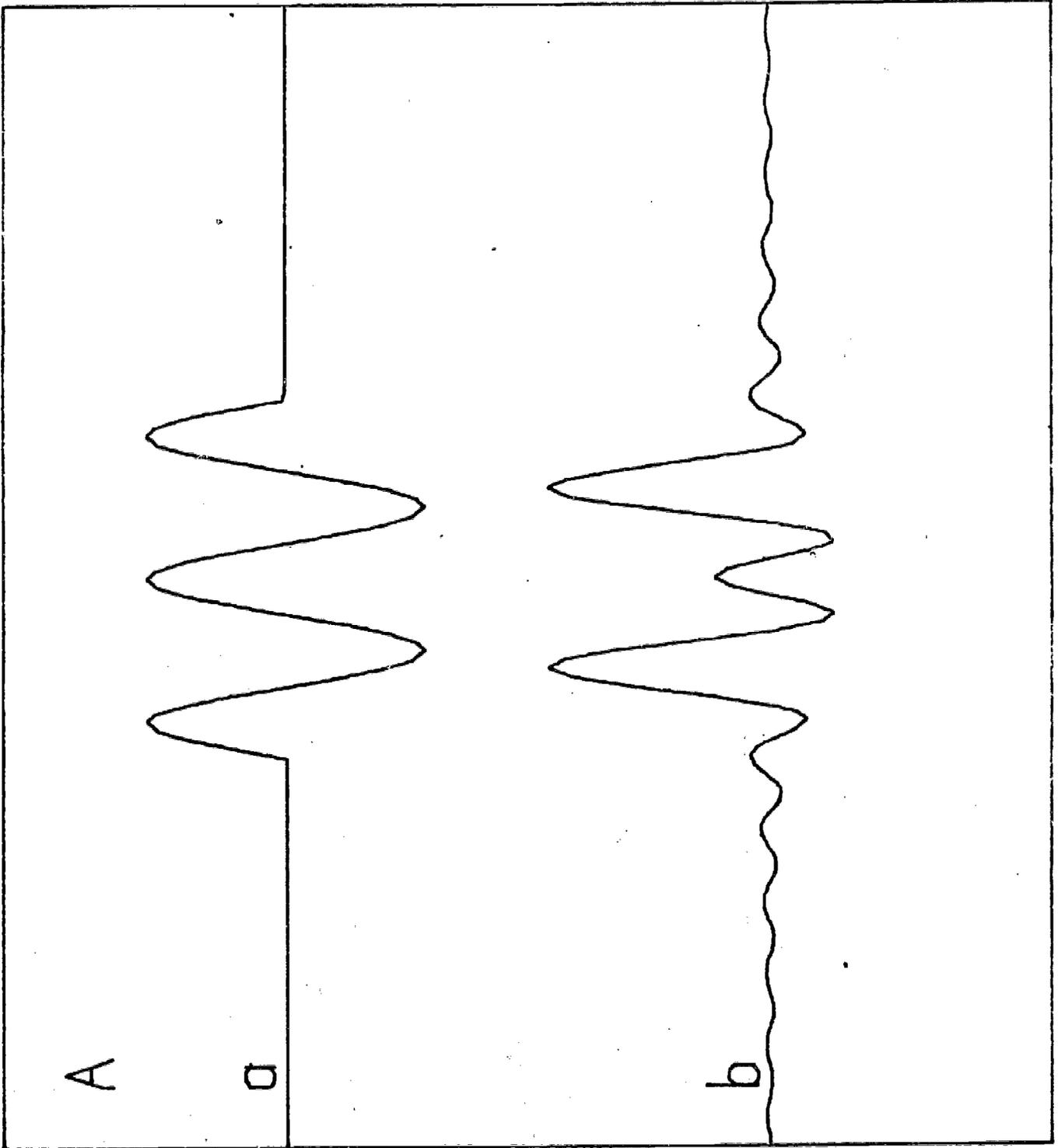


FIGURE 3B

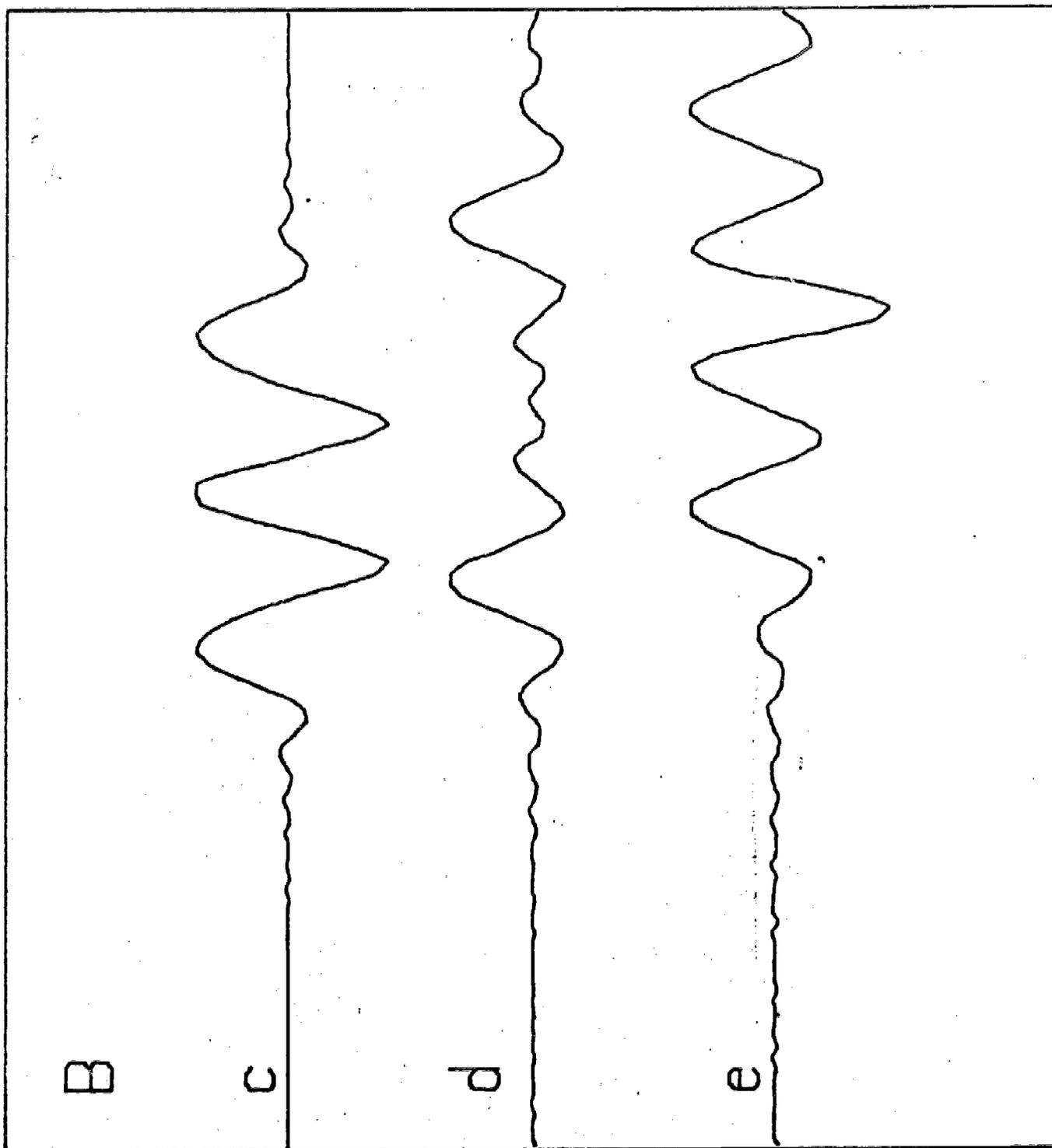


FIGURE 3C

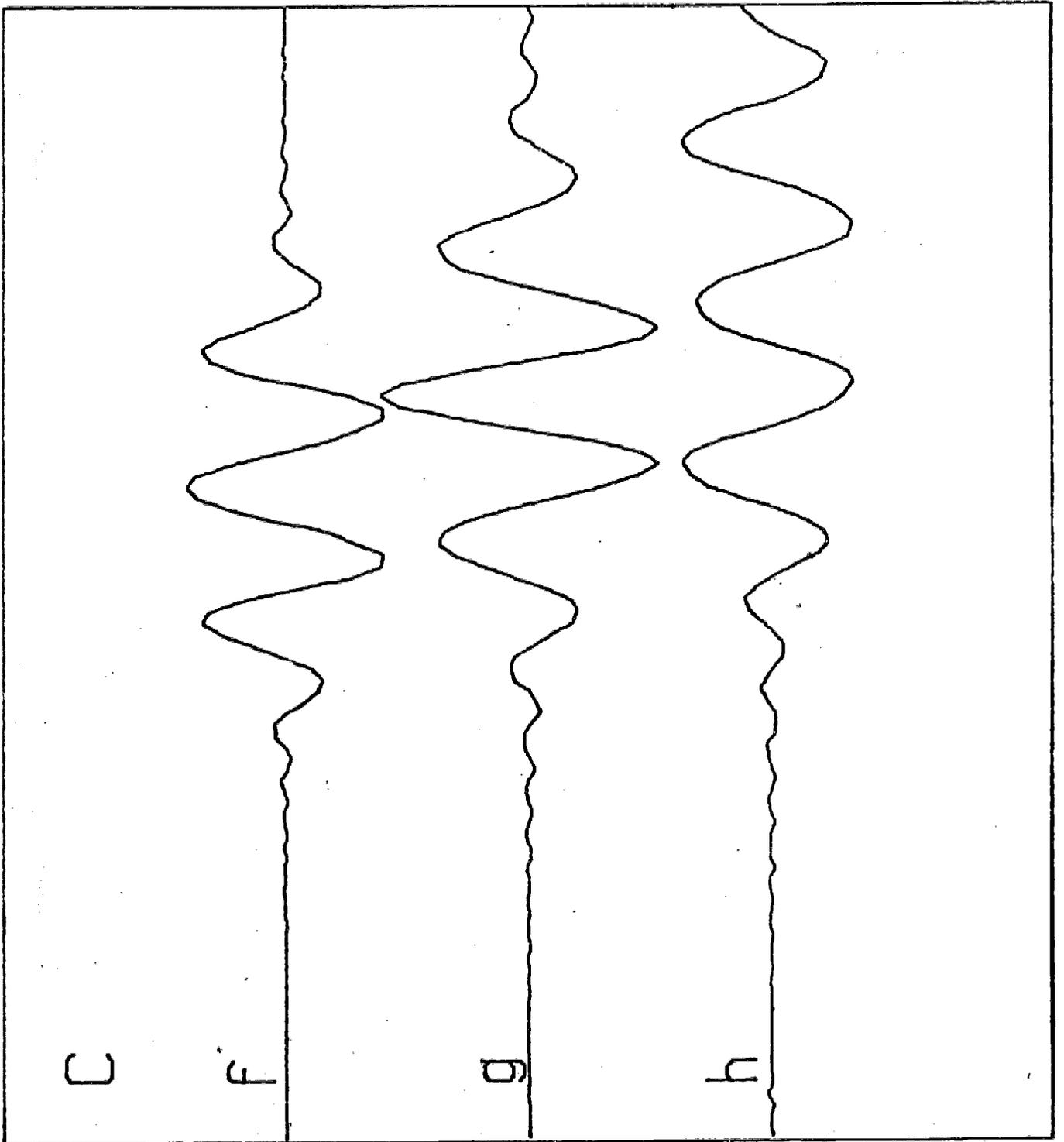


FIGURE 4A

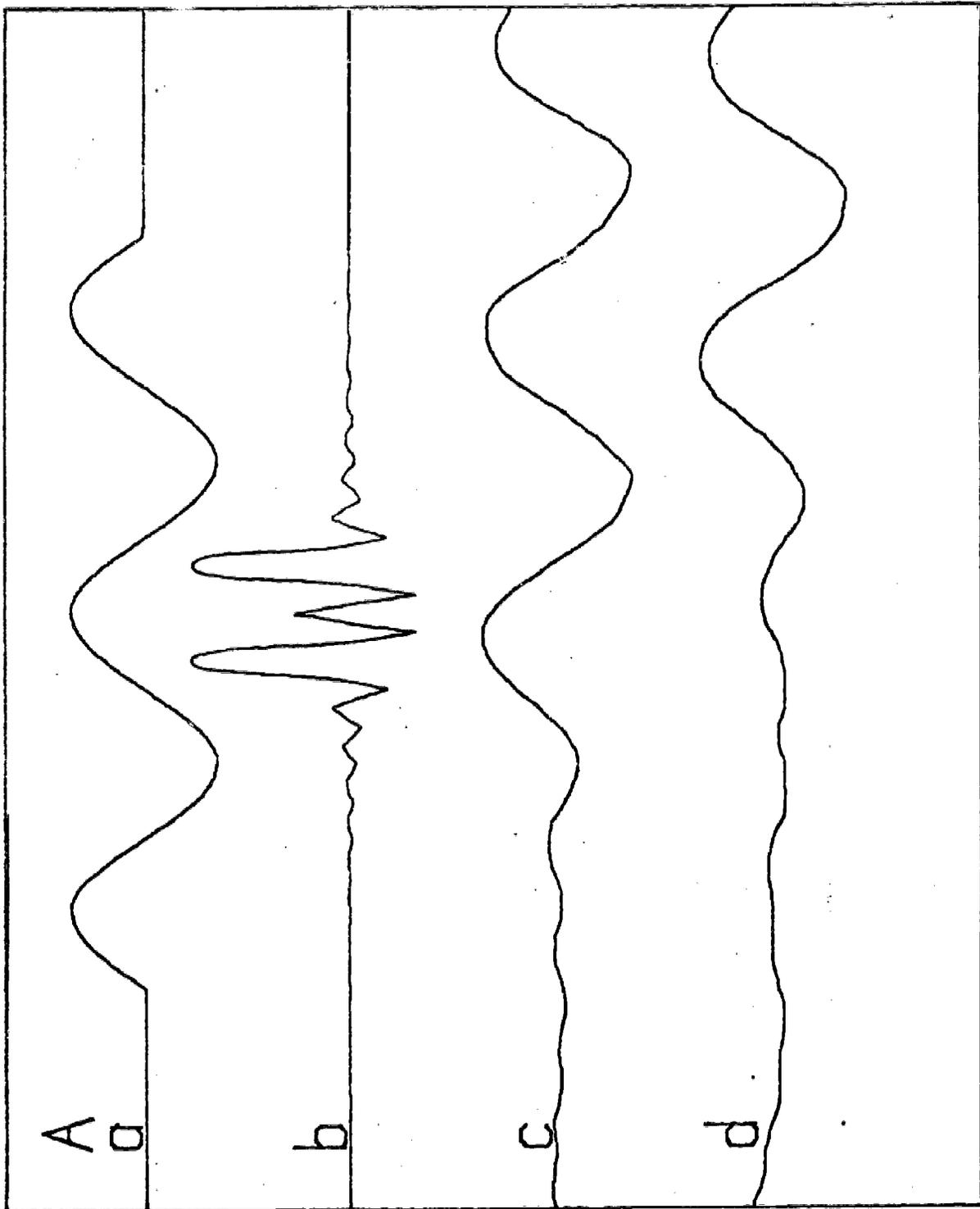


FIGURE 4B

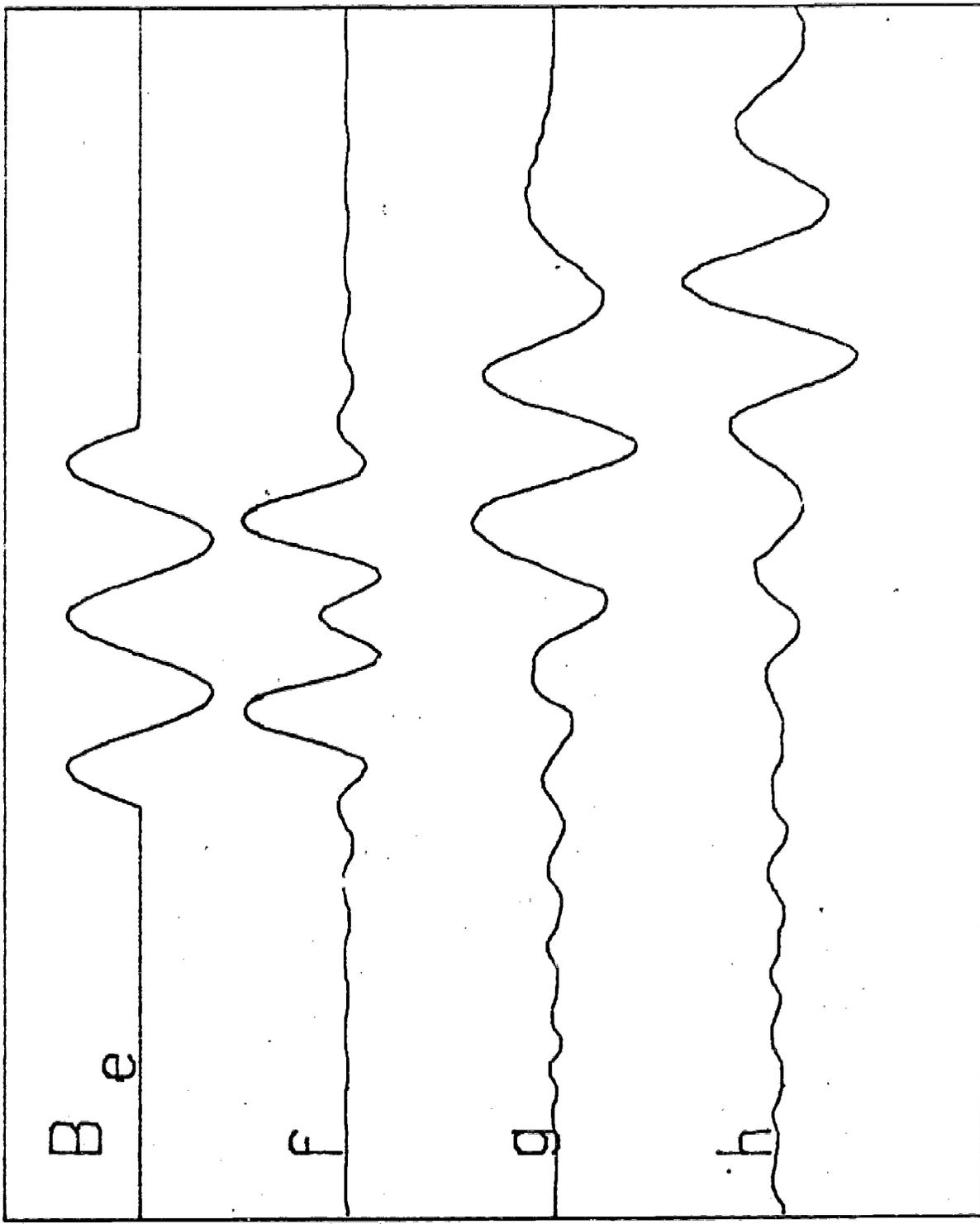


FIGURE 4C

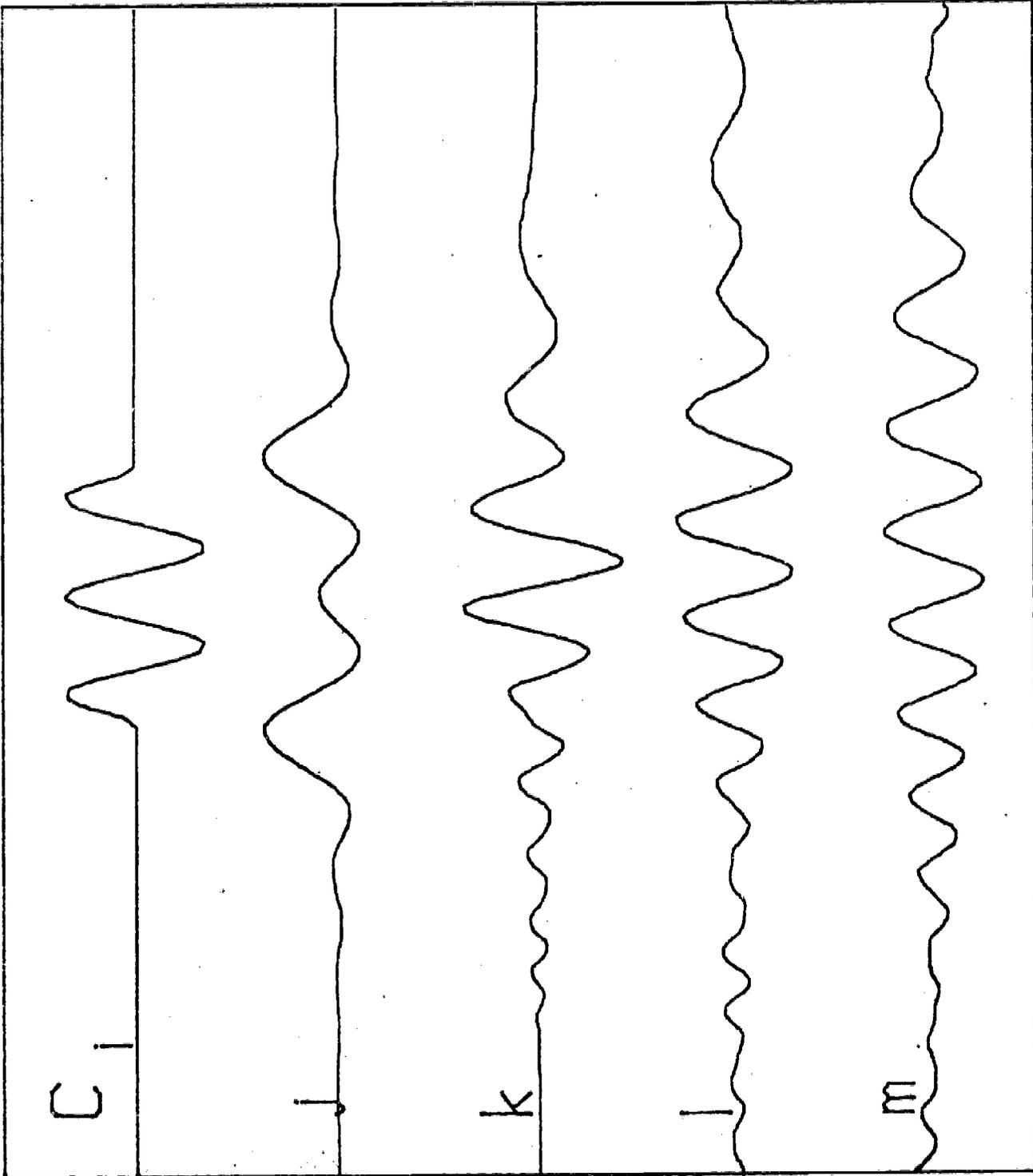
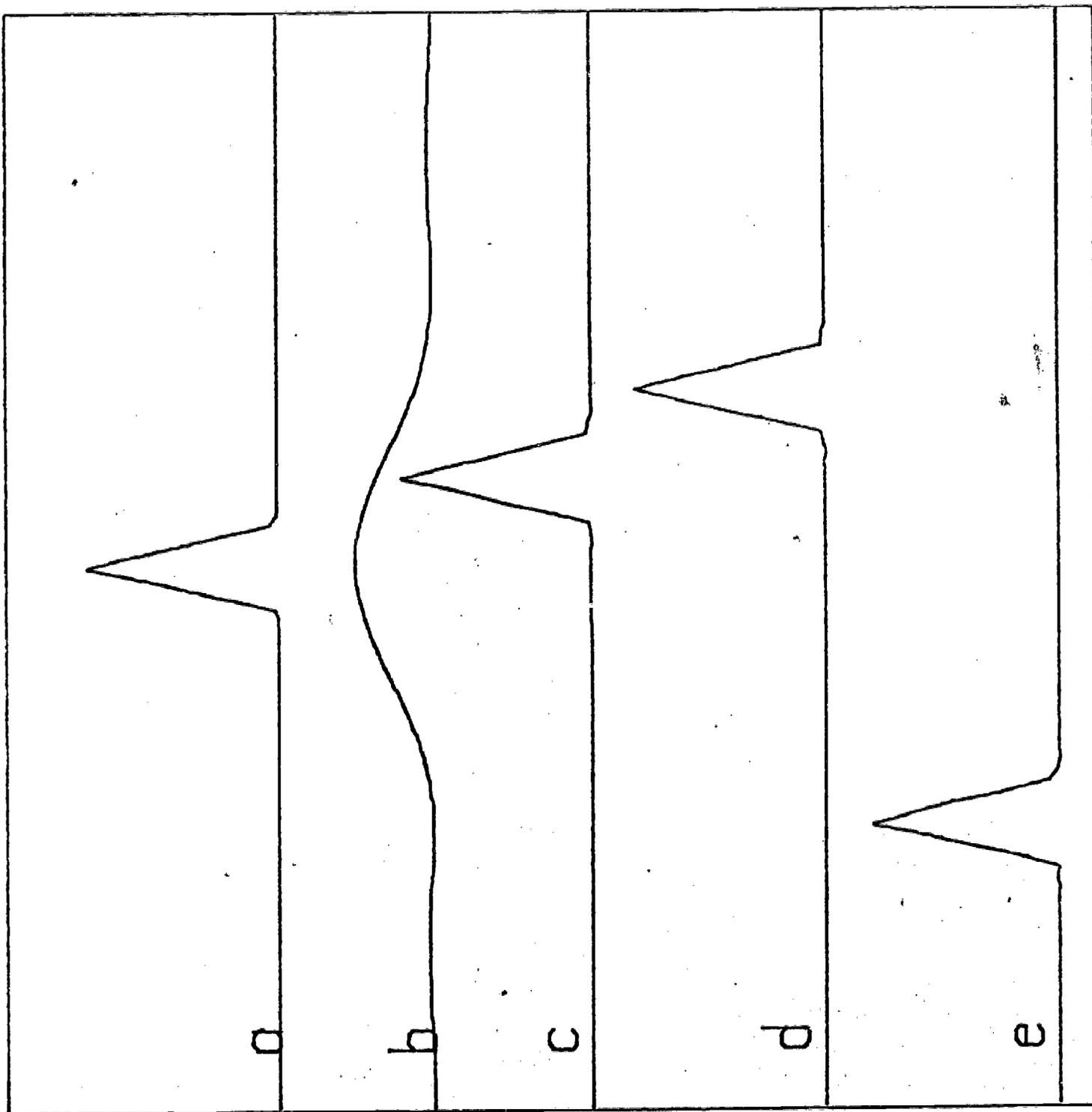


FIGURE 5



APPENDIX

-1-

WAVES

```
100 REM PROGRAM FOURIER TRANSFORMS A WAVE PULSE AND THEN PROPAGATES EACH
110 REM FOURIER COMPONENT SEPARATELY IN TIME. THE VELOCITY CAN BE WAVE-
120 REM NUMBER DEPENDENT SO THAT THE RESULT IS A DISPERSIVE MEDIUM OF
130 REM PROPAGATION. WRITE THE INITIAL PULSE SHAPE INTO FNR,FNI = THE
140 REM REAL & IMAGINARY PARTS OF THE PULSE, AND WRITE THE (K DEPENDENT)
150 REM VELOCITY IN THE PLACE INDICATED.
160 PRINT "PROGRAM CALCULATES THE FOURIER TRANSFORM (BOTH REAL AND"
170 PRINT "IMAGINARY PARTS) FOR THE WAVE PULSE DEFINED IN FNR & FNI."
180 PRINT "IT PRINTS OUT THE FOURIER TRANSFORM AND THEN THE RESULT"
190 PRINT "OF PROPAGATING THE PULSE THROUGH A DISPERSIVE MEDIUM."
200 PRINT
210
220 REM FNR,FNI=RE,IM PARTS OF FN. TO BE TRANSFORMED
230 DEF FNR(X)
240 LET FNR=0
250 LET X2=1
260 IF (X-X2)*(X+X2)>0 THEN 280
270 LET FNR=1-ABS(X/X2)
280 FNEND
290 DEF FNI(X)=0
300
310 REM DEFINE SEVERAL PARAMETERS RELATED TO PI
320 LET P9=3.14159265
330 LET P8=2*P9
340 LET P7=P9/16
350 LET P6=SQR(P8)
360 LET P5=5*P9
370
380 REM FILL FUNCTION VECTORS
390 DIM R(500),I(500)
400 LET I0=0
410 FOR X0=-P5 TO P5 STEP P7
420 LET I0=I0+1
430 LET R(I0)=FNR(X0)
440 LET I(I0)=FNI(X0)
450 NEXT X0
460
470 REM FILL SIN & COS LISTS
480 DIM C(360),S(360)
490 LET P0=P8/360
500 LET C1=COS(P0)
510 LET S1=SIN(P0)
520 LET C(0)=1
530 LET S(0)=0
540 LET C2=1
550 FOR I=1 TO 360
560 LET C3=C2
570 LET C2=C2*C1-S2*S1
580 LET S2=S2*C1+C3*S1
590 LET C(I)=C2
```

-2-

WAVES (CONTINUED)

```
600 LET S(I)=S2
610 NEXT I
620
630 REM CALC. FOUR. TRANSF. FOR RANGE OF K'S
640 PRINT "K","RE(F.T.)","IM(F.T.)"
650 DIM F(500),G(500)
660 LET I9=0 'COUNTER
670 FOR K0=-P5 TO P5 STEP P7
680 LET I9=I9+1
690 LET I1=0 'REAL F.T.
700 LET I2=0 'IMAG F.T.
710 LET I0=0
720 FOR X0=-P5 TO P5 STEP P7
730 LET I0=I0+1
740 LET K9=K0*X0
750 LET K8=INT((K9-INT(K9/P8)*P8)/P0)
760 LET C0=C(K8)
770 LET S0=S(K8)
780 LET R8=R(I0)
790 LET R9=I(I0)
800 LET R1=C0*R8-S0*R9
810 LET R2=C0*R9+S0*R8
820 LET I1=I1+R1
830 LET I2=I2+R2
840 IF (X0-P5)*(X0+P5)<>0 THEN 870
850 LET I1=I1-R1/2
860 LET I2=I2-R2/2
870 NEXT X0
880 LET I1=I1*P7/P6
890 LET I2=I2*P7/P6
900 LET F(I9)=I1
910 LET G(I9)=I2
915 IF INT((I9-1)/8)<(I9-1)/8 THEN 930
920 PRINT K0,I1,I2
930 NEXT K0
940
950 REM RESYNTHESIS AFTER PROPAGATING EACH FOUR. COMPONENT
960 REM BY AN AMOUNT V(K)*T
970 PRINT
980 PRINT " TIME";
990 INPUT T1
995 PRINT "X","WAVE(COS)","WAVE(SIN)"
1000 FOR X1=-5 TO 5 STEP .5
1010 LET I1=0
1020 LET I2=0
1030 LET I0=0
1040 FOR K0=-P5 TO P5 STEP P7
1050 LET I0=I0+1
1060 REM ***PUT V(K) BETWEEN HERE
1070 LET V0=1+.01*K0
```

WAVES (CONTINUED)

```
1080 REM ***AND HERE
1090 LET K9=K0*(X1-V0*T1)
1100 LET K8=INT((K9-INT(K9/P8)*P8)/P0)
1110 LET C0=C(K8)
1120 LET S0=S(K8)
1130 LET R8=F(I0)
1140 LET R9=G(I0)
1150 LET R1=C0*R8+S0*R9
1160 LET R2=C0*R9-S0*R8
1170 LET I1=I1+R1
1180 LET I2=I2+R2
1190 IF (K0-P5)*(K0+P5)<>0 THEN 1220
1200 LET I1=I1-R1/2
1210 LET I2=I2-R2/2
1220 NEXT K0
1230 LET I1=I1*P7/P6
1240 LET I2=I2*P7/P6
1250 PRINT X1,I1,I2
1260 NEXT X1
1270 GOTO 980
1280 END
```

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Computers and Introductory Interference Phenomena[†]

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ABSTRACT

This note presents a simple program which can be used to calculate a large number of interference and diffraction patterns. Several applications of the method are discussed; radio antennas are emphasized. In class use, the student writes his own program and calculates intensity patterns for interference systems of interest to him.

[†]Work supported by the National Science Foundation Foundation (NSF-GJ-650)

Introduction

This note describes some uses of the computer in practical applications of wave interference. Although the applications discussed are complicated to handle in closed, analytic form, they are easy to understand with the computer. The computer program propagates waves out from any number of wave sources to some point on a large sphere. The program then adds the amplitudes of all the waves (including phase) at that point, squares the result to get the total intensity, and averages over a complete cycle of the sources. One straightforward practical application of this method is to "broadside arrays" of radio antennas.¹

Most students have seen broadside arrays. A radio station will place a number of antennas in an equally spaced row, the plane of the antennas facing a city. The station feeds the antennas with radio frequency currents of certain relative amplitudes and phases. The result is a highly directional transmission of the station's power, usually directly toward the city.

The simplest broadside array feeds equal amplitude, in-phase currents to the N antennas. The antennas are often one-half wavelength apart. The transmission pattern is the N slit diffraction pattern. It is common to express the transmission pattern as a polar plot of intensity versus angle around the sources. Plotting the results in this way affords the student a comparison to typical diffraction patterns in physics which show the intensity pattern across a screen placed parallel to the plane of wave sources (or slits).

Results

Figure 1 shows the polar plot of the transmission pattern for two antennas separated by two wavelengths and fed with equal amplitude, in-phase currents. There are two sets of three maximum intensity lobes in the forward and backward directions; there are broad maxima in the side directions. This is also a polar plot for the intensity pattern of a double slit diffraction experiment (narrow slits placed $\lambda/2$ apart).

Figure 2A shows a more common broadside array - four antennas placed half wavelengths apart and fed equal, in-phase currents. The increased directionality is clear from the polar plot of intensity. Figure 2B is the polar plot for a "binomial broadside array" in which the currents fed to the antennas are in the ratio of binomial coefficients.¹ The transmission pattern has no power wasted in side lobes; all the intensity is radiated in the forward and backward directions.

More complicated arrays are sometimes used. The "optimal array" has a complicated set of relative amplitudes of the feed currents. Two dimensional arrays are sometimes used, usually at high radio frequencies. The student can even consider Yagi-Uda arrays such as those used in TV reception antennas. The reception pattern of an antenna system is simply related to its transmission pattern. The method presented here can also be applied to interferometric radio telescopes, interference patterns through thin films, or the diffraction pattern of the sound emitted from a loud speaker. Using secondary waves, the student can model intensity patterns in auditoria. In all these problems, the method adds up waves from a finite (but sometimes large) number of distinct sources having different relative amplitudes and phases.

Program

All the cases mentioned above can be treated by a very simple computer program. Figure 3 is such a program in BASIC. The relative amplitudes of the N wave sources are stored in the vector $A()$; the relative phases are stored in $P()$; and the positions of the sources are stored in $X()$ and $Y()$. The wavelength of the waves is L . The program calculates the intensity I_0 (averaged over a period of the wave) at 10 degree intervals (angle T) around a circle of radius 10 . The average over one cycle in phase is performed by the FOR-NEXT loop on $P0$. The fundamental loop which adds the wave amplitudes from the N sources is lines 230 through 290 (7 statements). As written, the program calculates the intensity as a function of angle for two source interference. Figures 1 and 2 were plotted directly from output of a program such as that shown in Figure 3.

Conclusion

The program discussed in this note can be used with the smallest computers. The method is easy to explain even to the most mathematically unsophisticated students. The method of the program is entirely general and covers a very large number of applications of interference and diffraction phenomena.

References

- ¹See Reference Data for Radio Engineers, H.P. Westman, ed., International Telephone and Telegraph Corp., N. Y., N. Y. (1967).

Captions

- Figure 1. Polar plot of the intensity pattern for two sources, two wavelengths apart. The program allows any number of sources to be placed anywhere in the plane; the program then calculates a polar intensity pattern.
- Figure 2. Polar plot of the intensity pattern for four element radio antenna broadside arrays. The antennas are placed half wavelengths apart so maximum transmission is in the forward and backward directions. A) Simple broadside array.
B) Binomial broadside array.
- Figure 3. BASIC program to calculate interference patterns. The positions $X()$, $Y()$ of the N wave sources which emit waves of wavelength L , relative amplitudes $A()$, and phases $P()$ are READ in from DATA. The fundamental loop adding the waves from the sources is lines 230 through 290.

FIGURE 1

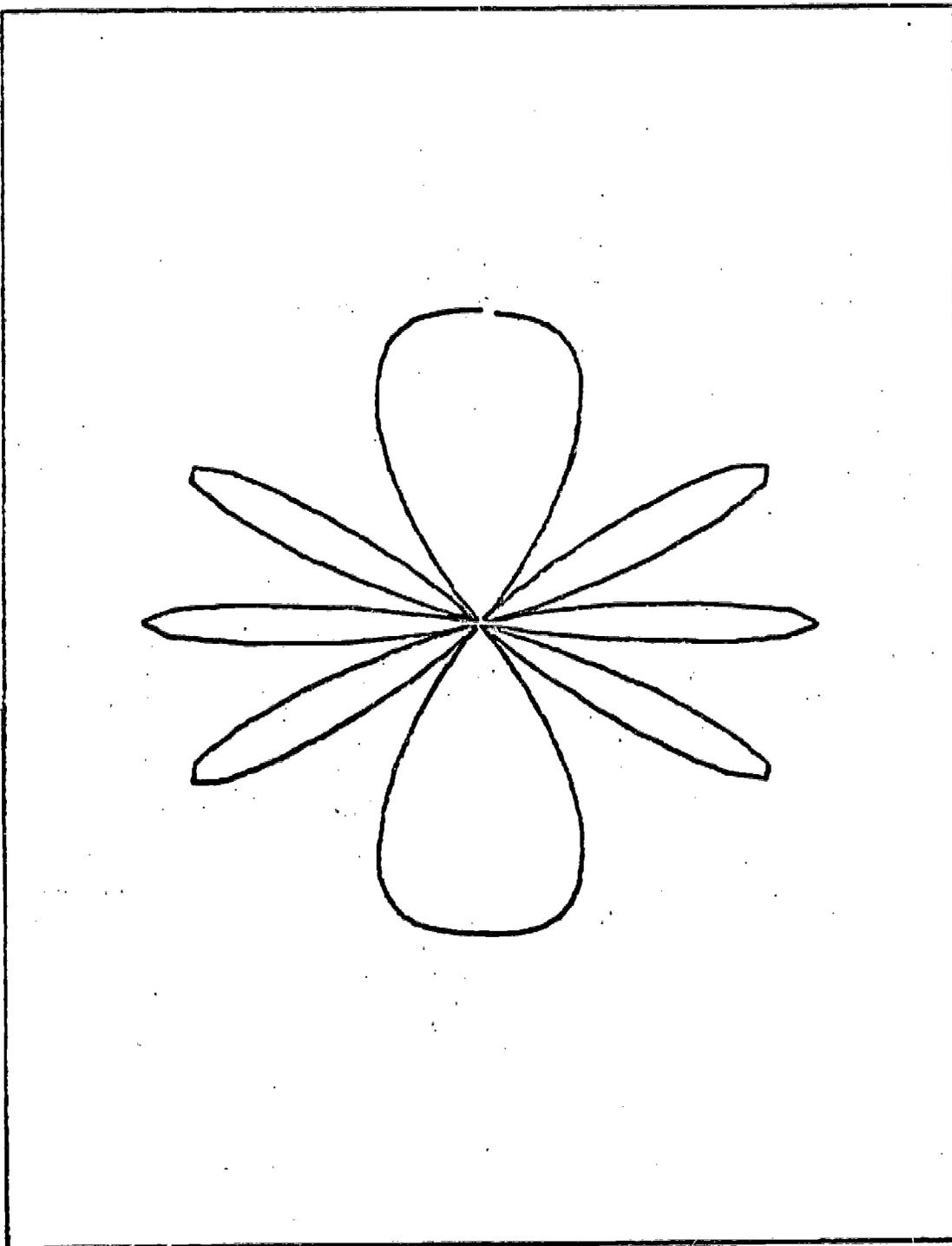


FIGURE 2

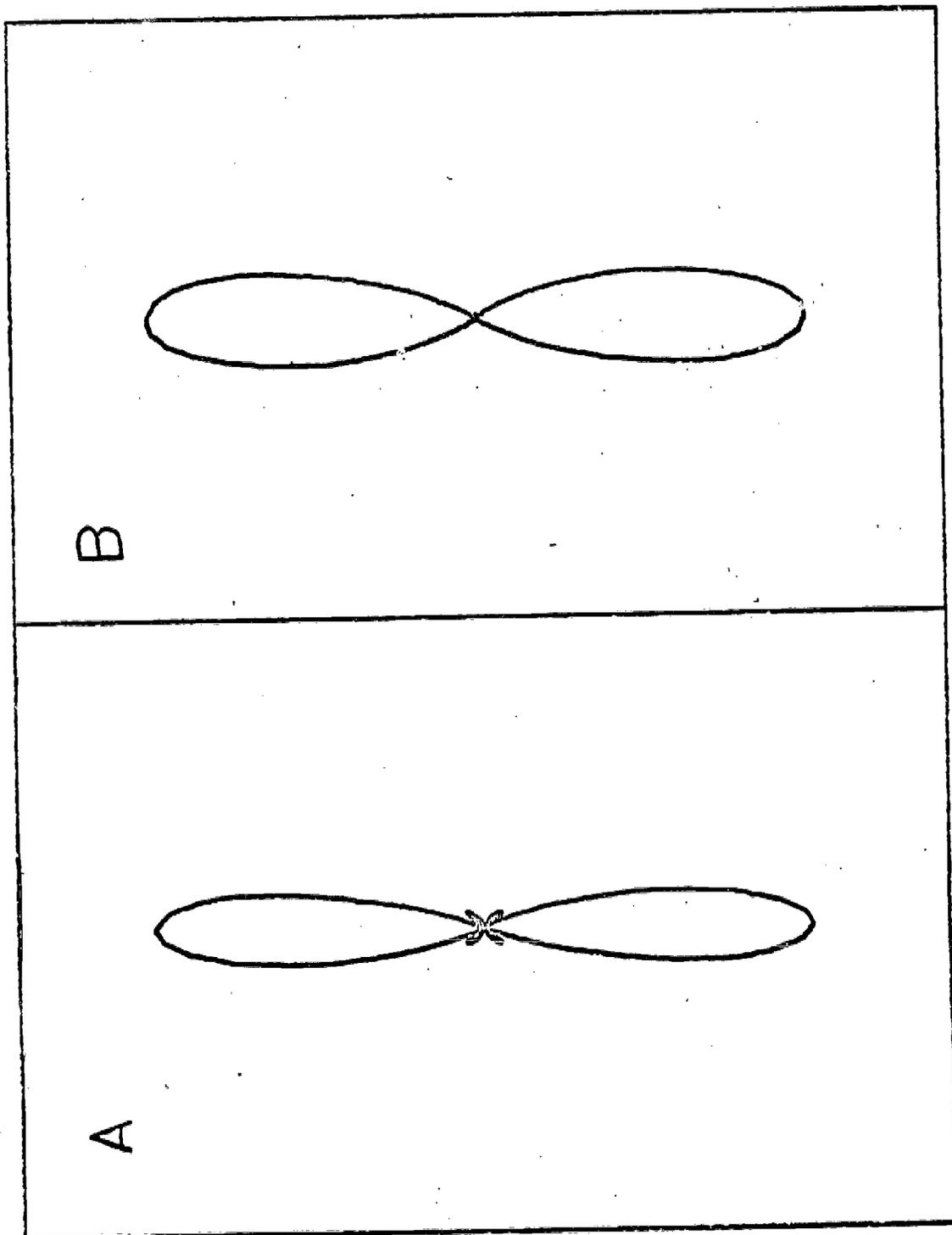


FIGURE 3

```
100 REM SIMPLE VERSION OF I VS ANGLE
110 READ N,L
120 FOR I=1 TO N
130 READ X(I),Y(I),A(I),P(I)
140 NEXT I
150 DATA 2,1
160 DATA .5,0,1,0, -.5,0,1,0
170 PRINT "ANGLE","INTENSITY"
180 FOR T=0 TO 6.28318 STEP 3.14159/18
190 LET XO=10*COS(T)
200 LET YO=10*SIN(T)
210 LET IO=0
220 FOR PO=0 TO 6.28318-3.14159/8 STEP 3.14159/8
230 LET A=0
240 FOR I=1 TO N
250 LET X=XO-X(I)
260 LET Y=YO-Y(I)
270 LET R=SQR(X*X+Y*Y)
280 LET A=A+A(I)*SIN(6.28318*R/L + PO)
290 NEXT I
300 LET IO=IO+A*A
310 NEXT PO
320 PRINT 180*T/3.14159,IO/8
330 NEXT T
340 END
```

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SOME USES OF COMPUTERS IN INTRODUCTORY ELECTRIC AND MAGNETIC FIELD MAPPING

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INTRODUCTION

Past publications concerning the uses of the computer in field mappings have stressed particular geometries for the charge distributions¹. This note presents general methods to find and map field patterns for general distributions of charges and current loops. Two fundamental programs are presented with illustrations of the student's uses of both. Both programs use subroutines as building blocks so that the student can write programs using very simple calls to subroutines. The programs are given in appendices in the language BASIC as implemented on Dartmouth's time-sharing computer system.

GENERAL ELECTROSTATIC FIELDS

The first program allows students to map electric field lines and equipotentials for an arbitrary number of point charges placed anywhere in the plane. The program could also map fields of line charge distributions or any combination of line charge and point charge distributions. The program just needs an expression for the electric field \vec{E} (due to the charge distribution) everywhere in space. Thus the program can perform the calculations for uniformly charged spheres, if one wishes

The strategy of the program is as follows:

The program to follow electric field lines first chooses the starting point for the field line; second, calculates the electric field in the X and Y directions at that point; third, uses the differential equation for a field line to take a small step (along the field line) to a new point in space. Finally, the program goes back to the second step and repeats the calculation.

For equipotentials, the program first chooses the starting coordinates for the equipotential; then, second, calculates the electric field at that point; then, third, moves a small step perpendicular to the electric field \vec{E} to find a new point on the equipotential. Finally the calculation goes back to the second step and repeats itself.

The method only needs to calculate the electric field \vec{E} at each point in space. The steps taken along the field lines or equipotential surfaces must be small enough to be treated as differentials. This latter demand is more simply stated by saying that the numerical approximation to the integration of the differential equation must converge. The initial choice of starting coordinate may be a set of inputted coordinates X, Y or could be the result of a hunting routine to find, say, some point on the 2 volt equipotential.

Figures 1 thru 4 show the results of these calculations for several configurations of point charges. Figure 1 is the field lines and equipotentials for three, equal, positive charges placed on the corners of an equilateral

triangle. Notice that the starting points for the equipotentials were chosen in such a way that equal steps in potential occurred. Figure 2 shows the field lines and equipotentials for a system of four, equal, positive charges placed on the corners of a square. Figure 3 shows the field lines and equipotential surfaces in the plane of a two dimensional quadrupole (two positive and two equal, negative charges on opposing corners of a square). Notice that the starting points for the field lines were not chosen quite symmetrically. Figure 4 shows the field lines and equipotential surfaces in the plane of a one dimensional quadrupole (two back-to-back dipoles).

Charge distributions even as simple as these are not usually given in introductory physics courses simply because of the complication of the closed form solutions to these problems. Using the iterative techniques, outlined above, the problem is not only tractable but even easy for the introductory student to understand and to compute by himself.

CRITICAL PARTS OF THE STRATEGY

Two separate parts of these calculations deserve a little attention. First, how does one calculate movement along a field line? Consider taking a step ΔS from a point X, Y at which the electric field has components E_x , and E_y . Using the fact that the triangle with sides dX , dY , and dS is similar to the triangle having sides E_x , E_y and $\sqrt{E_x^2 + E_y^2}$

$$\Delta X = \Delta S (E_x / \sqrt{E_x^2 + E_y^2})$$

$$\Delta Y = \Delta S (E_y / \sqrt{E_x^2 + E_y^2})$$

Finally, then, the new coordinates X, Y are just the old coordinates X, Y plus ΔX and ΔY . The fact that E lines are everywhere tangent to the electric field \vec{E} leads to these simple equations for integrating along a field line.

This process is easily introduced to a student. The student can then use the procedure as a subroutine, which is general enough to be available for any field mapping problem.

The second part of the calculation which deserves a little attention is following an equipotential. Consider stepping the distance ΔS perpendicular to the electric field \vec{E} at the point X, Y . Use the fact that the slope of a line perpendicular to a line of slope K has, in turn, the slope $-1/K$. Then for a step ΔS along the perpendicular to the electric field one has

$$\Delta X = -\Delta S (E_y / \sqrt{E_x^2 + E_y^2})$$

$$\Delta Y = +\Delta S (E_x / \sqrt{E_x^2 + E_y^2})$$

Finally, again the new X, Y is just the old X, Y plus ΔX and ΔY .

Using subprograms such as these, the student can write his own programs to perform more complicated calculations of various types. Appendix I shows such a program finding electric field lines and equipotentials for an arbitrary point charge distribution. The program is written in the Dartmouth form of the language BASIC. Notice that, since this form of the language BASIC has global variables, the calls to subroutines are more cumbersome than they are in languages such as FORTRAN. This is one of the few cases in which FORTRAN is easier for the student to use than is the language BASIC. Some newer forms of BASIC will use local variables in subroutines.

GENERAL MAGNETOSTATIC FIELDS

The second fundamental program reported in this note calculates the magnetic field \vec{B} at any point in space due to a current loop (which is parallel to the X, Y plane at some point Z). The program simply uses the Biot-Savart law and integrates around the current loop. The student then uses

this program (as a subroutine) to calculate magnetic fields due to such current loop configuration as Helmholtz pair, or even a short solenoid (treated as a number of separate loops placed next to each other along the Z axis). Another interesting program calculates the field at some point X,Y,Z due to a straight wire segment. When used as a subroutine, this straight wire program can do another set of interesting current geometries.

After calculating the magnetic field \vec{B} at some point, the student can call the field line subroutine, considered above, and then plot field lines for the coil configuration. Figures 5 and 6 show plotted results from programs such as these. Figure 5 is a magnetic field line pattern for a single loop around the origin. This problem is sufficiently complicated that in closed form it is not normally given to introductory students. Again, since the calculation is, first of all, iterative and, second of all, based on using subroutines as building blocks in programs, the introductory student has no difficulty understanding this approach to a fairly complicated problem. Figure 6 is the magnetic field lines for a Helmholtz pair. Notice that the homogeneity in the central field region is clear, as is also the symmetry of the inhomogeneous part of the field. Other interesting figures can also be introduced. For example, if the student treats a short solenoid as a series of current loops placed near each other, not only does he observe (in the plotted field lines) the obvious homogeneity and additive character of the field from the various loops, but he also sees immediately the effects of his approximation. Because the student has made discrete what is more closely approximated by a continuous current loop distribution, there is imposed on the homogeneous field an inhomogeneous ripple with the periodicity of his chosen loops.

MAGNETIC LOOP SUBROUTINES

The strategy of the subroutine which calculates the magnetic field at a point X,Y,Z due to a current loop is as follows: The program, first, breaks the loop into segments. The program then takes the cross product of the loop segment and the X,Y,Z vector from the origin to the observation point. The program then divides by R^3 and sums the result over the loop segments. This subroutine is very easy to program and is also very easy for the student to understand. Having written the subroutine, the student simply calls this subroutine (and perhaps others) to plot field lines. The student uses a building block approach, putting blocks together to form the structure he wishes. Appendix II contains a loop subroutine and a program which calls this subroutine and calculates the magnetic field at any point in space due to a single loop.

CONCLUSION

This note has presented several programs to solve general field mapping problems in electrostatics and magnetostatics. Students are encouraged to write programs as blocks using the subroutine capabilities of even simple languages such as BASIC. The student can then write driver programs (main programs) which are both particularly simple and also intuitively easy to understand. The student response to systems such as this has been very good. Calculations based on these programs have instilled in the students a much deeper, and more intuitive understanding of field patterns due to electric charge distributions and magnetic fields.

FIGURE 1

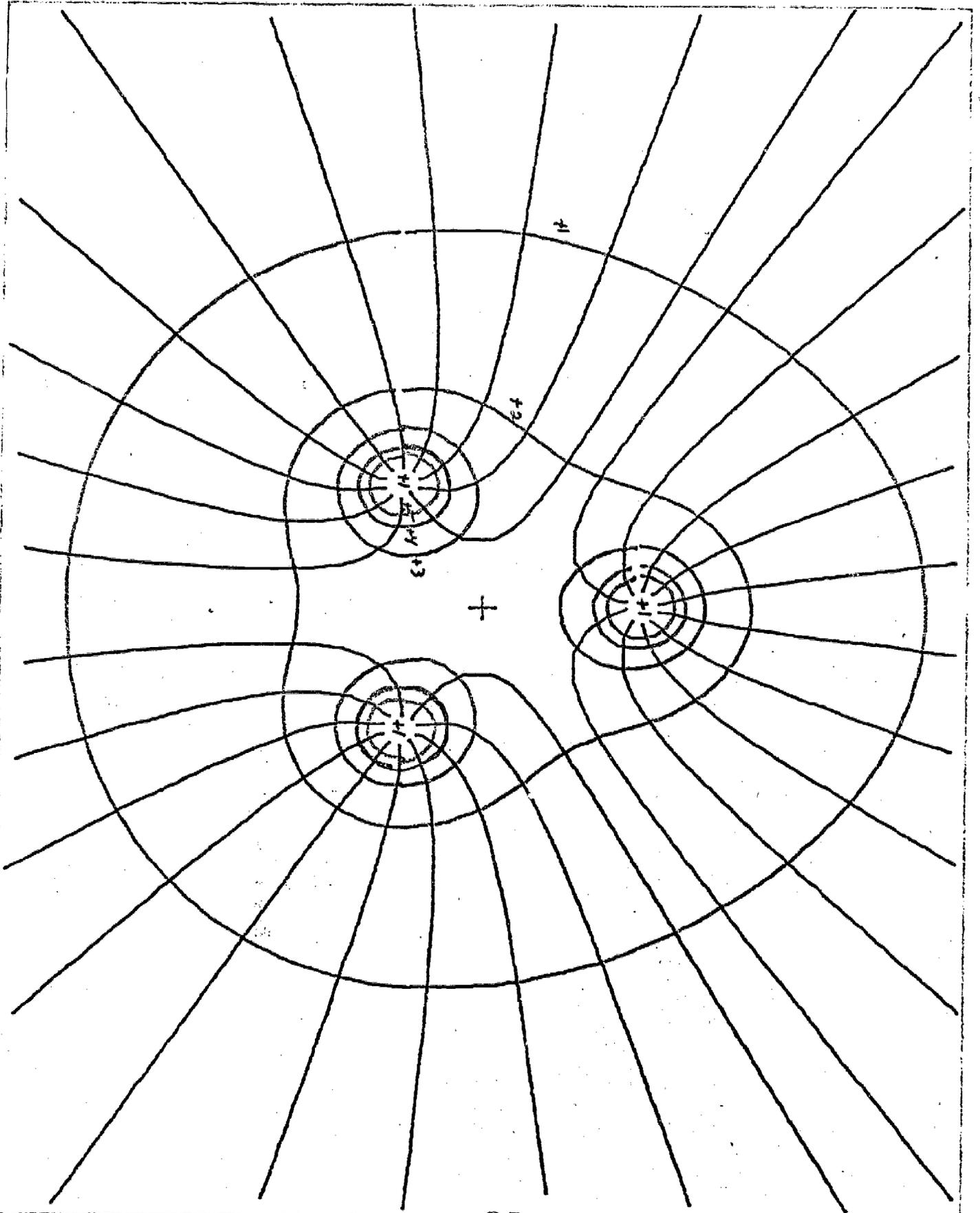


FIGURE 2

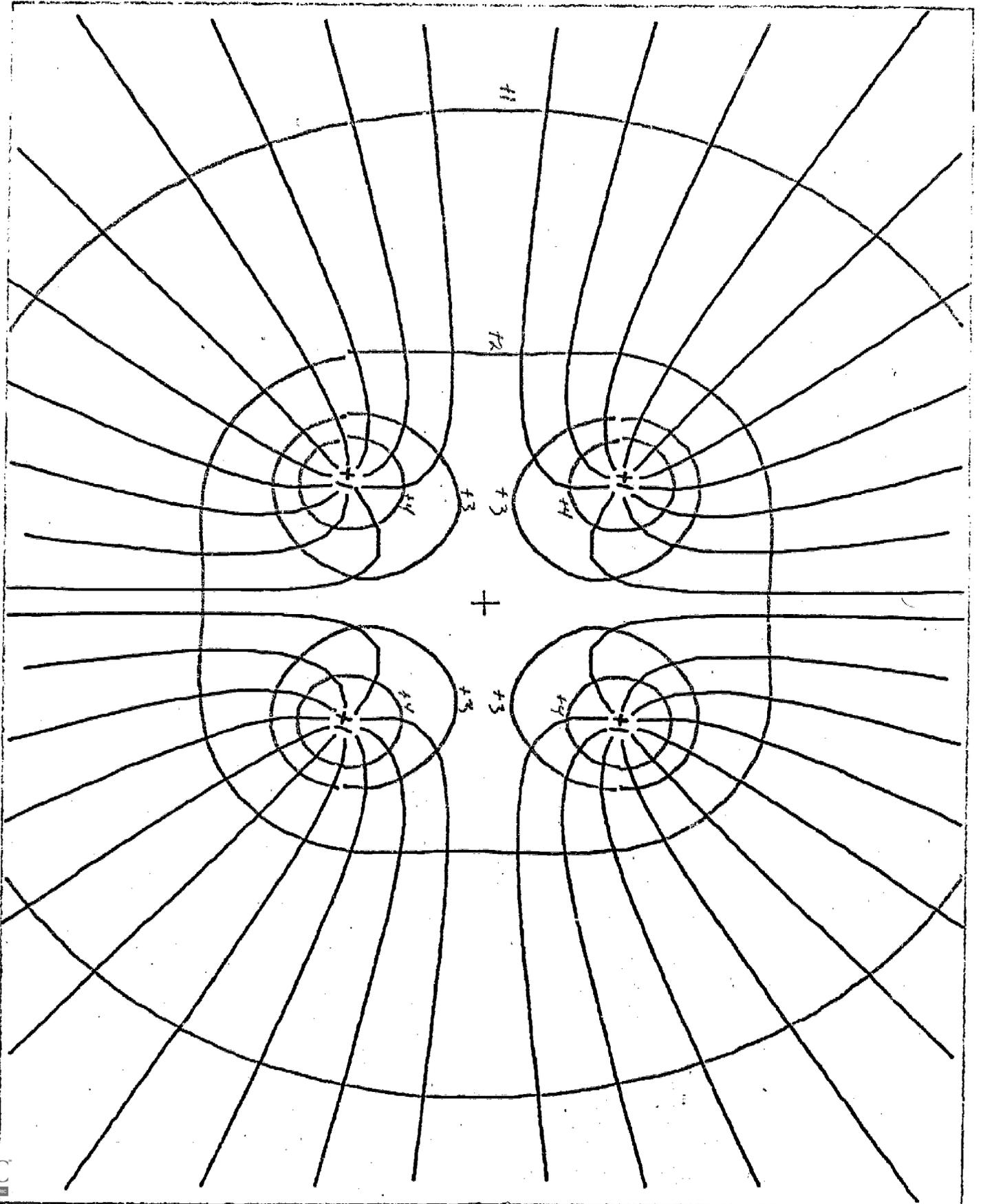


FIGURE 3

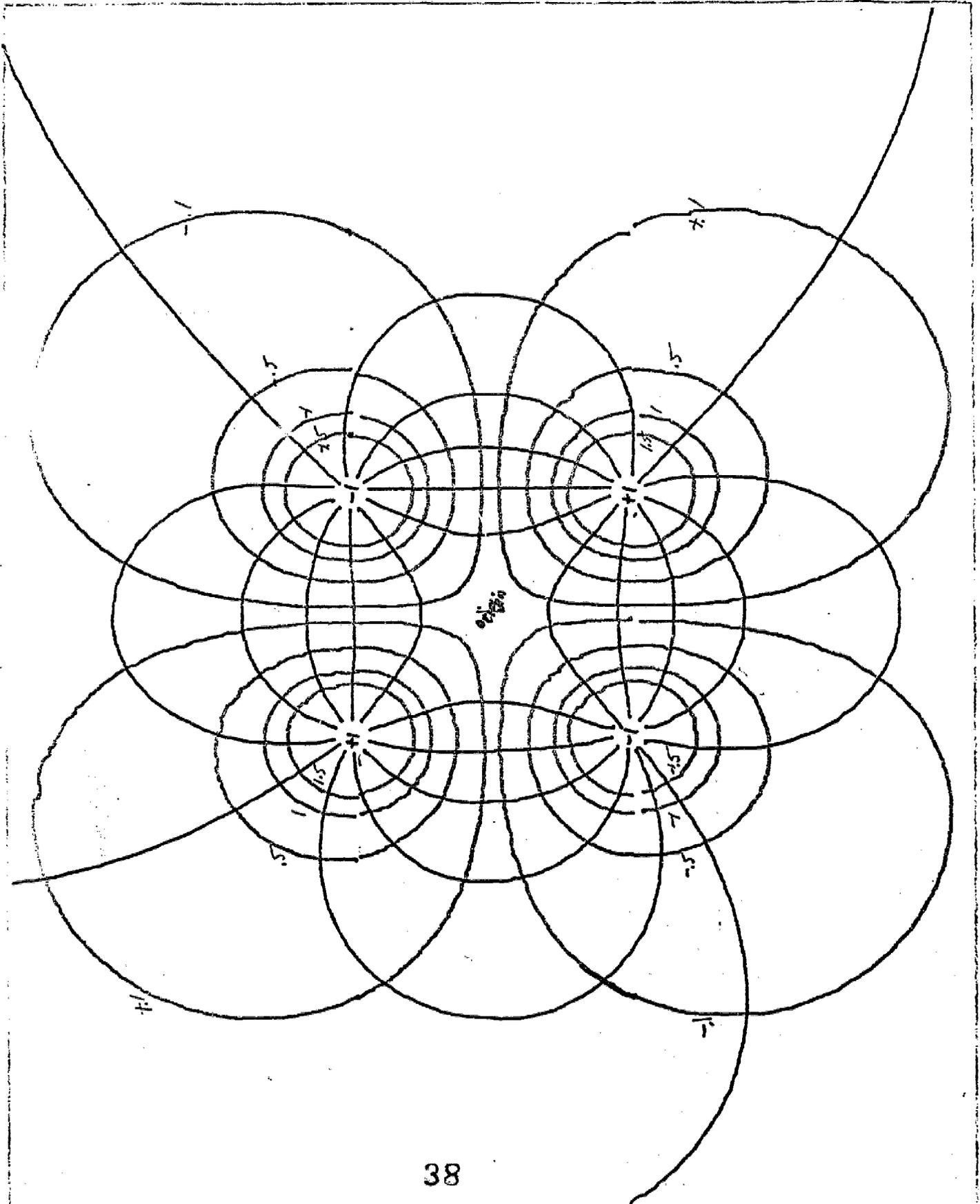


FIGURE 4

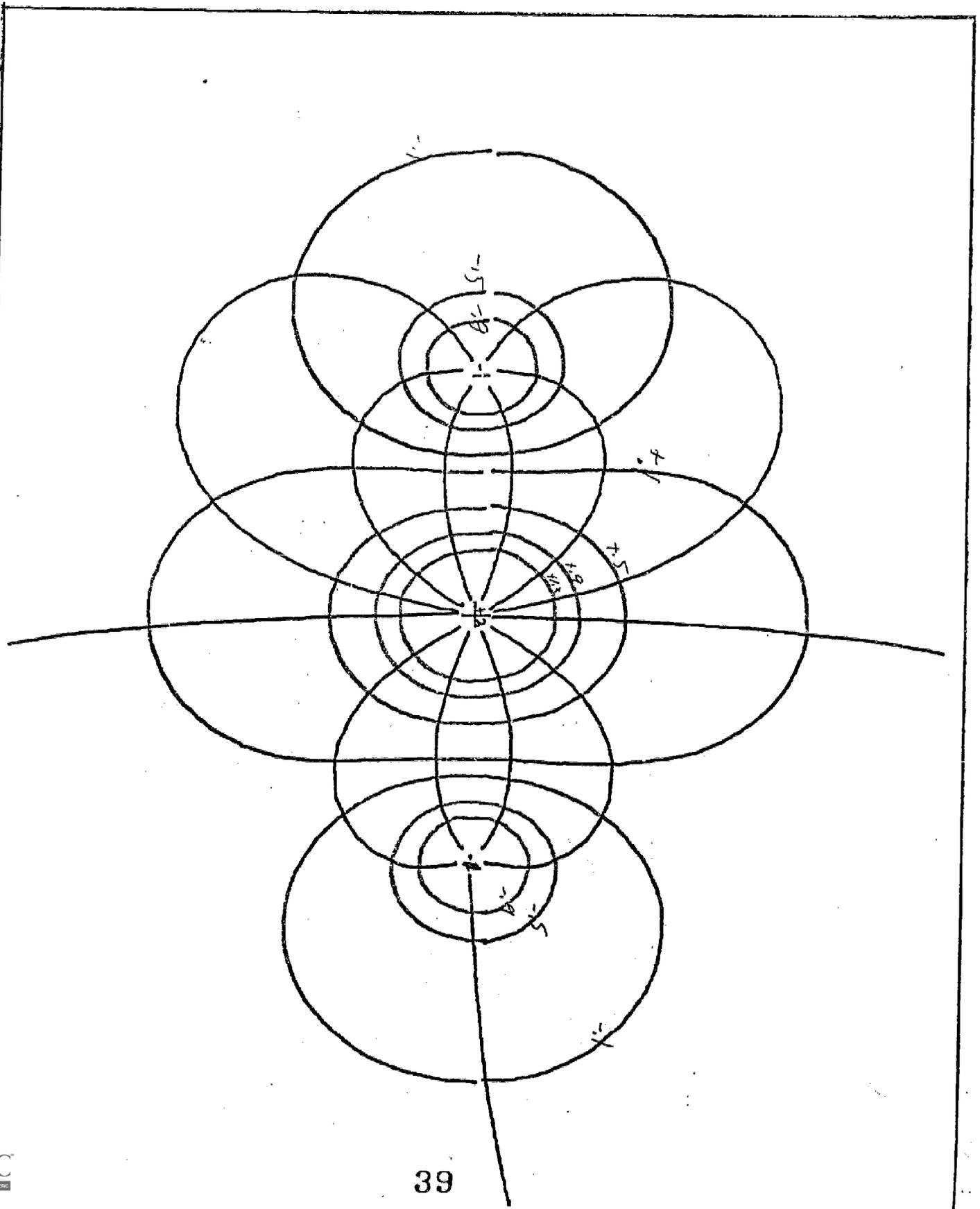


FIGURE 5

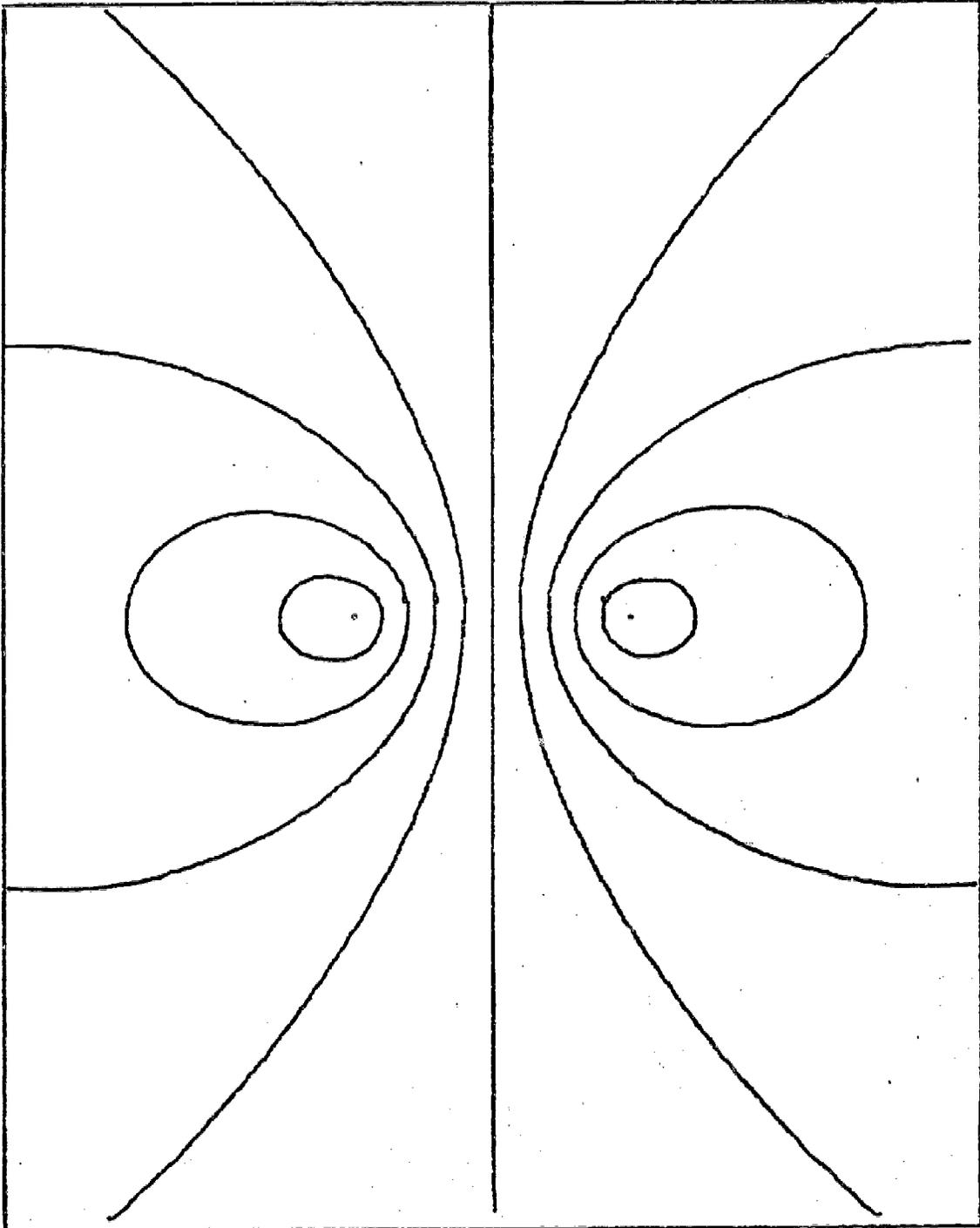
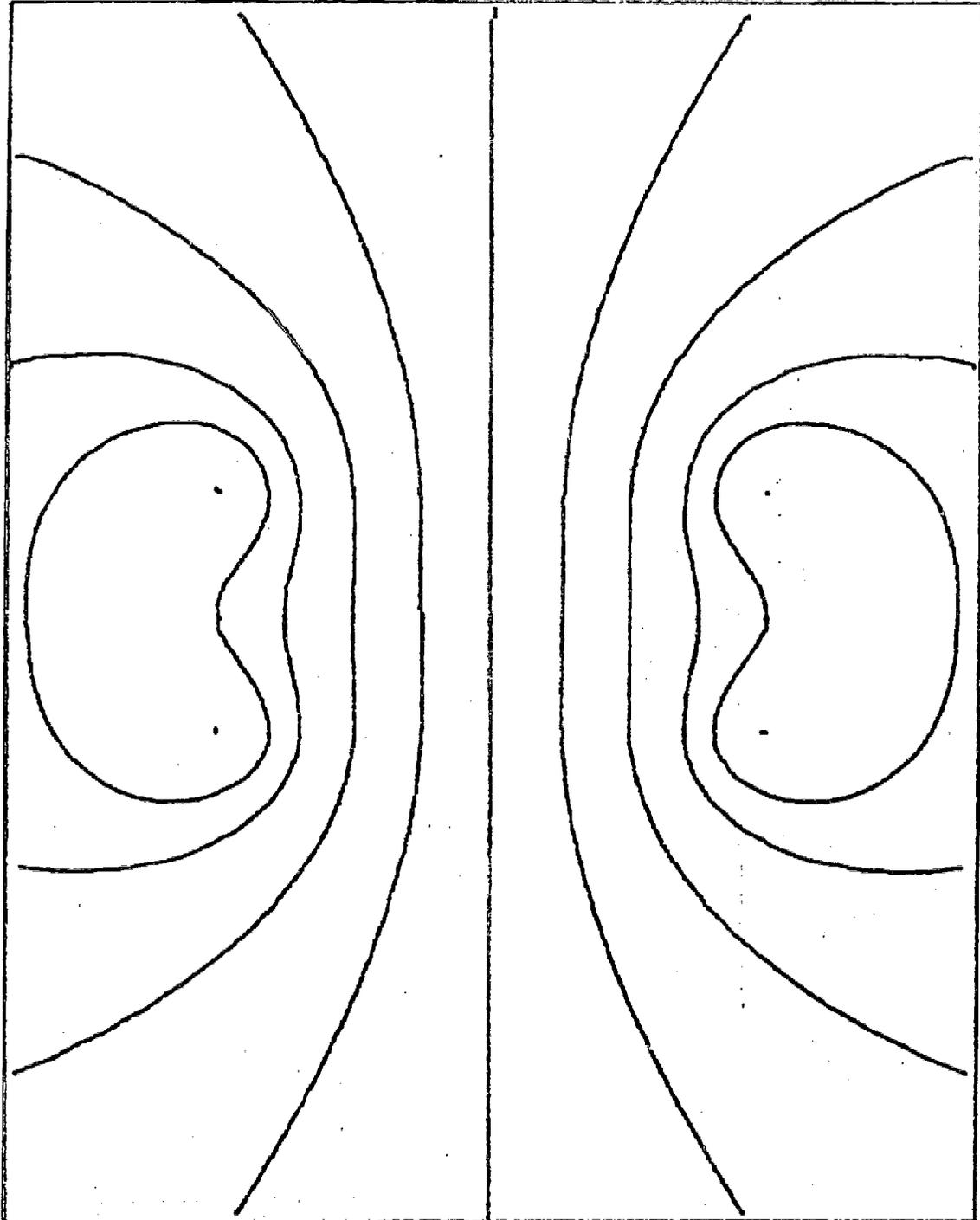


FIGURE 6



References

¹J. R. Merrill American Journal of Physics, 37, 837 (1969)

Captions

- Figure 1 Electric field lines and equipotentials in the plane of three, equal point charges on the corners of an equilateral triangle. The equipotentials are in equal steps (+1,2,3,4 and 5 in normalized units); the field lines start at equal angles around each charge. The center of the figure is marked with a cross.
- Figure 2 Electric field lines and equipotentials in the plane of four, equal, point charges on the corners of a square. The equipotentials are in equal steps (+1,2,3 and 4 in normalized units); the field lines start symmetrically at equal angles around each charge. The center of the figure is the cross.
- Figure 3 Electric field lines and equipotential surfaces in the plane of a two-dimensional quadrupole (equal but opposite point charges on alternating corners of a square). The equipotentials are in equal steps except for the outermost set; the equipotentials displayed are $\pm .1, .5, 1.0, 1.5$. The electric field lines do not start precisely symmetrically and their shape far from the charges is sensitive to the asymmetry.
- Figure 4 Electric field lines and equipotentials in a plane containing a one-dimensional quadrupole (two dipoles head-to-head). Again the field lines are very sensitive in the far region to small asymmetries in the choice of starting point.

Figure 5 Magnetic field lines in a central plane due to a circular current loop. The loop is perpendicular to the page and is centered on the middle; two dots mark the places where the loop cuts the page. The pattern is symmetric under rotations around the central field line.

Figure 6 Magnetic field lines in a central plane of a Helmholtz pair. The pair is perpendicular to the page; four dots mark the points where the loops cut the page. The central homogeneity of the field pattern is clear as is the symmetry of the inhomogeneous part of the pattern.

Appendix I

-1-

E&V SUBS

```

100 REM E FIELD LINES & EQUIPOTENTIALS USING SUBROUTINES
110 SUB FELDLINE;MOVEPERP
120 REM (FNX,FNY)=(EX,EY)
130 DEF FNX(X,Y)=X/(R*R*R)
140 DEF FNY(X,Y)=Y/(R*R*R)
150 PRINT "X","Y"
160 REM FIELD LINE PART
170 PRINT "INITIAL POINT (X,Y: 999 TO DO EQUI-V)":
180 INPUT X1,Y1
190 IF X1=999 THEN 370
200 LET N=0
210 LET N1=0
220 LET F1=0
230 LET F2=0
240 LET F0=.1
250 LET R=1
260 LET F3=FNX(X1+F1/2,Y1+F2/2)
270 LET F4=FNY(X1+F1/2,Y1+F2/2)
280 GOSUB #1
290 LET N1=N1+1
300 IF N1<5 THEN 340
310 LET N1=0
320 PRINT X1,Y1
330 LET N=N+1
340 IF N<10 THEN 260
350 GOTO 160
360 STOP
370 REM EQUIPOTENTIAL PART
380 PRINT "INITIAL POINT ON EQUI-V (X,Y: 999 TO END)":
390 INPUT X1,Y1
400 IF X1=999 THEN 560
410 REM FOLLOWS EQUI-V BY MOVING PERP. TO E
420 LET N=0
430 LET N1=0
440 LET M9=.1
450 LET R=1
460 LET M7=FNX(X1+M5/2,Y1+M6/2)
470 LET M8=FNY(X1+M5/2,Y1+M6/2)
480 GOSUB #2
490 LET N1=N1+1
500 IF N1<10 THEN 540
510 LET N1=0
520 PRINT X1,Y1
530 LET N=N+1
540 IF N<10 THEN 460
550 GOTO 380
560 END

```

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FELOLINE

```
1 REM SUBROUTINE--CALCS. NEXT PT. ALONG A FIELD LINE
5 REM GIVE X1,Y1(PRESENT), F0=DIST. TO MOVE ALONG LINE, AND
11 REM F3,F4=X,Y COMPS. OF FIELD (ONLY RATIOS COUNT)
16 REM BETTER CONVERGENCE IF GIVE FIELD 1/2 STEP AHEAD OF PRES. PT.
21 REM BY USING LAST F1,F2=DX,DY RETURNED BY THIS SUBROUTINE
26 REM USES F0-F5
31 LET F5=SQR(F3*F3+F4*F4)
36 LET F1=F0*F3/F5
41 LET F2=F0*F4/F5
46 LET X1=X1+F1
51 LET Y1=Y1+F2
56 RETURN
60 END
```

-3-

MOVEPERP

```
1 REM SUBROUTINE--CALCS. NEXT X,Y ON EQUIPOTENTIAL BY GOING PERP TO F
6 REM CALCS NEW PT. A DIST. M9 ALONG PERP. TO A GIVEN LINE
11 REM AT GIVEN PT. (X1,Y1)
16 REM GIVE PROG.: X1,Y1 (PRESENT), M9=DIST TO MOVE, AND
21 REM (M7,M8)=VECTOR DEFINING GIVEN LINE AT POINT X1,Y1
26 REM PROGRAM RETURNS X1,Y1(NEW) AND M5,M6=(DX,DY)
31 REM PROGRAM USES M4,M5,M6,M7,M8,M9
36 LET M4=SQR(M7*M7+M8*M8)
41 LET M6=M9*(M7/M4)
46 LET M5=M9*(-M8/M4)
51 LET Y1=Y1+M6
56 LET X1=X1+M5
61 RETURN
66 END
```

Appendix II

- 1 -

LOOPFELD

```
100 REM GIVES FIELD LINES IN XZ PLANE FOR SINGLE LOOP
110 REM AROUND ORIGIN IN XY PLANE--USES SUBROUTINES
120 SUB LOOPB;FELDLINE
130 PRINT "CURRENT, & RADIUS";
140 INPUT I,A
150 LET LO=0
160 LET FO=.05
170 PRINT "INITIAL POINT (X,Z)";
180 INPUT X1,Z1
190 LET N=0
200 LET N1=0
210 PRINT "X","Z"
220 LET X2=X1+F1/2
230 LET Y2=0
240 LET Z2=Z1+F2/2
250 GOSUB #1
260 LET F3=L5
270 LET F4=L7
280 LET Y1=Z1
290 GOSUB #2
300 LET Z1=Y1
310 LET N1=N1+1
320 IF N1<5 THEN 360
330 LET N1=0
340 LET N=N+1
350 PRINT X1,Z1
360 IF N<10 THEN 220
370 PRINT
380 GOTO 170
390 END
```

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LOOPS

```

1 REM SUBROUTINE--CALCS. B OF LOOP AT GIVEN POINT
6 REM GIVE I(CURRENT), A(RADIUS), (X2, Y2, Z2)=FIELD PT., AND LO=Z OF LOOP
11 REM RETURNS L5, L6, L7=(BX, BY, BZ) AT (X2, Y2, Z2)
16 REM LOOP IS PARALLEL TO XY PLANE AT PT. Z=LO
21 REM USES K1-4; LO-9; MO-9
26 LET MO=1E-7*I
31 LET K4=3.14159265
36 LET L1=2*K4*A/32
41 LET L2=K4/16
46 LET L5=0
51 LET L6=0
56 LET L7=0
61 FOR M9=0 TO 2*K4-L2 STEP L2
66 LET L4=COS(M9)
71 LET L3=SIN(M9)
76 REM M1, 2, 3 = DL ON LOOP
81 LET M1=-L1*L3
86 LET M2=L1*L4
91 LET M3=0
96 REM L8, 9, 0 = COORDS. OF LOOP PT
101 LET L8=A*L4
106 LET L9=A*L3
111 REM M4, 5, 6 = R FROM LOOP PT. TO FIELD PT
116 LET M4=X2-L8
121 LET M5=Y2-L9
126 LET M6=Z2-LO
131 LET M7=SQR(M4*M4+M5*M5+M6*M6)
136 LET M8=M7*M7*M7
141 REM K1, 2, 3=CROSSPRODUCT
146 LET K1=M2*M6-M3*M5
151 LET K2=M3*M4-M1*M6
156 LET K3=M1*M5-M2*M4
161 REM L5, 6, 7=COMPS. OF B
166 LET L5=L5+MO*K1/M8
171 LET L6=L6+MO*K2/M8
176 LET L7=L7+MO*K3/M8
181 NEXT M9
186 RETURN
191 END

```

-3-

HELMHOLZ

```
100 REM HELMHOLTZ PAIR B FIELD USING SUBROUTINE LOOPB
110 SUB LOOPB
120 PRINT "CURRENT, LOOP RADIUS, & RIGHT SIDE COIL Z COORD.";
130 INPUT I,A,ZO
140 PRINT "FIELD POINT (X,Y,Z)";
150 INPUT X2,Y2,Z2
160 LET LO=ZO
170 GOSUB #1
180 LET B1=L5
190 LET B2=L6
200 LET B3=L7
210 LET LO=-ZO
220 GOSUB #1
230 LET B1=B1+L5
240 LET B2=B2+L6
250 LET B3=B3+L7
260 PRINT "B FIELD:"
270 PRINT " (";B1;" ,";B2;" ,";B3;")."
280 GOTO 140
290 END
```

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Computer Solutions to Some Simple 1D Schrodinger Equations[†]

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ABSTRACT

The Schrodinger equation solutions for the sequence of potentials $V(x) = |x|^n$ for $n = 1, 2, \dots$ is investigated. The eigenvalues and eigenfunctions are calculated numerically using a short program students write themselves. The program and its results are illustrated in the note. The ground state eigenvalues illustrate an interesting competition between kinetic energy (wavefunction curvature) and potential energy as the exponent n increases.

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Introduction

The Schrodinger equation for stationary states in one dimension is easily solved numerically using even the smallest computer. The problem is especially simple if the potential, $V(x)$, is symmetric so that each eigenfunction is either of even or odd parity. The method of solution is very similar to iterative numerical solutions for $\vec{F} = m\vec{a}$ mechanics problems.^{1,2} This note points out an interesting sequence of potentials which approximate an infinite square well but have rounded corners. Eigenfunctions and eigenvalues are reported for the sequence, and a simple program which students themselves write is presented. The sequence of lowest energies for these potentials demonstrate a balance between kinetic and potential energy to achieve the lowest total energy for the ground state.

Potentials

The infinite square well is a useful approximation to many physical problems, mostly because the problem is exactly solvable. Many physical situations, however, are more realistically modeled by a well with rounded corners. The sequence of potentials $V(x) = |x|^n$ for $n = 1, 2, 3, \dots$ approaches the infinite square well but rounds the corners of the potential.

Figure 1 shows several of these potentials. The curves for $n = 2, 6, 10,$ and 40 are shown for $x \geq 0$; the infinite square well is shown for comparison. All the potentials go through the points $(0,0)$ and $(1,1)$. As n increases, the corner for $x \lesssim 1$ sharpens, and a larger region for which $V(x)$ is essentially zero occurs. As n increases, the potential beyond $x = 1$ increases more sharply.

Program

Since all the potentials are symmetric around $x = 0$, the eigenfunctions have either even parity or odd parity. The ground state is even, and the excited states alternate odd, even, odd, ---. The program to integrate Schrodinger's equation to find an eigenfunction is very simple. The student demands that $\psi(0) = 1$ and $\psi'(0) = 0$ for even states (or $\psi(0) = 0$ and

$\psi'(0) = 1$ for odd states).³ He then picks an energy and integrates the Schrodinger equation $\frac{d^2\psi}{dx^2} = 2(V(x) - E)$ in a stepwise way out the x-axis. (All the problems discussed in this note will have $\hbar = m = 1$.) If E is an eigenvalue, the wavefunction will go to zero for large x; if not, the wavefunction will diverge. For energies on either side of an eigenvalue, the wavefunction diverges to opposite signed infinities. Hence, the student zeros in on an eigenvalue in three or four pairs of energies. Four figure accuracy of the energy eigenvalues is typical even for the simplest programs. The wavefunctions the student derives are unnormalized.

The programs the students write can be very short. The basic integration strategy is seven lines long. Figure 2A) shows a program which steps along the x-axis (X1) and calculates the wavefunction (P0) at each step. The program is in the language BASIC. The calculation of P0 uses the average of the two first derivatives (P3, P4) at the two ends of each interval Δx (L1). The calculations of the first derivatives use the average of the potentials (V1, V3) at the two ends of the interval. The wavefunction is assumed to vary slowly enough that its change over one step (of size L1) can be neglected. Figure 2B) shows changes in the program to achieve a more convergent numerical method. (One which is more accurate even for larger step sizes.)

Eigenvalues and Eigenfunctions

Figure 3 shows the energies of the ground state, E_1 , and the second excited state, E_3 (the third energy level), as functions of exponent, n, in the potential, $V(x) = |x|^n$. Table 1 gives numerical values for these energies. The sequence of energies is asymptotic to the infinite square well ($n = \infty$) for which $E_m = \frac{m^2\pi^2}{8}$ in the present units. The values calculated numerically for $n = 2$, the harmonic oscillator, agree with the exact solution, $E_m = (m - 1/2) \sqrt{2}$, to six figure accuracy using the higher convergence program (four figures using the simple program). Figure 4 shows some of the wavefunctions calculated by the program. Even for an eigenvalue correct to six figures, the eigenfunction will still diverge for large enough x. For eigenvalues correct to three or more figures, the wavefunction in the region of interest ($0 \leq |x| \leq 1.5$) is not significantly changed by higher eigenvalue accuracy.

The minimum in the values of the ground state energy, E_1 , as a function of exponent n has an interesting physical basis. For n between 1 and about 5, the major effect on states of low energy ($E \lesssim 1$) includes not only the more steeply increasing potential beyond $x = 1$, but also the substantial broadening of the region (for $x < 1$) where V is essentially zero. The increasing breadth of this $V \sim 0$ region allows the wavefunction to spread out and hence to decrease its curvature in the central area. This decrease in curvature is a decrease in kinetic energy, and, for small n , is larger than the increased potential energy experienced by the tails of the wavefunction in the classically forbidden region. Thus, initially as n increases from 1, the total energy of the ground state, E_1 , decreases.

After $n \sim 6$, most of the broadening of the $V \sim 0$ region has been accomplished and the further broadening is progressively smaller. For larger exponents, n , then, the cost of the increased penetration of the classically forbidden region rises sharply, and the total energy of the ground state rises accordingly. By attempting to cut off the eigenfunction tails sharply, the wavefunction's curvature and hence the kinetic energy increase again.

For states with energies substantially greater than one, the increased $V \sim 0$ region is of much less importance. For these states, the dominant effect, as n increases, is always the steepening of the potential beyond $x = 1$. For these higher energy states, the total energy should increase monotonically with n . The energy of the second excited state, E_3 , which is shown in Figure 3, illustrates the dependence for these higher energy states upon the exponent n . Figure 3 also shows that the dependence of E_1 on n approaches that of higher energy states after the broadening effect of $V \sim 0$ has become negligible.

Conclusion

The sequence of potentials $V(x) = |x|^n$ for $n = 1, 2, 3, \dots$ has interesting properties. Not only does this sequence approach the infinite square well (but with rounded corners), but also the stationary state energies of this sequence illustrate the effects of competing changes in kinetic energy (wavefunction curvature) and potential energy as the exponent n increases. This note has presented a simple program to find eigen-

functions and eigenvalues for one dimensional Schrodinger equation problems. The method is easy to explain and is very general. This use of the computer in introductory quantum mechanics has removed much of the mystery of solving the Schrodinger equation, and has allowed the students to concentrate on the physics of what is happening.

Acknowledgments

The authors would like to thank Arthur W. Luehrmann, co-director of Project COEXIST, for many helpful conversations on this problem.

References

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- ²E. Huggins, The Computer in First Semester Physics, Project COEXIST, Dartmouth College, Hanover, N. H. 03755.
- ³For potentials that are not symmetric, the student can be led to find asymptotic solutions for the wavefunctions, and then the student can integrate in from the asymptotic region.

TABLE 1

Ground state energy, E_1 , and second excited state energy, E_3 , for $V(x) = |x|^n$.
 $\hbar = m = 1$.

| <u>n</u> | <u>E_1</u> | <u>E_3</u> | |
|----------|-------------------------|-------------------------|--|
| 1 | .809 | 2.58 | |
| 2 | .707 | 3.54 | (E ₅ = 6.36; E ₇ = 9.19) (harmonic oscillator with k = 2) |
| 3 | .675 | 4.20 | |
| 4 | .668 | 4.70 | |
| 5 | .672 | 5.08 | |
| 6 | .681 | 5.40 | |
| 7 | .692 | 5.66 | |
| 8 | .704 | 5.89 | |
| 9 | .717 | 6.08 | |
| 10 | .729 | 6.26 | (E ₅ = 16.3; E ₇ = 29.9) |
| 12 | .753 | 6.57 | |
| 14 | .776 | 6.82 | |
| 16 | .796 | 7.05 | |
| 18 | .814 | 7.24 | |
| 20 | .831 | 7.41 | |
| 30 | .898 | 8.05 | |
| 40 | .942 | 8.48 | |
| ∞ | 1.234 | 11.10 | (E ₅ = 30.8; E ₇ = 60.5) (∞ square well) |

Captions

- Figure 1. Potentials $V(x) = |x|^n$ for $n = 2, 6, 10,$ and 40 . The infinite square well of width 2 is shown for comparison. For n up to about 6, the breadth of the region where $V(x)$ is nearly zero increases substantially.
- Figure 2. Program to solve 1D, stationary state, Schrodinger equation problems. A) The program is in the language BASIC. The fundamental calculations are in lines 230-330. B) Replacement lines for a form of the program having faster convergence.
- Figure 3. Energy levels as a function of the exponent, n , in the potential. E_1 is the ground state energy; E_3 is the third energy level (the second excited state). The minimum in E_1 near $n = 6$ is discussed in the text. Both curves are asymptotic to the infinite square well ($n = \infty$).
- Figure 4. Several wavefunctions for the potentials $V(x) = |x|^n$. Top) Ground state wavefunctions for $n = 2, 10$ and 40 . The traces are halted just as the wavefunctions start to diverge. Bottom) Second excited state wavefunctions for $n = 2, 10$ and 40 . All traces are drawn directly by the computer from data calculated by the program of Figure 2.

FIGURE 1

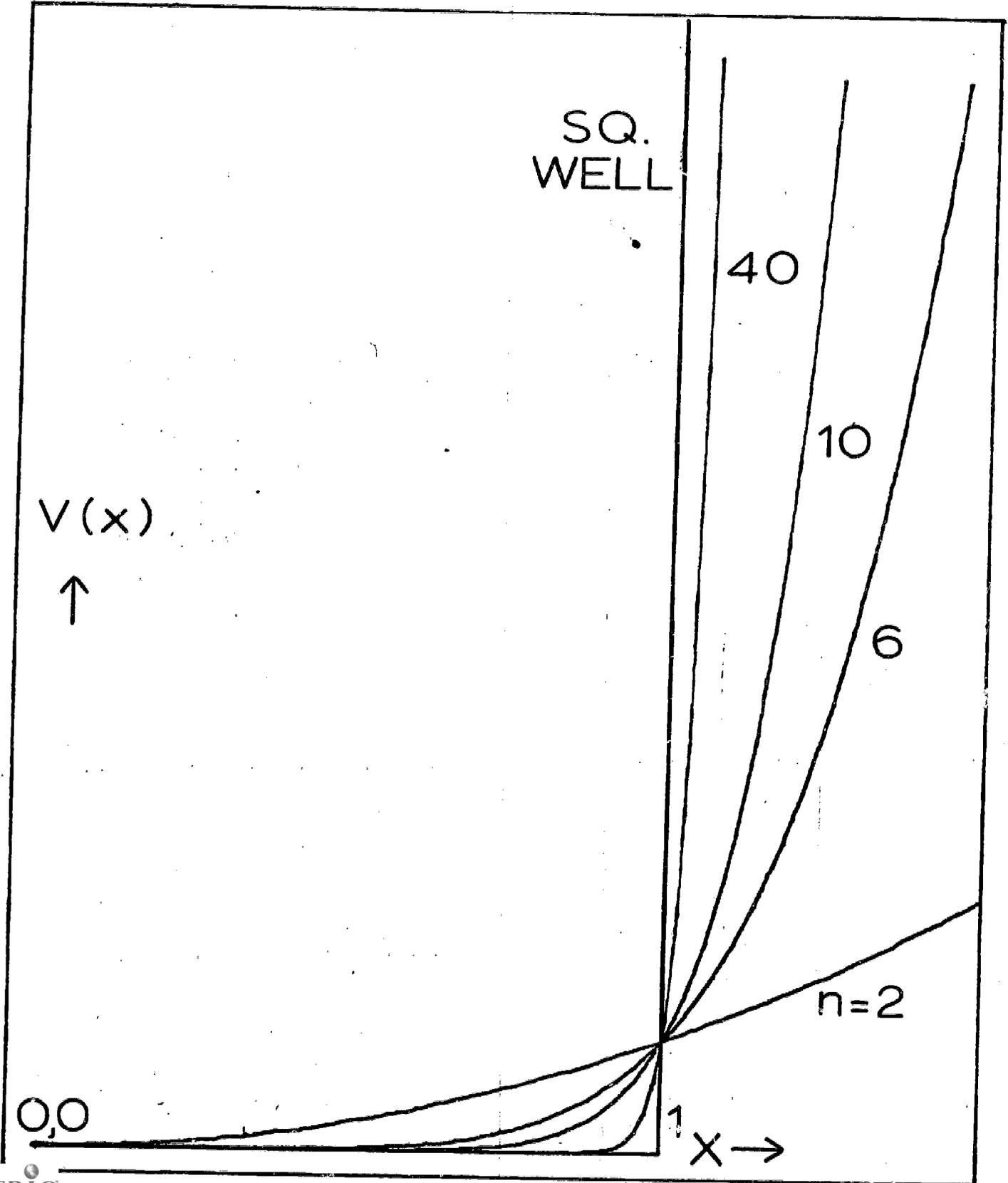


FIGURE 2

A) SIMPLE PROCEDURE TO SOLVE 1D SCHRÖDINGER EQN.

```

100 DEF FNV(X)=X+N9
110 PRINT "N";
120 INPUT N9
130 PRINT "END OF INTERVAL, STEP SIZE";
140 INPUT L,L1
150 PRINT "INITIAL WAVEFN., DERIV.";
160 INPUT P8,P9
170 PRINT "ENERGY";
180 INPUT E
190 LET P0=P8
200 LET P4=P9
210 LET X1=0
220 LET V1=FNV(0)
230 LET V3=V1
240 LET V1=FNV(X1+L1)
270 LET P2=2*((V1+V3)/2 - E)*P0
280 LET P3=P4
310 LET P4=P4+P2*L1
320 LET P0=P0+L1*(P4+P3)/2
330 LET X1=X1+L1
340 LET N=N+L1
350 IF N<L/10 THEN 230
360 LET N=0
370 PRINT X1,P0
380 IF X1<L THEN 230
390 GOTO 170
400 END

```

B) FOR FASTER CONVERGENCE

```

240 LET V1=FNV(X1+L1)
250 LET V4=FNV(X1+L1/4)
260 LET V2=FNV(X1+L1/2)
270 LET P2=2*((V1+V3)/2+V2)/2 - E)*P0
280 LET P3=P4
290 LET P5=2*((V2+V3)/2+V4)/2 - E)*P0
300 LET P6=P4+P5*L1/2
310 LET P4=P4+P2*L1
320 LET P0=P0+L1*((P4+P3)/2+P6)/2

```

FIGURE 3

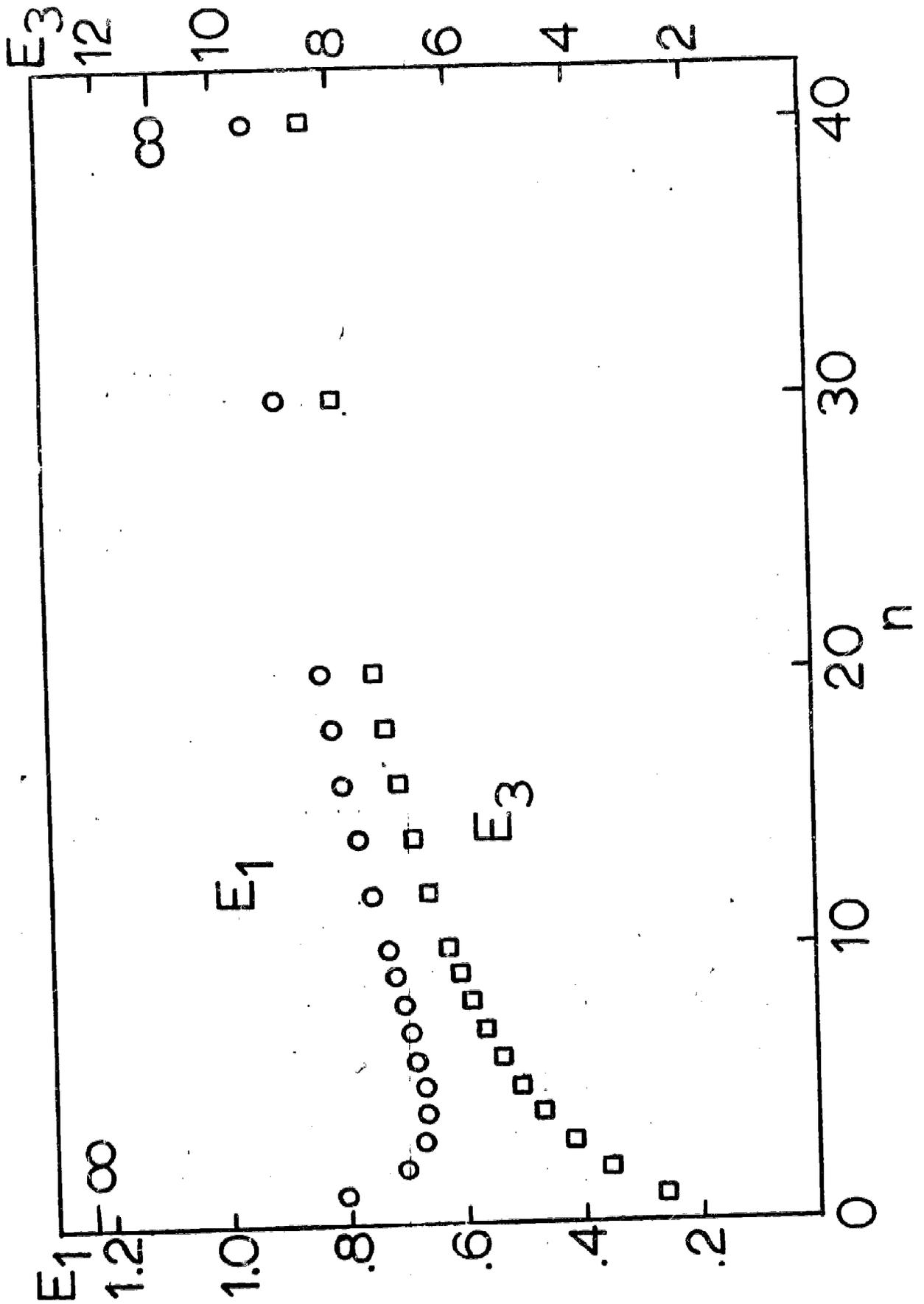
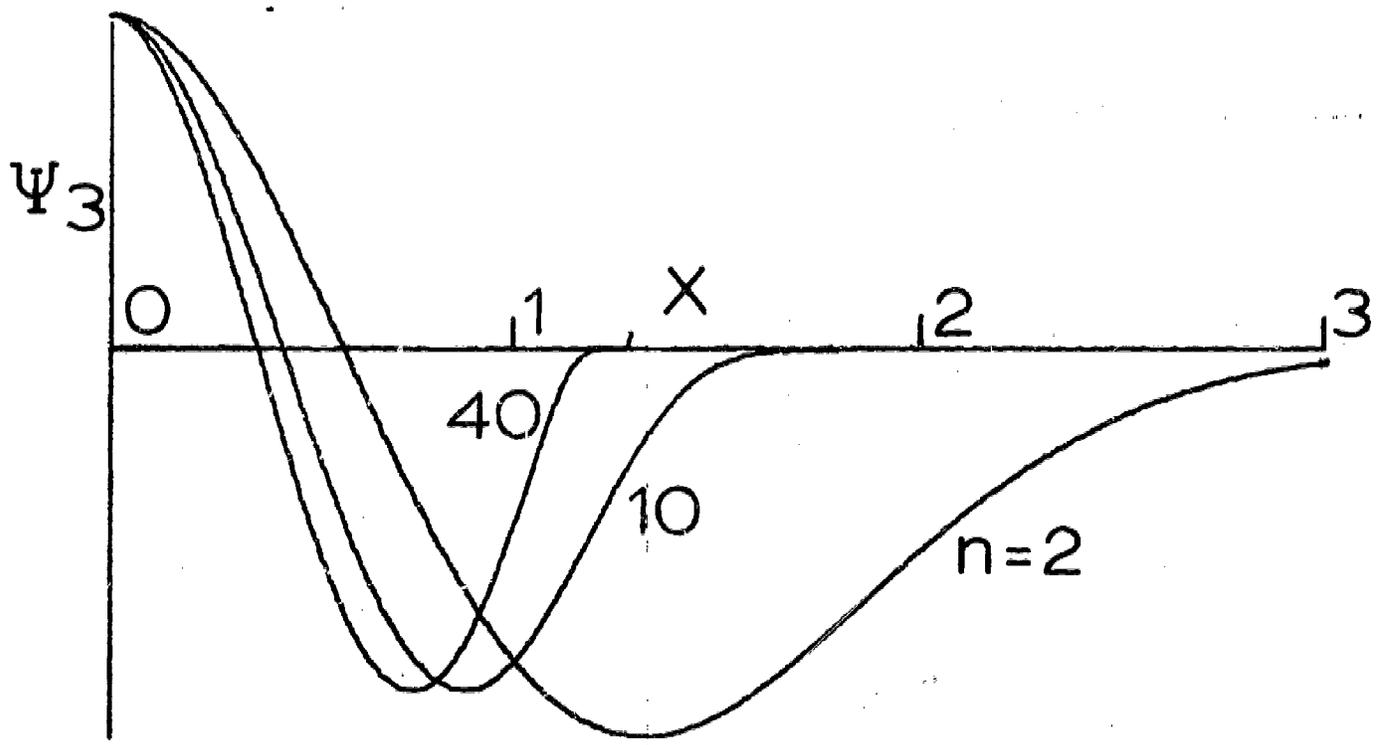
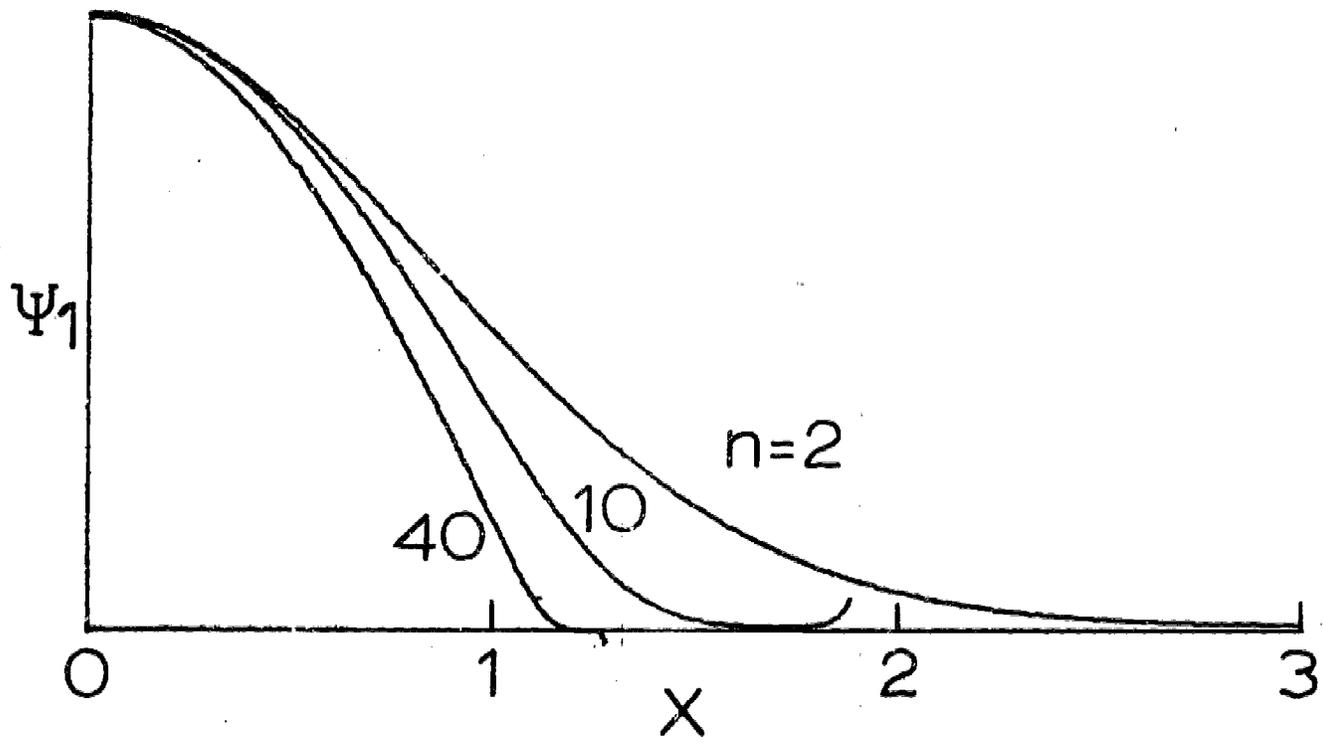


FIGURE 4



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INEXPENSIVE, INTERACTIVE GRAPHICS ON
TELEPHONE-CONNECTED, TIME-SHARED COMPUTERS

John R. Merrill
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This paper presents some of the preliminary results of Project COEXIST at Dartmouth College. Project COEXIST is an NSF sponsored project to investigate ways to use computers in introductory physics and mathematics teaching. The computer opens up areas of study not previously available at introductory levels. Students use the computer in a number of ways on homework, on individual projects, and in the laboratory. Students, whenever possible, write their own programs. On occasion, it is more useful to have the students programs written and saved by the teacher.

Project COEXIST has made wide use of computer-connected graphic display devices such as X-Y plotters and cathode ray terminals. This paper presents illustrations of the Project's uses of these devices. Illustrations from a broad range of study areas are introduced to show the versatility of these display devices.

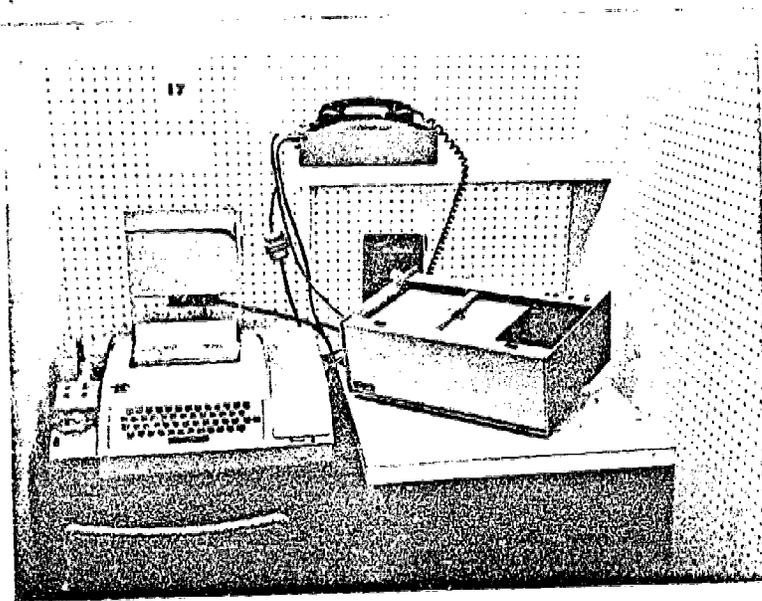
EQUIPMENT USED

X-Y plotters of the type used are made by several companies. They utilize a regular X-Y analog recorder with an interface between the recorder and the computer. The interface converts digital characters coming from the computer over a telephone line into voltage positions on an X-Y page. The computer software converts calculated values of X-Y coordinates to sets of ASCII characters. The ASCII characters are the elements actually sent over the telephone line. Such an analog X-Y recorder is considerably faster in real time (and in CPU time) than, for example, a Cal Comp incremental system. The most important attribute of X-Y plotter systems and graphic systems, in general, is that the graphic or plotted output is usually much more useful than tabulated numbers. While graphic displays do not have the resolution of tabulated numbers, they nevertheless convey a great deal more information in a short time. The cost on one of these inexpensive X-Y plotter systems is about \$3300, of which the cost of the interface itself is about \$2000. A typical X-Y plotter system connected to a teletype and to an acoustical coupler is shown in figure 1.

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FIGURE 1

Teletype and X-Y plotter as used with the time-shared Dartmouth GE-635 system. Software saved in the computer can be called from any program to position the X-Y pen anywhere on the page. The final output can then be a hard copy paper plot, graph or picture.



A second graphic display device is the cathode ray Tektronix 4002 terminal. This terminal is similar to an X-Y plotter except that it incorporates the keyboard. Also, hard copy can not be obtained from the cathode ray terminal without photographic techniques or a hardware attachment. However, the cathode ray terminal is often very much faster than an X-Y plotter, which makes the terminal useful for debugging, and for those situations where the student must observe large numbers of curves. Since no inexpensive hard copy is available from the CRT display device, the CRT will not be emphasized. Nonetheless, everything in this paper has been performed on the CRT device. The Tektronix 4002 cathode ray system is shown in figure 2.

ILLUSTRATIONS

Illustrations from classical mechanics, fluid fields, electrostatic fields, geometrical optics, and physical optics have been chosen. The ways in which graphic display devices have been used, in as broad a range of introductory physics topics as possible, are shown. In classical mechanics, students have written and used programs on such areas as trajectory motion, strobe photograph labs (including non-closed integrable force laws), Keplerian and non-Keplerian orbits, relativistic dynamics (including relativistic motion of charged particles), accelerator simulation, and a number of scattering situations. The following are results of one sophomore-level scattering simulation laboratory.

Figure 3 shows the results of the classical scattering of point positrons off a model of S-state hydrogen. The atom is modeled as a point nucleus surrounded by a uniform negatively charged sphere. The total negative charge in the sphere exactly cancels the total charge of the point nucleus. The scattered particle is repelled from the nucleus. The figure shows the trajectories of positrons with an energy of .25 of the ionization energy (13.7 volts) and for various impact parameters. The scattering is entirely classical. The student becomes familiar with the concepts of impact parameter, angular momentum, differential cross section, total cross section, and effective potential, in a classical system. The student then finds these concepts much easier to understand in quantum mechanical cases. Figures such as figure 3 are used in a laboratory simulation experiment. The student starts with hard spheres. After plotting and understanding the trajectories of hard sphere scattering, the student then plots trajectories such as these shown in the figure. The student measures the angle of deviation and then counts the number of particles scattered into 20° intervals of scattering angle

FIGURE 2

Cathode Ray Display terminal as used with the time-shared Dartmouth GE-635 system. Software saved in the computer can be called from any program to position the light spot anywhere on the screen. The keyboard is part of the display terminal and letters are "printed" by the light spot on the screen. Hard copy is only available by photographic techniques or from a hardware attachment.

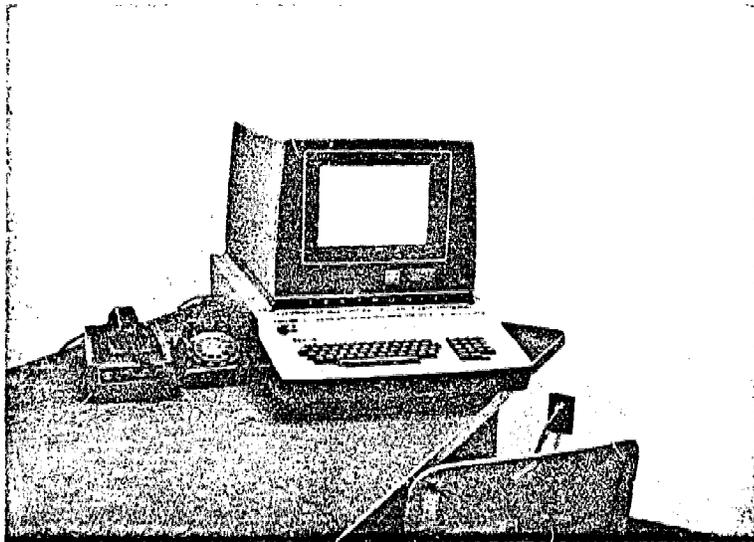
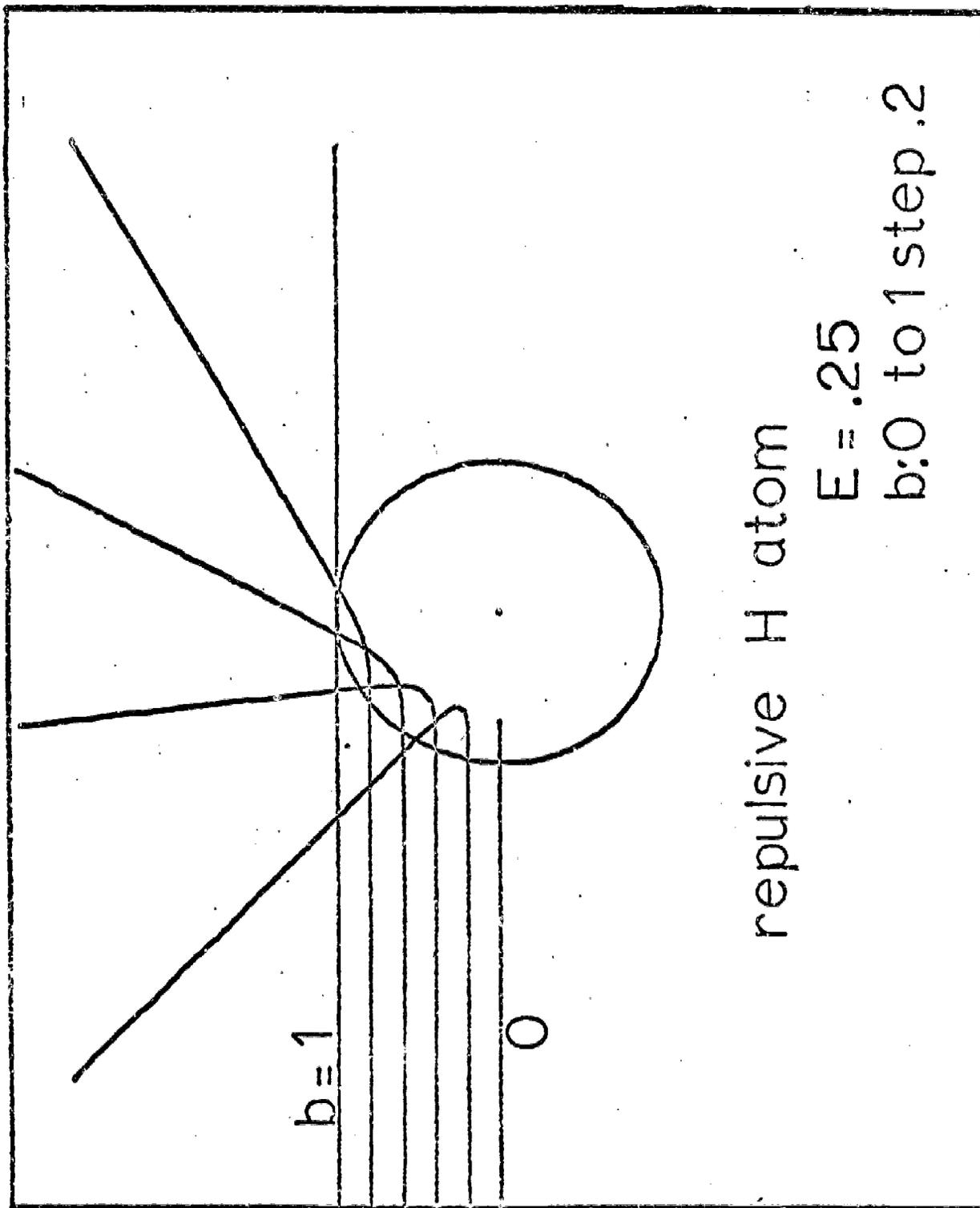


FIGURE 3

Classical scattering of a point positron off a model of an S-state hydrogen atom. The model is a point nucleus surrounded by a uniformly oppositely charged cloud. The whole structure is neutral. The units are normalized so that the circle is the outside of the cloud and is one spatial unit; energy is in units of 13.7 ev. The student plots many such trajectories and measures angles of deviation. b is the impact parameter. The program illustrates a classical mechanics use of display devices.



as a function of the angle of deviation. The plot is normalized in such a way as to make it a plot of differential cross section. The student gets results like those shown in figure 4. This figure shows the number of particles scattered into a given angle as a function of scattering angle. Notice the large number of small angle scatterings. Since the potential is cut off by the electron screening, the number of small angle scatterings is large but not infinite. The student gets even better data than this shown by using smaller bin sizes and more trajectories. The total cross section in the normalized units used in these plots should be approximately π since the normalized radius of the model atom is 1, and the total cross section should be essentially πR^2 . If the student adds up the results for the differential cross section, he typically gets a total cross section between 3.12 and 3.15. The data from this figure gives a value of 3.12. So, in general, students do at least as well as shown in the figure.

Figure 5 shows this same S-state hydrogen model for electron scattering. That is, the scattered particles are attracted to the central nucleus. Notice the peculiar looping orbits. These orbits are correct. They are not due to a calculational error. The student must explain these effects. The answer is seen, most easily, in the effective potential. Figure 6 shows the effective potential for various impact parameters. The physical situation is that of figure 5. Near an impact parameter of .9 (for a normalized energy of .25), the negative charge just makes it over the bump. Since the radial velocity squared is proportional to the total energy minus the effective potential, the particle slows down radially while passing over the bump in V_{eff} . Conservation of the angular momentum demands that the charge wind around the nucleus a number of times. Ultimately the electron leaves the atom, but for angular momenta very near .9 it may take an arbitrarily long time to get away.

In COEXIST, graphic displays have been very useful with various field patterns. The concept of vector fields has been introduced by means of flow patterns in hydrodynamics. Figure 7 shows the pattern of the velocity field around a cylindrical object placed in a uniform stream. Students plot such flow patterns for a number of objects. Then they find densities and directions of lines to derive the relative velocities at different points in the pattern. In this way the student not only acquires some information about fluid flow, but also about various ways to represent vector fields. Vortex fields in fluid flow can often motivate curl discussions very well.

Figure 8 shows the plot of the electric field lines and equipotentials around a two dimensional quadrupole. This program allows placing point charges anywhere in the plane. The program then follows the field lines by integrating

FIGURE 4

Differential cross section as a function of scattering angle for trajectories such as those of figure 3. The scattering angles are grouped in 20 degree intervals. The differential cross section is then the number in a bin times the impact parameter b , divided by $\sin\theta\Delta\theta$. The small angle scattering is large but not infinite since the potential is cut-off by the charged cloud.

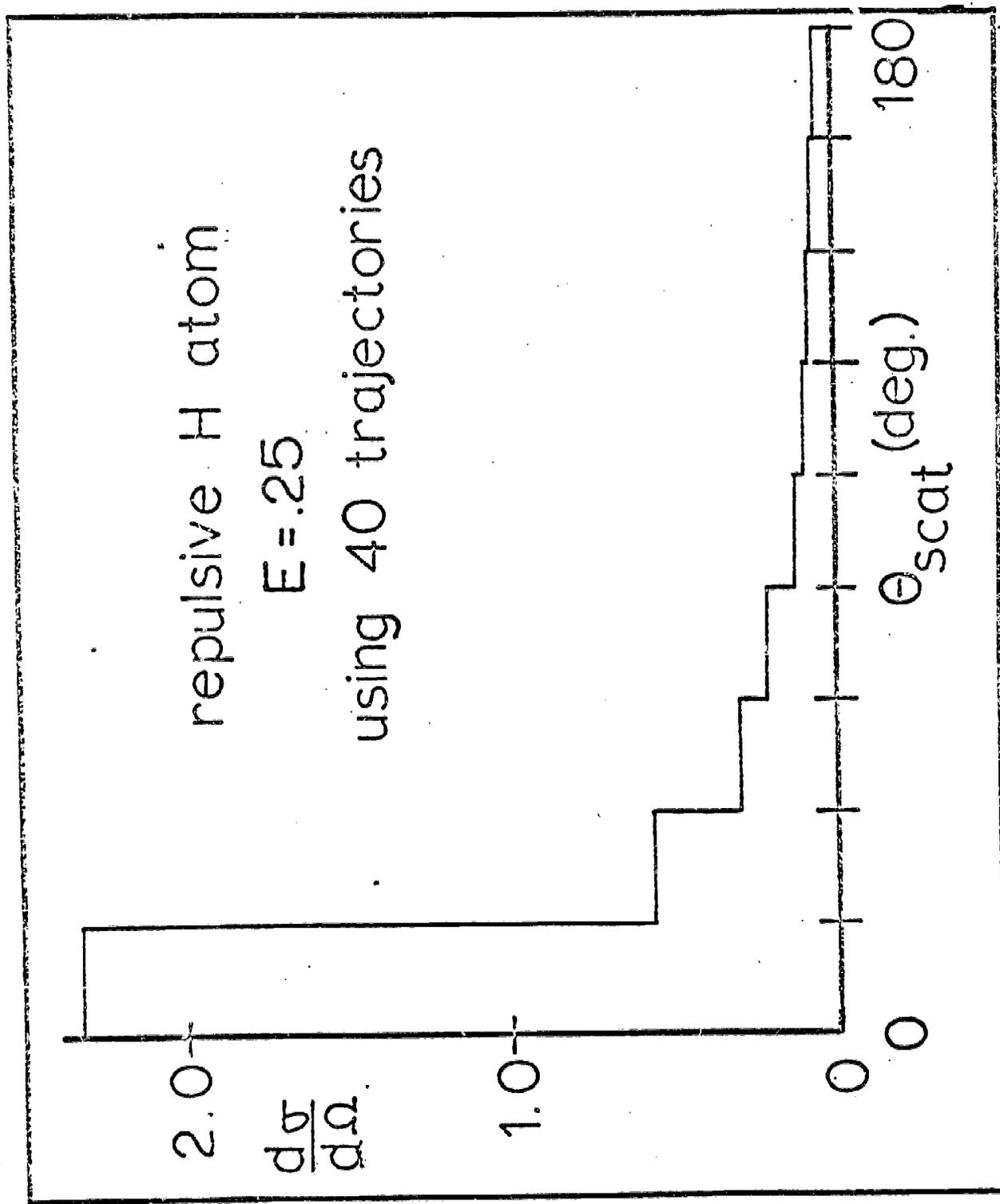


FIGURE 5

Classical scattering of a point electron off the model of S-state hydrogen. The looping orbits are real. Near an impact parameter of .9 for energy of .25 (normalized units) the particle takes an arbitrarily long time to escape from the atom. The program illustrates another of many uses of computer graphics in classical mechanics.

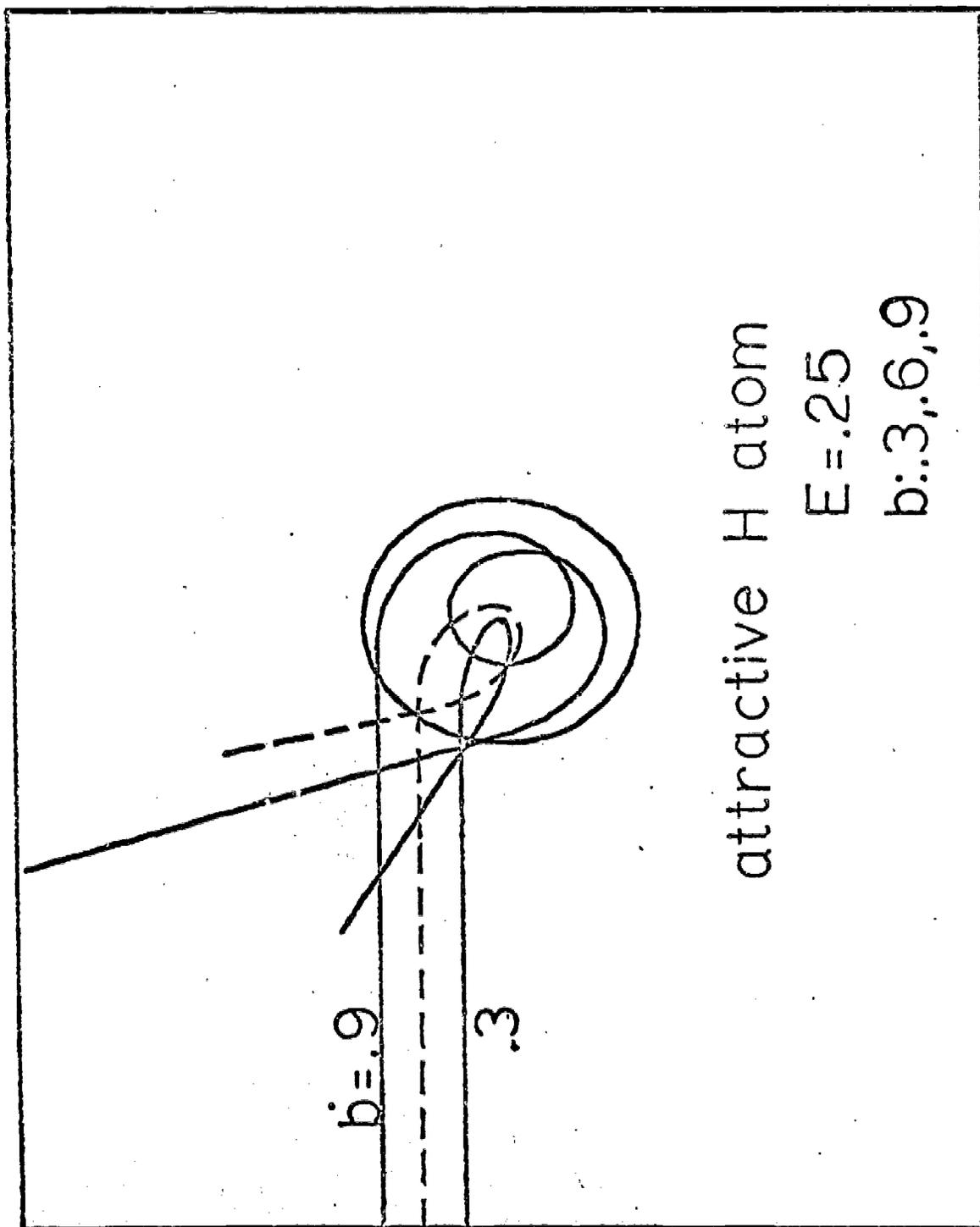
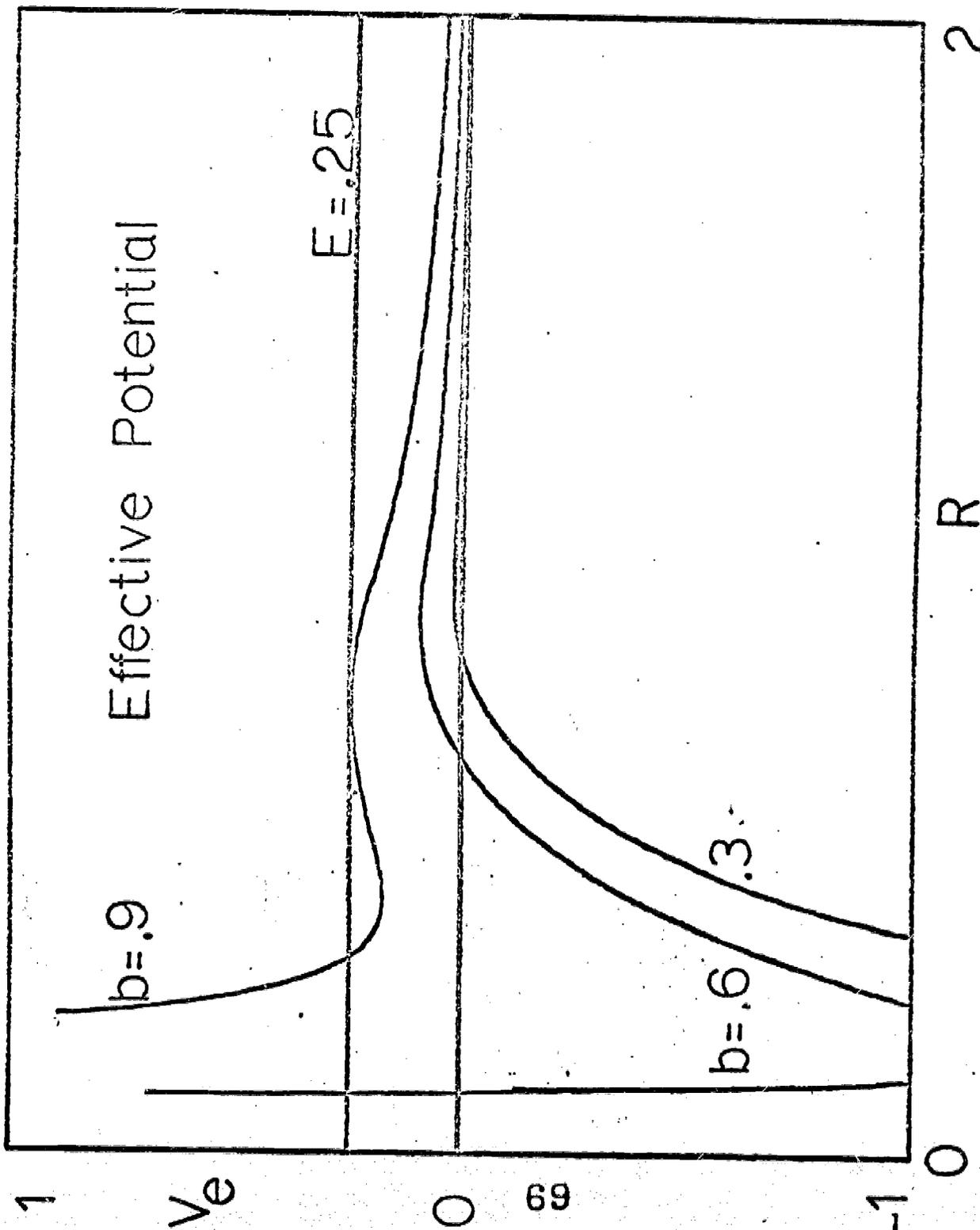


FIGURE 6

Effective potential for several impact parameters for electron scattering off hydrogen. The curves correspond to the trajectories shown in Fig. 5. Since the (radial velocity)² is proportional to $(E - V_{\text{eff}})$, the particle can take a long time moving in or out over the bump in V_{eff} . During this time, conservation of angular momentum forces the particle to wind many times around the nucleus.



Flow By Cylindrical Object

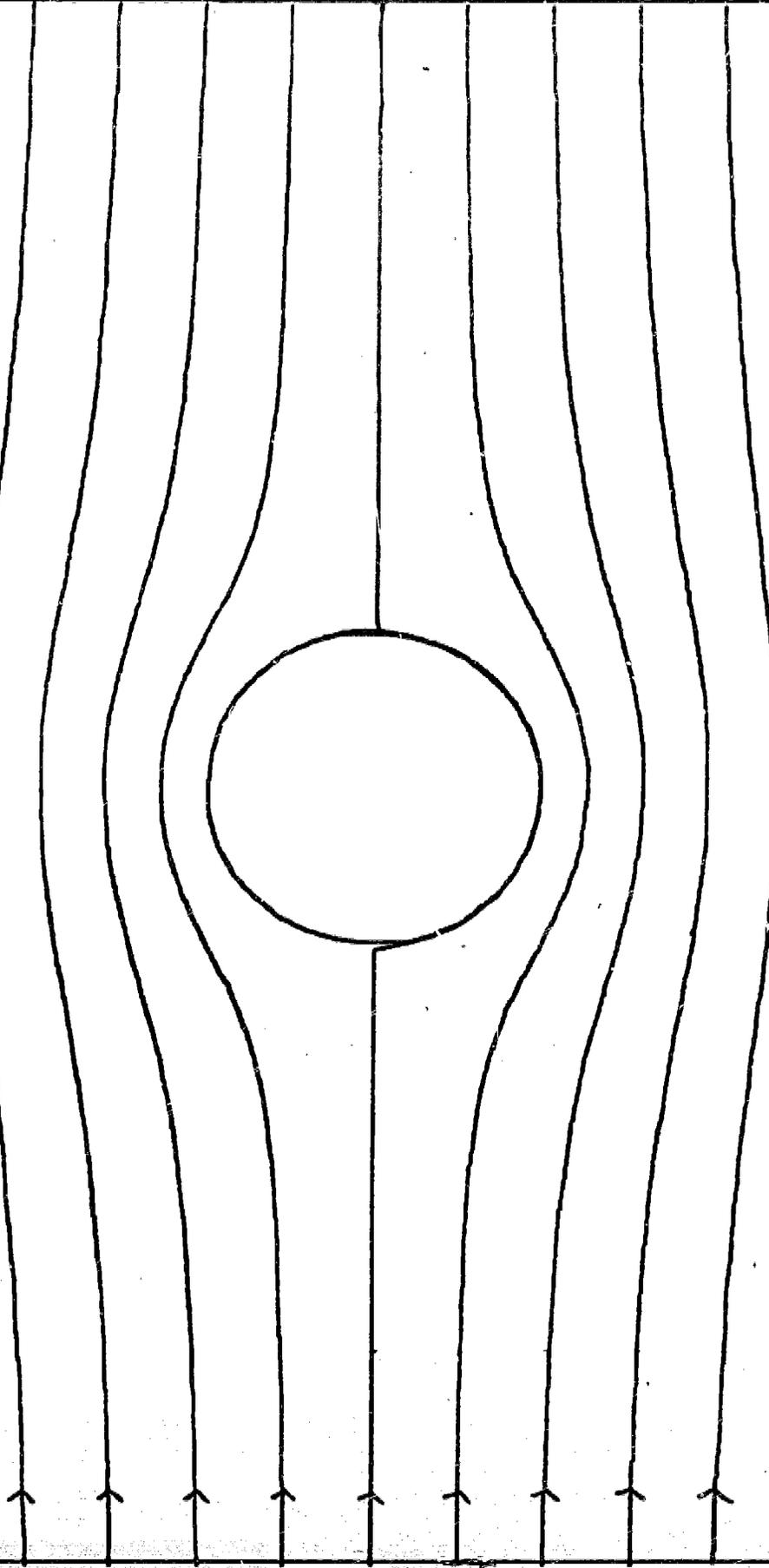
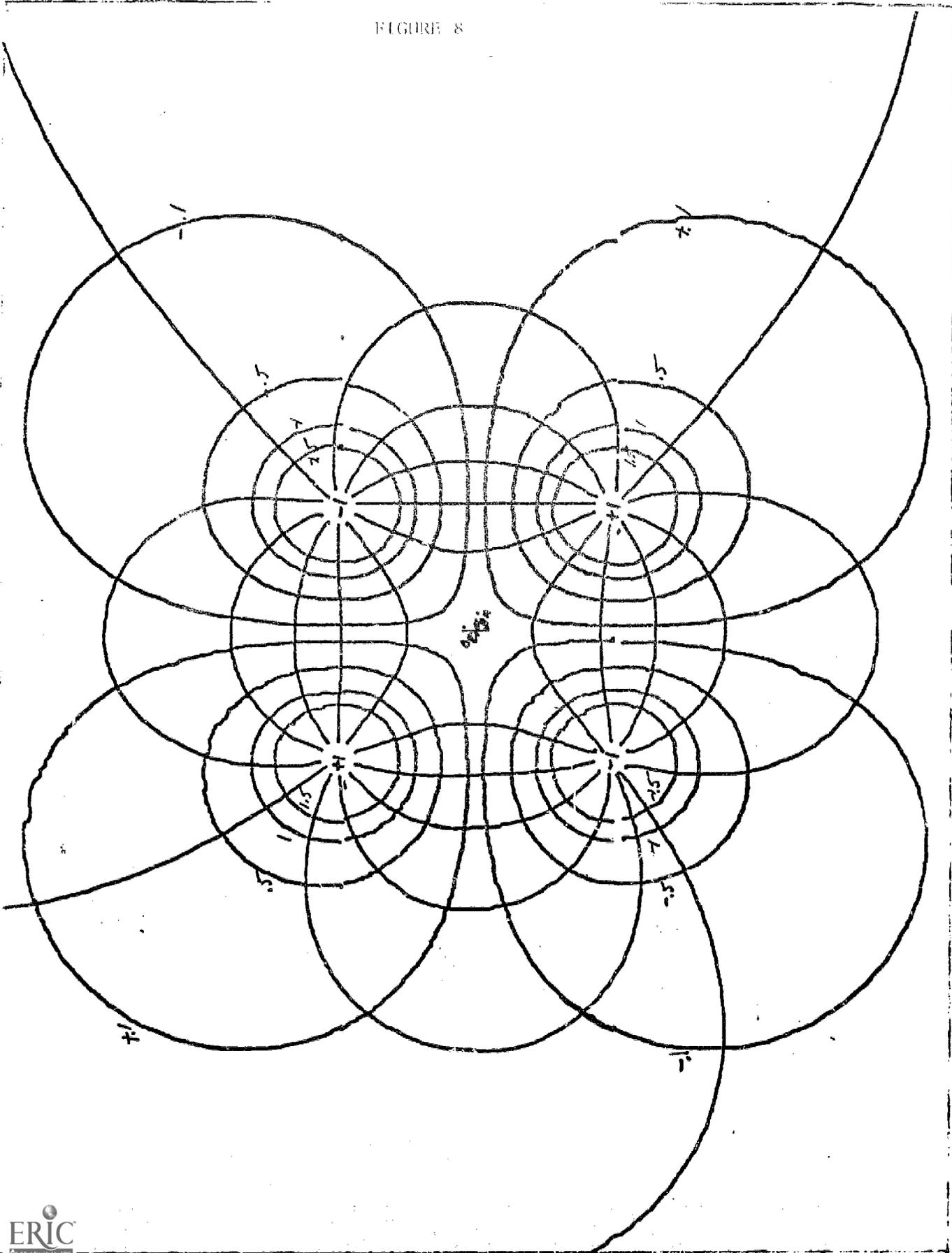


FIGURE 7

Velocity flow lines for fluid flow around a cylindrical object. The student becomes used to field line concepts by measuring the [relative] velocities at various points in the velocity field. The program is one of several dealing with fluid flow and velocity fields.

FIGURE 8



Electric field lines and equipotential surfaces in the plane of a two-dimensional quadrupole. The program allows placement of charges anywhere in the plane. Field lines are followed by integrating $dx/E_x = dy/E_y$; equipotential surfaces are followed by hunting. The program illustrates one of many ways computer graphic displays are used to enhance the student's intuition about electrostatic field problems.

$dx/E_x = dy/E_y$. The program follows the equipotential by a hunting routine which follows the equipotential contour. Programs have also been developed which follow the equipotential by moving everywhere perpendicularly to the local electric field lines. These programs and plots are useful in that the student very quickly gains an intuitive grasp of the meaning of the abstract concepts of field lines and equipotential surfaces. Figures 9, 10 and 11 show other charge distributions that students have found interesting and useful.

In geometrical optics we have developed programs to illustrate tracing principal rays through a thin lens or spherical mirror optical system. By plotting rays for several systems the student understands imaging much more quickly. We have also developed true ray tracing programs in which the student can place any number of spherical interfaces between media anywhere in the plane. The student then starts the ray at some angle and at some position, and the program traces the ray through the system. This program demonstrates nicely the various forms of aberration, as shown in figure 12. The shift in focal point due to spherical aberration is apparent.

Figure 13 shows another application of the computer to introductory geometrical optics - mirages. The program allows the index of refraction of the medium to be a function of height. The figure shows the results for a model index of refraction near heated ground. The sheet of less dense air near the ground produces a second, inverted, virtual image of any object above the surface. One observes two objects - one at the true position of a tree; the second a mirage image. This program can also be used to demonstrate "looming". Looming is an upside down mirage and probably explains most sightings of the "Flying Dutchman". Looming is due to a layer of warm air sandwiched between layers of cold air. The program also illustrates reflections of radio waves off the ionospheric F layer.

In physical optics, we have programmed a number of applications of Huygen's Principle. The student, for example, actually shows that an N-slit diffraction pattern is produced by adding up circles centered on the slits. One can even produce a fairly good single slit pattern with relatively short times.

Such programs have also led to more applied physical optics. Students have dealt with arrays of radio antennas placed to maximize the directionality for transmission or reception. They have studied broadside arrays and interferometric radio telescope arrays. In these programs the student compares plots of intensity versus angle, and intensity versus position on a screen. Figure 14 is a plot of intensity versus angle for three line sources placed on an equilateral triangle of side length = $1/2$ wavelength.

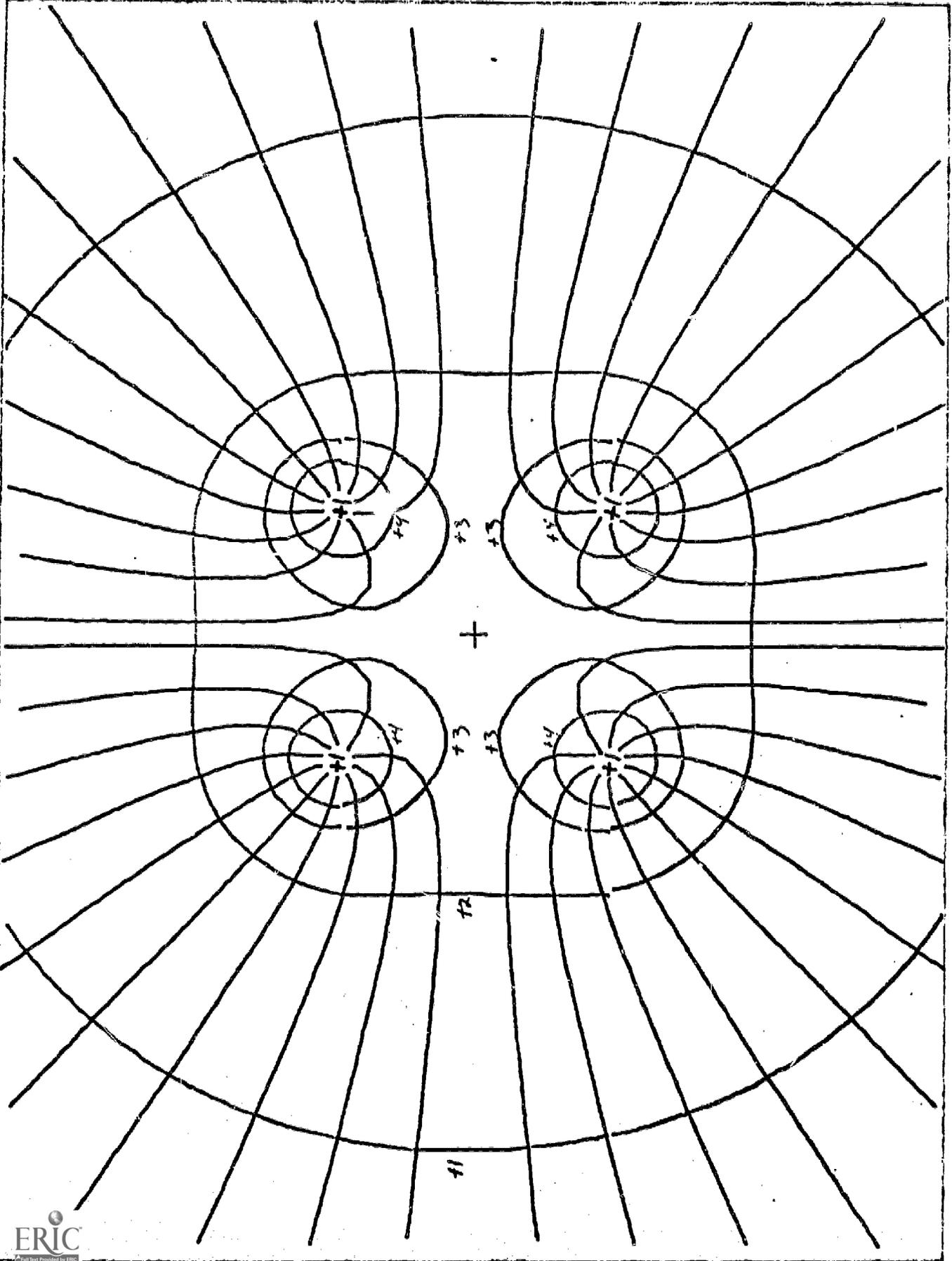


FIGURE 9

Field lines and equipotential surfaces in a plane containing four equal positive point charges on the corners of a square. Notice that close to the charges and far from the charges the equipotentials are circles. At intermediate distances the equipotentials in the plane take the general shape of the charge distribution.

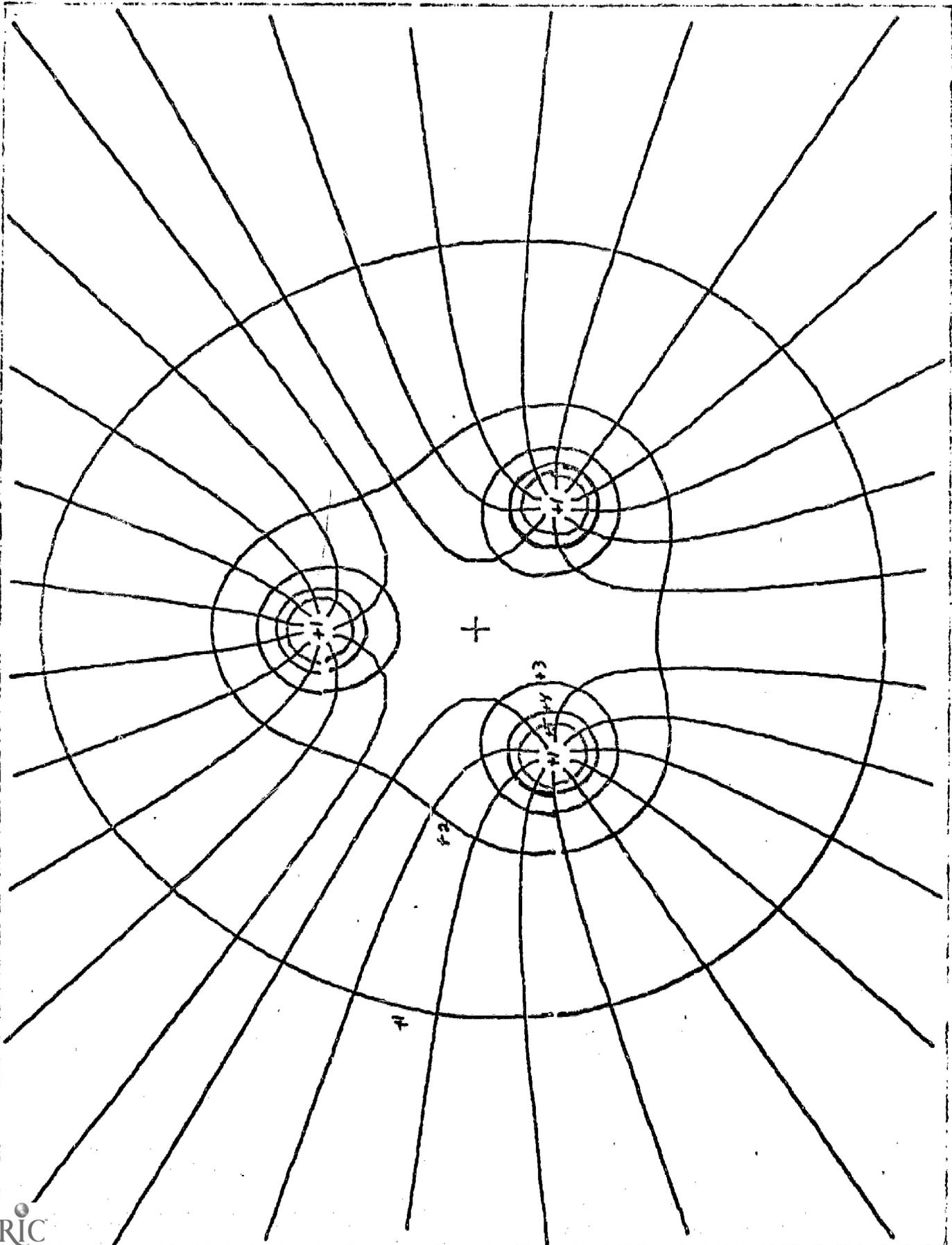
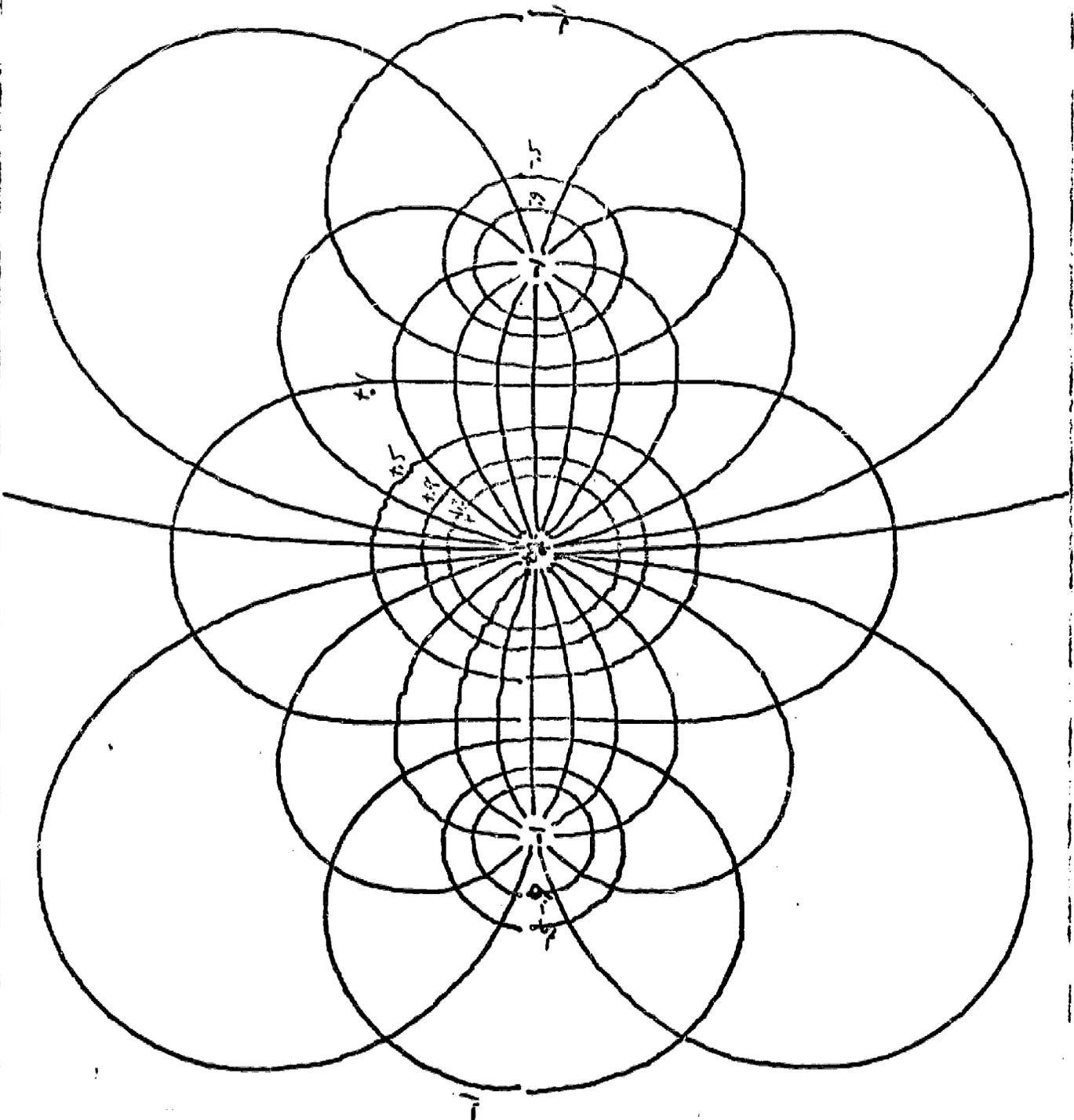


FIGURE 10

Field lines and equipotential surfaces in a plane containing three equal positive point charges on the corners of an equilateral triangle.

FIGURE 11



Field lines and equipotential surfaces for two back-to-back linear dipoles. The complete set of surfaces are generated by rotating the figure about an axis through the charges.

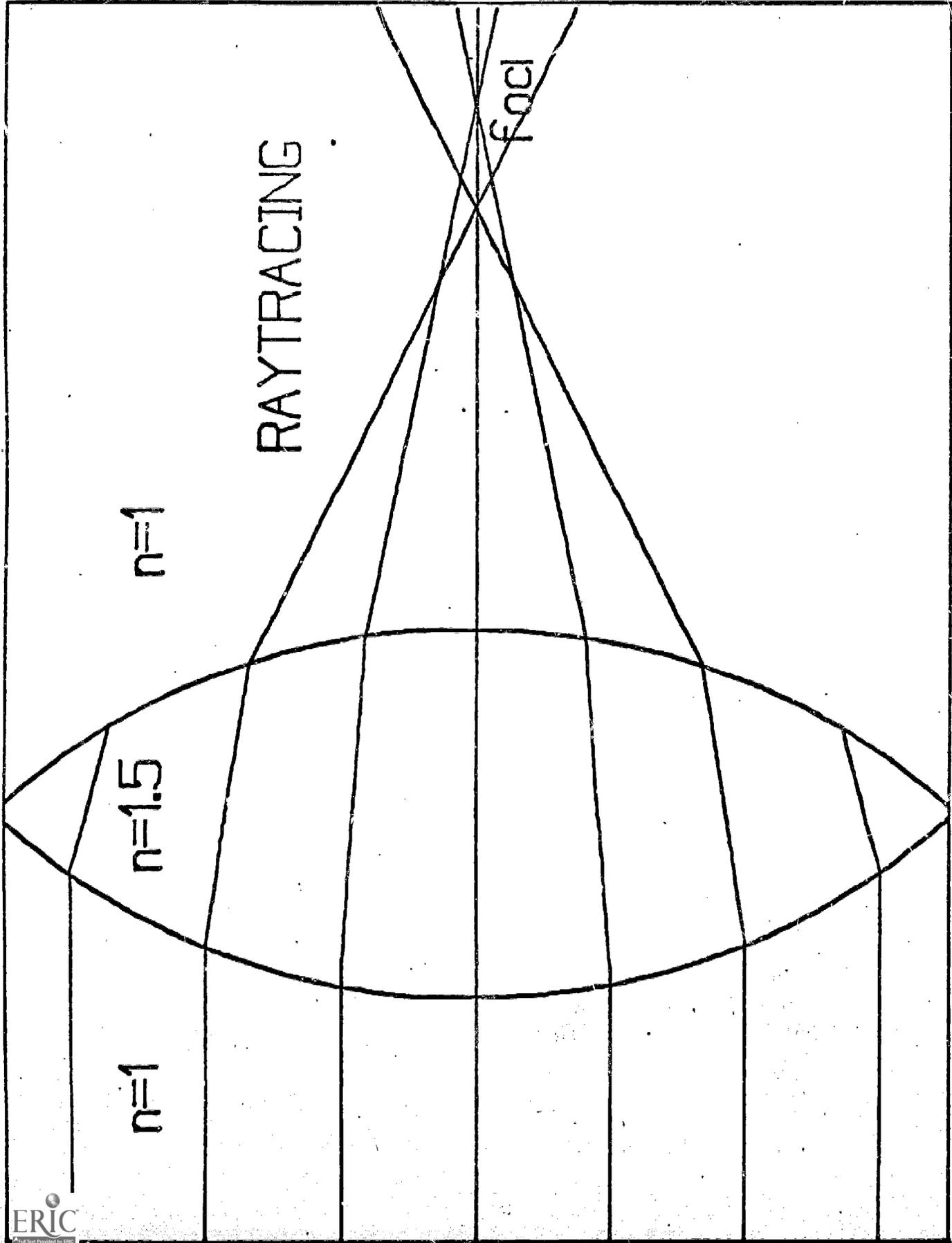


FIGURE 12

Rays traced through a thick lens. The effects of aberration are apparent in the focal point. The program allows any number of spherical interfaces between media to be placed anywhere in the plane. Rays are then started at any position and angle to the axis and are traced through the system.

FIGURE 13

Mirage effects when the index of refraction varies with height above the ground. Due to total internal reflection in the heated air layer, an observer sees two objects - one above the ground; one below. The program is one of a series of various ray-tracing illustrations.

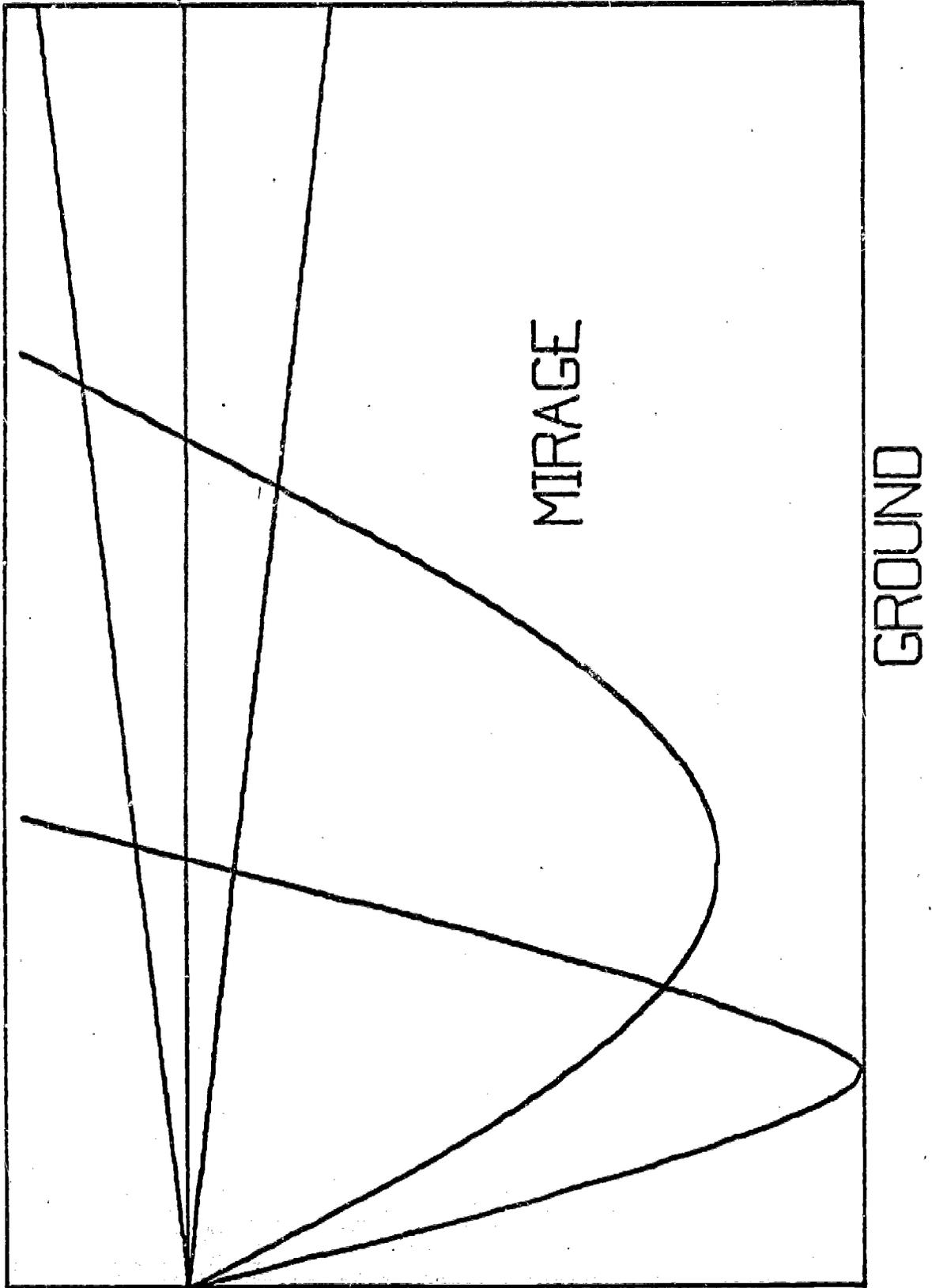
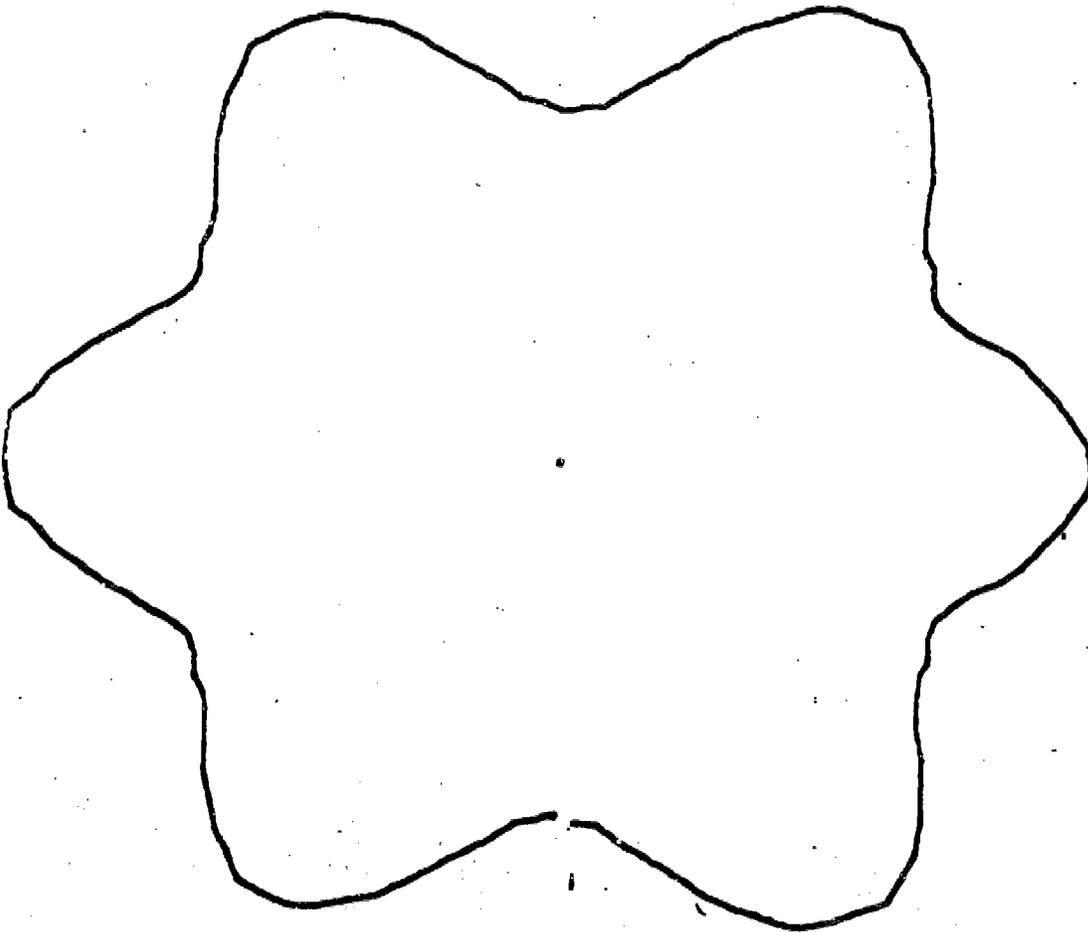


FIGURE 14

Intensity of emitted radiation versus angle from three synchronous sources placed at the corners of an equilateral triangle of side $\lambda/2$. The program allows the student to place any number of sources anywhere in the plane and to choose relative intensities and phases.



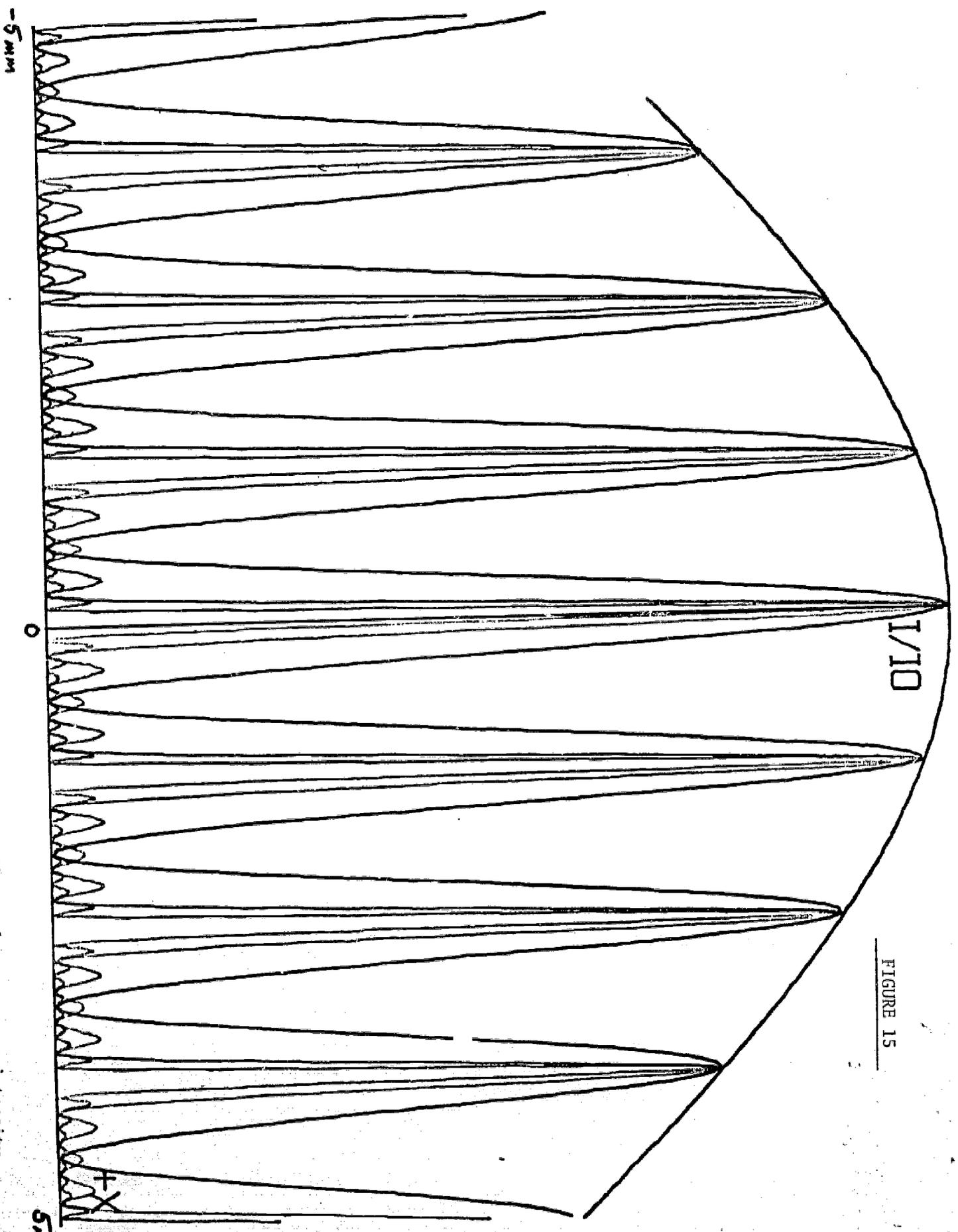
A laboratory application of the computer in introductory physical optics is shown in figure 15. This figure shows (normalized) N-slit diffraction patterns from 1, 2, 5 and 10 slits using the geometry and wavelength given for an introductory lab. The student measures the intensity versus position across the observation screen of an N-slit experiment using a photoresistor and a He-Ne laser. He plots his results on top of a theoretical plot such as figure 15. The agreement is good.

CONCLUSION

This paper has illustrated a number of uses for graphic display devices in introductory physics teaching. All the illustrations used inexpensive X-Y plotter systems connected to the computer. The programs have also been performed on a CRT terminal. Some of the plots also have been performed on the teletype itself. Hopefully, a large number of examples of the use of graphic display devices illustrates the importance of these devices better than volumes of words and perhaps these examples will trigger other examples in the reader's mind. A glance at a plot often leads to more understanding than a long look at a series of numbers in tabular form.

A short comparison of the three methods of plotting we have used might be helpful. The CRT device is faster than either the X-Y system or the teletype. It is useful for debugging and for situations where large numbers of curves must be displayed quickly. The CRT is, incidentally, essentially silent when compared to a teletype, but also relatively expensive when compared to a teletype and an X-Y plotter. The X-Y recorder plotting system is much faster, in general, than a teletype and has much higher resolution. It automatically gives the student a hard copy of his results for further deduction. It could well become the work horse of introductory teaching applications. The plots are easy to handle, scale and even label on the computer if the student wishes. The teletype itself can be used to plot some curves; often however, the resolution available is insufficient to show anything but coarse behavior. Nonetheless teletype plotting is a useful way to introduce students to plotting in general and can be very useful in debugging plotting routines fairly quickly.

FIGURE 15



1, 2, 5 and 10. slit diffraction patterns for data from a student laboratory. The student measures intensity versus position on the screen by using a photoresistor and a Simpson meter; he then compares his results to plots such as these. The program illustrates one of many ways computer display devices are used in physical optics.