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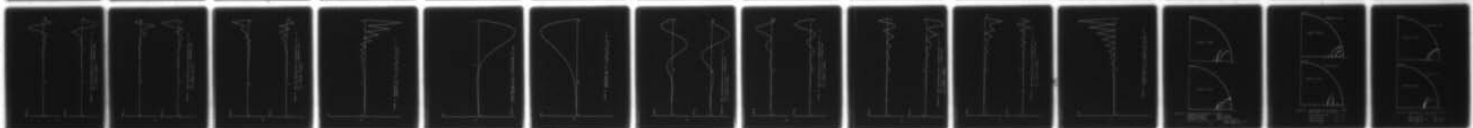
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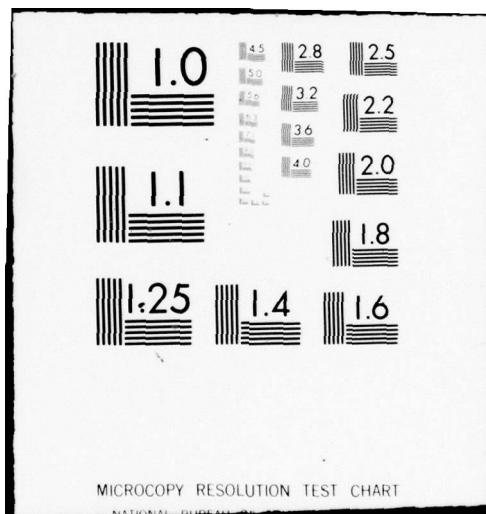
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THE MARTIN-LOMAX ITERATION FOR THE COMPUTATIONS OF
TRANSONIC FLOW FIELDS - SOME OBSERVATIONS.

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Karl G./Guderley and Donald S./Clemm

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Charles L. Keller

CHARLES L. KELLER
Project Engineer
Applied Mathematics Group
Analysis & Optimization Branch

Charles A. Bair, Jr.

CHARLES A. BAIR, Jr, Major, USAF
Chief, Analysis & Optimization Br
Structural Mechanics Division

FOR THE COMMANDER

Ralph L. Kuster, Jr.

RALPH L. KUSTER, Jr, Colonel, USAF
Chief, Structural Mechanics Division

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pertaining to the elliptic operator used in the Martin-Lomax iteration, with those of a hyperbolic problem is discussed. The one-dimensional difference procedure gives rise to a linear eigenvalue problem. The distribution of the eigenvalues and the form of the eigenvectors explains the convergence behavior of solutions obtained with different initial conditions. The influence of certain arbitrary parameters which occur in the Martin-Lomax procedure is briefly discussed. An attempt is made to improve the convergence of the iterations by the application of Aitken-Shanks formulae of different orders. A direct derivation of the concept underlying these formulae is given. In the present examples, the Aitken-Shanks extrapolation failed to accelerate the convergence.

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FOREWORD

The work was performed in 1978 under Grant AFOSR 78-3524 to the University of Dayton with K.G. Guderley as Principal Investigator. The work of Donald S. Clemm was carried out in the Air Force Flight Dynamics Laboratory under Project 2304N102, Mathematical Problems in Fluid Dynamics.

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SECTION I

INTRODUCTION

This article studies some simple examples which illustrate the working of the Martin-Lomax iteration (Ref. 1) for the computation of transonic flow fields. They deal with flow fields linearized for the vicinity of a fixed Mach number or (in the discussion of the shock operator) linearized with respect to a subsonic and to a supersonic Mach number, both assumed to be fixed. Martin (Ref. 2) has carried out similar discussions but only in a rudimentary form; this suffices to develop and motivate his ideas. His discussions merely serve to suggest that a stable iteration scheme for flow computations can be obtained if one chooses certain parameters in a suitable manner, while the actual test of convergence is carried out in a more realistic setting. For a justification of the Martin-Lomax procedure, the present more detailed study is therefore unnecessary. Nevertheless, it may have a certain interest because it provides an insight into the working of the method. In addition, there are certain difficulties of an intuitive character which a novice to this procedure is likely to have and which the author hopes to dispel by the present study. To be specific: in each iteration step the Martin procedure solves a problem closely related to Poisson's equation, the solutions satisfy the boundary conditions of an elliptic problem. It is not immediately clear how the solution to a hyperbolic problem, which has different boundary conditions and regions of influence can be built up in this manner. Of a similar nature is the question how such a procedure can lead to shocks, for one is inclined to ascribe a smoothing tendency to an elliptic operator, but for a shock a sudden change of velocity is characteristic. These objections may appear less serious if one interprets the iterations as a time dependent process, as is done

in Ref. 2. Then one deals with a three dimensional problem (two space dimensions and the time) for which the solution in the long time limit happens to satisfy the desired two dimensional problems, which are governed by elliptic or hyperbolic operators.

Martin's stability analysis of the difference equation is carried out by means of a substitute partial differential equation which arises from the three dimensional difference formulation by a Taylor development with respect to space and time. Strictly speaking, such a development is valid only if the wave length of the perturbations is large in comparison to the grid size, and if the changes with respect to time are only small. It is sufficient to establish consistency of the difference scheme with the original two dimensional partial differential equation. But the stability analysis cannot be restricted to perturbations of this character. Short waves (down to a wave length of twice the distance between grid points) cannot be disregarded. It is true, in the limit of zero grid size such waves are unimportant in a smooth starting approximation for elliptic problems. Still they may be excited by rounding errors. In supersonic flows and in flows with shocks, short waves will be excited even by the starting approximation.

In the author's opinion an independent analysis of the shock point operator is inappropriate. In a shock one has a rapid change of the gradient of the potential within a few mesh points. The number of mesh points where this happens does not increase as the mesh is refined. Moreover, the shock point operator is applied only at the shock points, that is along a line of the two dimensional flow field. It is therefore necessary that the shock is considered as imbedded in a supersonic-subsonic flow field.

The present report investigates questions of this kind.

SECTION II

DESCRIPTION OF SAMPLE PROBLEMS

Martin and Lomax use the velocity components as independent variables. For the present discussion, it is equally convenient to work with the velocity potential. We consider the linear differential equation

$$-\frac{\partial}{\partial x} (u_\ell \phi_x) + \phi_{yy} = 0 \quad (1)$$

here u_ℓ denotes the local deviation of the x-velocity from 1, ϕ is the perturbation potential. In our example u_ℓ is considered as constant. In studying the parabolic operator it would be necessary to allow u_ℓ to change continuously with x . Equation (1) arises, if one carries out a Prandtl-Glauert coordinate distortion for a subsonic Mach number in a linearized differential equation for subsonic or supersonic flow. The local Mach number is allowed to be different from the Mach number for which the Prandtl-Glauert coordinate distortion is carried out. The velocity field represented by ϕ gives a small perturbation to the local velocity u_ℓ . The potential ϕ is assumed to be of period L in the y direction. Let the number of subdivisions per period in the y direction be N , then one has a grid size

$$h = L/N. \quad (2)$$

We have assumed that a Prandtl-Glauert transformation has already been carried out in Equation (1); it is therefore reasonable to assume that the grid size in the x and y direction is the same. In analyzing the procedure we consider particular solutions

$$\phi(x, y) = \tilde{\varphi}(x) \exp(i n 2\pi \frac{y}{L}) \quad (3)$$

This solution has n full waves within the period L . In a finite difference approximation one obtains

$$\begin{aligned} \phi_{yy} &= -\frac{1}{h^2} \tilde{\phi}(x) \exp(i n 2\pi \frac{y}{L}) 4 \sin^2(\pi n \frac{h}{L}) \\ &= -\frac{1}{h^2} \tilde{\phi}(x) \exp(i n 2\pi \frac{y}{L}) 4 \sin^2(\pi \frac{n}{N}) \end{aligned}$$

Thus, one obtains

$$-\frac{\partial}{\partial x} (u_{\frac{1}{2}} \tilde{\phi}_x) - \frac{4}{h^2} \sin^2(\pi \frac{n}{N}) \tilde{\phi} = 0 \quad (4)$$

Here, n assumes values from 0 to $N/2$; $n = 0$ gives a one dimensional flow. Let

$$\bar{\phi}_k = \tilde{\phi}(kh)$$

The difference form of Equation (4) for an elliptic problem (with constant $u_{\frac{1}{2}} = -|u_{\frac{1}{2}}|$) is then given by

$$|u_{\frac{1}{2}}| [\bar{\phi}_{k+1} - 2\bar{\phi}_k + \bar{\phi}_{k-1}] - 4 \sin^2(\pi \frac{n}{N}) \bar{\phi}_k = 0 \quad (5)$$

Let the beginning and the end in the x direction of the region under consideration be given as $k = 0$ and $k = K$. The values of ϕ_0 and ϕ_K are prescribed as boundary conditions. For the hyperbolic region the difference operator expressing ϕ_{xx} is displaced by one mesh in the upstream direction (here to the left)

$$-|u_{\frac{1}{2}}| [\bar{\phi}_k - 2\bar{\phi}_{k-1} + \bar{\phi}_{k-2}] - 4 \sin^2(\pi \frac{n}{N}) \bar{\phi}_k = 0 \quad (6)$$

Here the values of $\bar{\phi}$ and $\bar{\phi}_x$ are prescribed at the initial point ($k=0$). To the first order in h these quantities are expressed by $\bar{\phi}_0$ and $\bar{\phi}_{-1}$. Equation (6) expresses $\bar{\theta}_k$ in terms of $\bar{\theta}_{k-1}$ and $\bar{\phi}_{k-2}$. The initial conditions are of a nature which allows the problem to be solved by a marching procedure.

A flow containing a shock is hyperbolic upstream (to the left) of the shock and elliptic downstream of it. In the Murman procedure (Reference 3) the point at which the shock operator is to be applied is found by a separate test. In the present context we deal with perturbations to a flow which already contains a shock. These perturbations are assumed to be small enough so that the result of this test will not be affected by the perturbations. Accordingly, the shock point is considered as fixed. Let s be the subscript of the point at which the shock point operator is applied. To the left and to the right of this point one has respectively $u_\ell = |u_\ell| = \text{const}$ and $u_\ell = -|u_\ell| = \text{const}$. For $1 < k < s - 1$ and for $s + 1 < k < K - 1$, one applies respectively the hyperbolic form (6) and the elliptic form (5) of the difference operator. The shock point operator is obtained by replacing $\partial(u_\ell \phi_x) / \partial x$ by $(h)^{-1} ((u_\ell \phi_x)_{s+1/2} - (u_\ell \phi_x)_{s-1/2})$. One has $u_{\ell, s-1/2} = |u_\ell|$; $u_{\ell, s+1/2} = -|u_\ell|$ and

$$(\tilde{\phi}_x)_{s+1/2} = h^{-1} (\bar{\phi}_{s+1} - \bar{\phi}_s)$$

and because of the shift by one mesh to the left in the hyperbolic region

$$(\tilde{\phi}_x)_{s-1/2} = h^{-1} (\bar{\phi}_{s-1} - \bar{\phi}_{s-2})$$

One thus obtains for the shock point

$$|u_\ell| \{ (\bar{\phi}_{s+1} - \bar{\phi}_s) - (\bar{\phi}_{s-1} - \bar{\phi}_{s-2}) \} - 4 \sin^2(\pi \frac{n}{N}) \bar{\phi}_s = 0$$

We shall not carry out a study of problems containing a parabolic point. In such a case one would assume that u_ℓ changes continuously from a negative to a positive value. Let $k = p$ be the point where the parabolic operator is to be applied. A simple choice for u_ℓ is

$$u_\ell = \text{const} (x - x_p)$$

Then one would have for a point of the elliptic region, that is for

$$1 \leq k \leq p-1$$

$$\text{const } h \{ (k + 1/2 - p)(\bar{\phi}_{k+1} - \bar{\phi}_k) - (k - 1/2 - p)(\bar{\phi}_k - \bar{\phi}_{k-1}) \} - 4 \sin^2(\pi \frac{n}{N}) \bar{\phi}_k = 0$$

and in the hyperbolic region, that is for $p+1 \leq k < K$

$$\text{const } h \{ (k - 1/2 - p)(\bar{\phi}_k - \bar{\phi}_{k-1}) - (k - 3/2 - p)(\bar{\phi}_{k-1} - \bar{\phi}_{k-2}) \} - 4 \sin^2(\pi \frac{n}{N}) \bar{\phi}_k = 0$$

At the parabolic point, one obtains by a procedure corresponding to that of a shock point

$$(u_2 \phi_x)_{p+1/2} = u_{2,p-1/2} (\bar{\phi}_p - \bar{\phi}_{p-1})$$

$$(u_2 \phi_x)_{p-1/2} = u_{2,p-1/2} (\bar{\phi}_p - \bar{\phi}_{p-1})$$

Hence

$$\frac{\partial}{\partial x} (u_2 \phi_x)_p \sim 0$$

and because of Equation (4)

$$\bar{\phi}_p = 0$$

Notice that the parabolic operator provides a boundary condition for the elliptic region. It is therefore possible to compute the elliptic region independently. Of course, this holds only for the present example where the transition from the elliptic to the hyperbolic region occurs along a line $x = \text{const}$.

SECTION III

THE MARTIN-LOMAX ITERATION

Let us denote by ϕ_k^i the values ϕ_k obtained by the i^{th} iteration. Assume that the ϕ_k^i 's are known, that is, that the i^{th} iteration is completed. To obtain the equations for the $(i+1)^{\text{th}}$ iteration the difference approximation for $\partial^2\phi/\partial y^2$ is expressed in terms of the unknown values ϕ_k^{i+1} ; while the difference approximations for the x derivatives are computed for the ϕ_k^i 's. Martin and Lomax include in the equations further expressions which are linear in the ϕ_k , evaluated once with the ϕ_k^{i+1} and a second time with the opposite sign with the ϕ_k^i . If the iterations converge, that is, if $\phi_k^{i+1} = \phi_k^i$ in the limit $i \rightarrow \infty$, these terms cancel and one is left with the difference approximation to the problem. These additional expressions are of such a nature that the resulting difference equations for the ϕ_k^{i+1} 's have constant coefficients. Martin's preliminary analysis suggests that for a suitable choice of certain parameters which are left arbitrary, the procedure will converge. The equations ultimately to be solved are:

$$\begin{aligned}
 & (1-\alpha_1)(\phi_{k+1}^{i+1} - \phi_k^{i+1}) - (1+\alpha_2)(\phi_k^{i+1} - \phi_{k-1}^{i+1}) - 4 \sin^2\left(\frac{\nu}{N}\pi\right)\phi_k^{i+1} \\
 & = (1-\alpha_1)(\phi_{k+1}^i - \phi_k^i) - (1+\alpha_2)(\phi_k^i - \phi_{k-1}^i) \\
 & + \begin{cases} |u_\ell|(-\phi_{k+1}^i + 2\phi_k^i - \phi_{k-1}^i) & \text{for elliptic points} \\ |u_\ell|(\phi_k^i - 2\phi_{k-1}^i + \phi_{k-2}^i) & \text{for hyperbolic points} \\ |u_\ell|(-\phi_{s+1}^i + \phi_s^i - \phi_{s-1}^i + \phi_{s-2}^i) & \text{for shock points} \end{cases} \quad (7)
 \end{aligned}$$

Similar equations arise in problems containing a parabolic point except that then one has to take the fact into account that u_ℓ is not constant.

SECTION IV

DISCUSSION OF EQUATION (7)

Martin's discussion amounts to an application of the von Neumann stability criterion to a simplified form of this equation. It is assumed that the region extends in the x direction from $-\infty$ to $+\infty$. The elliptic and the hyperbolic problem will be studied separately. The difference equation for the ϕ_k^{i+1} 's has constant coefficients. Therefore, it is natural to study particular solutions of Eq. (7) of the form

$$\phi_k^{(i)} = \exp(i\mu 2\pi kh) \rho_\mu^i \quad (8)$$

where μ is a real constant, which ranges from 0 to 1/2. The smallest wave length (namely $2h$) occurs for $\mu = 1/2$. The hypothesis Eq. (8) guarantees that these particular solutions remain bounded for $k \rightarrow \pm\infty$. The constant ρ_μ , so far unknown, is the (complex) factor by which each particular solution is multiplied as one proceeds from one iteration step to the next one. One obtains immediately from Eq. (7)

$$\begin{aligned} & (\rho_\mu - 1) \left[(1 - \alpha_1) (\exp(i\mu 2\pi h) - 1) - (1 + \alpha_2) (1 - \exp(-i\mu 2\pi h)) \right] - 4\rho_\mu \sin^2\left(\frac{n}{N}\pi\right) \\ & + \begin{cases} |u_\ell| (-\exp(i\mu 2\pi h) + 2 - \exp(-i\mu 2\pi h)) & \text{for elliptic problems} \\ |u_\ell| (1 - 2\exp(-i\mu 2\pi h) + \exp(-2i\mu 2\pi h)) & \text{for hyperbolic problems} \end{cases} \end{aligned} \quad (9)$$

From this equation, one readily computes the ρ_μ 's for each choice of α_1 , α_2 , $|u_\ell|$, n/N , and h . In order for the procedure to converge in a general case, it is necessary that one finds values of the parameters α_1 and α_2 in such a manner that $|\rho_\mu| < 1$ for all values of $|u_\ell|$, n/N and μ which occur in the flow field.

To be somewhat more specific: one starts with an assumed vector ϕ_k^0 which satisfies the boundary conditions of the elliptic or hyperbolic problem. It can be considered as a linear combination of the desired solution (for which $\phi_k^{i+1} = \phi_k^i$) and homogeneous particular solution of the form Eq. (8). The contributions of these homogeneous

particular solutions become small as the iterations proceed, if $|\rho_\mu| < 1$ for $0 < \mu < 1/2$, because they are multiplied in each iteration step with respective values of ρ_μ . Finally, the desired solution of the inhomogeneous problem is left.

The analysis described so far agrees with that of Martin except that he assumes n and μ to be small. Such an analysis does not provide an insight into the effect of boundary conditions at the beginning and at the end of a finite region; the conditions of boundedness at $x \rightarrow \pm\infty$, which take their place, are somewhat vague. For the homogeneous particular solutions, one has the boundary conditions $\phi_0 = 0$ and $\phi_K = 0$, for hyperbolic as well as for elliptic problems. For the elliptic problem, these conditions do not offer any conceptual difficulty, for they agree with those of the original partial differential equation. For the hyperbolic problem, one postulates that ϕ_0 and ϕ_{-1} assume the values given as initial conditions in all iterations (including the starting approximation); besides one sets $\phi_K = 0$. The boundary values for ϕ_{-1} and ϕ_K are used when one computes the right hand side for the $(i + 1)^{\text{th}}$ iteration from the values of ϕ_k^i . In the computation of ϕ_k^{i+1} only the values of ϕ_0^{i+1} and ϕ_k^{i+1} appear as boundary conditions.

If the homogeneous particular solutions die out in the course of the iterations, then the final solution will, of course, have the prescribed values of ϕ_{-1} and ϕ_0 . That is, it will satisfy the boundary conditions of the hyperbolic problem. There is, however, a question about the meaning of the condition $\phi_K = 0$. Certainly there is no room in a hyperbolic problem to satisfy this condition. This discrepancy resolves itself in the following manner. It was mentioned above that the hyperbolic problem can be solved by a marching procedure. The expression Eq. (6) allows one to compute the value of ϕ for some point k from points preceding k ; it expresses the requirement that the differential equation in its finite difference form be satisfied at point k . This requirement is met for all interior points of the region, that is, for $1 < k < K - 1$. At the point K , no such requirement is imposed. It follows that the value of $\phi_K = 0$ imposed in computing a new iteration need not coincide with the values of ϕ_K which one would obtain at point K if one solves the original difference equation (by the marching procedure). A

curve drawn through the points ϕ_k will, in general, have a break at the point K-1. The starting approximation cannot be expected to have the correct value of ϕ_{K-1} , for this value is not known in advance. The contribution of the homogeneous particular solutions to the starting solution will therefore be finite at the point K-1, while it is zero at point K. One sees that homogeneous particular solutions of short wave length will play an important role in the hyperbolic problems. In elliptic equations, a corresponding jump tends to zero as the mesh is refined.

SECTION V

STABILITY

The stability of the procedure for a certain choice of the parameters $\alpha_1, \alpha_2, u_\ell$, and n/N can be studied by assuming arbitrary initial conditions for ϕ which satisfy the boundary conditions of the homogeneous problem and by carrying the iteration out. The system of equations for the ϕ_k^{i+1} , is actually a three-point recurrence relation with constant coefficients. It can be efficiently solved by the method of cyclic reduction.

(Because of this method we have chosen $K = 32 = 2^5$). Such computations have been carried out for a number of cases. The ϕ_k^i have been plotted for different values of i . A sample of these plots is shown in Figures 1 and 2. The initial conditions chosen are $\phi_k = 0$ for all points except either the point $k = 1$ or $k = K-1$. Such initial conditions could be represented by a linear combination of the eigensolutions of the problem (with none of the coefficients being zero). Therefore, it cannot happen that an eigensolution which might cause instability (that is for which the eigenvalue has an absolute value larger than one) is inadvertently excluded from the initial condition. In spite of this fact, one finds practically no similarity in the convergence behavior for these two kinds of initial conditions.

A more detailed insight is obtained by computing the eigenfunctions and eigenvalues which determine the iteration process. Let

$$\phi_k^{(i)} = u_k \rho^i, \quad k = 1, 2, \dots, K-1$$

The u_k 's are combined into a vector \vec{u} . Then one obtains from Equation (7) the following matrix eigenvalue problem.

$$[A + B]\vec{u} - \rho [A + C]\vec{u} = 0$$

A, B and C are matrices of dimension $K-1$ by $K-1$. Our examples have been computed for $K = 32$.

$$A = \begin{bmatrix} b & c & & & \\ a & b & c & & \\ & a & b & c & \\ & & & \dots & \\ & & & & a & b \end{bmatrix}$$

with $a = 1 + \alpha_2$

$$b = -(1 - \alpha_1) - (1 + \alpha_2)$$

$$c = (1 - \alpha_1)$$

$$C = -4 \sin^2\left(\frac{\pi n}{N}\right) I_{31}$$

where I_{31} is the 31 by 31 identity matrix

$$B = |u_\ell| \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & & \dots & \\ & & & & -1 & 2 \end{bmatrix}$$

for the elliptic case

In our computations the 15th point has been taken as the shock point. The eigenfunctions and eigenvalues are computed using the Q-Z Algorithm Ref. (4, 5)*.

The case $|u_\rho| = .5$; $n/N = 0.05$; $\alpha_1 = 0$; $\alpha_2 = 1$ has been taken as the starting point of the explorations.

For $K = 32$ one has 31 eigenvalues and eigenfunctions, most of them occur in conjugate complex pairs. Figures 3 and 4 show for the elliptic and the hyperbolic problem the eigenvalues which lie in the first quadrant of the complex ρ plane. They lie rather close to each other. Accordingly, one will not have an outspoken dominance of a single eigenvalue (or rather, in this case, of a pair of conjugate complex eigenvalues) even after a fairly large number of iterations. Figures 6 through 17 show some of the eigenfunctions for the elliptic and for the hyperbolic cases. They are ordered according to the absolute value of ρ . The waviness of the eigenfunctions increases as the absolute value of ρ decreases. It is somewhat disturbing that at the left end of interval the eigenfunctions are extremely small. To represent an initial condition in which all values of ϕ_2 are zero except for ϕ_1 , requires a linear combination of the eigenfunctions with very large coefficients. In contrast if $\phi_{K-1} = 1$ and all others are zero the coefficients of this linear combination will be of moderate size. This explains the difference of the results in Figures 1 and 2.

In Figures 3 and 4 some values of ρ which hold for an infinite interval are included. To obtain some similarity of the problem for an infinite interval with the eigenvalue problem for a finite region, we assumed that one has the same interval but with periodicity conditions for $k = 0$ and $k = 32$. This then selects 32 discrete eigenvalues from the continuous set given by Equation (9). The values of μ in Equation (9) are

*The algorithm is part of the EISPACK library, but it is not yet contained in the second edition of the EISPACK Guide.

found from the periodicity requirement

$$\mu 2\pi K h = m 2\pi$$

hence

$$\mu h = m/K$$

where

$$-K/2 < m \leq +K/2$$

The eigenvalues for periodicity conditions lie in the vicinity of those obtained with $\phi = 0$ at both ends of the region, but not in a close vicinity. The discrepancies are particularly large for the longest and for the shortest wave lengths. To recognize the influence of the length of the region under consideration, we have carried out the computations with boundary conditions $\phi = 0$ also for $K = 16$ (Fig. 5). All eigenvalues so obtained are close to some of the eigenvalues of the problem for $K = 32$. One sees that the stability analysis for an infinite interval gives results which are different from those for a finite interval (even though 32 is a rather large number). In the present example, the stability criteria obtained for an infinite interval are conservative.

Figure 18 shows the eigenvalues for an elliptic, a hyperbolic operator, and a problem with a shock. The number of eigenvalues is, of course, the same for the three cases. In this particular case one finds the remarkable result that the eigenvalues for the shock are close either to elliptic or hyperbolic eigenvalues. The same trend, but less pronounced, is found in Figure 18 for $n/N = 0$. In any case, one observes that the presence of the shock has no adverse effect on the stability of the procedure.

Figures 19, 20 and 21 give some indication of what happens if the parameters of the problem are changed. This part of the study is by no means exhaustive. One sees that a decrease in n/N and of u_0 has a destabilizing effect, an increase in α_2 makes the problem less stable in the elliptic case and more stable in the hyperbolic case.

These graphs can be used to discuss the influence of over or under relaxation between the relaxation steps. Let \vec{u}_k be the k^{th} eigenvector and let the difference between the values of ϕ in a certain iteration step and in the final solution be

expressed as $\sum_{k=1}^{K-1} C_k \vec{u}_k$. Then one obtains in the next iteration

step for this difference $\sum_{k=1}^{K-1} C_k \rho_k \vec{u}_k$. The change of this difference from one step to the next is given by $\sum_{k=1}^{K-1} C_k (1-\rho_k) \vec{u}_k$.

If one uses a relaxation factor β then this change is applied only partially, that is, one takes as a result of the next iteration step

$$\sum_{k=1}^{K-1} C_k \vec{u}_k - \beta \sum_{k=1}^{K-1} C_k (1-\rho_k) \vec{u}_k = \sum_{k=1}^{K-1} C_k (1-\beta(1-\rho_k)) \vec{u}_k$$

For a relaxation with a relaxation factor β , one therefore has as effective eigenvalues

$$\rho_k^* = 1 - \beta(1-\rho_k)$$

One will try to choose β in such a manner that $\max_k |\rho_k^*|$ is as small as possible; β is of course real. Since, for the critical eigenvalues, $\rho_k - 1$ is nearly imaginary, one can attain only very little improvement by the choice of a relaxation factor β .

SECTION VI

THE "SECOND" METHOD OF MARTIN AND LOMAX

Martin and Lomax recommend an extrapolation procedure for the results of subsequent iteration steps based on the Aitken-Shanks formula. This formula is correct if the differences between the results of the iteration steps behave like a geometric series. To be specific, let the results of 3 subsequent iterations be given by ϕ_k^1 , ϕ_k^2 , and ϕ_k^3 and assume that the differences

$(\phi_k^2 - \phi_k^1)$, $(\phi_k^3 - \phi_k^2)$ (and also subsequent differences) form a geometric series. Then one obtains

$$\lim_{l \rightarrow \infty} [\phi_k^{(1)}, \phi_k^{(2)}, \phi_k^{(3)} \dots \phi_k^{(l)} \dots] = \phi_k^{(1)} + (\phi_k^{(2)} - \phi_k^{(1)}) / [1 - (\phi_k^{(3)} - \phi_k^{(2)}) / (\phi_k^{(2)} - \phi_k^{(1)})] \quad (10)$$

$$= \frac{\phi_k^{(1)} \phi_k^{(3)} - \phi_k^{(2)2}}{\phi_k^{(1)} - 2\phi_k^{(2)} + \phi_k^{(3)}}$$

This is the Aitken-Shanks formula. Accordingly, starting with an initial value ϕ_k^1 , one carries out two iteration steps and then uses this formula to extrapolate. This gives a new initial condition which is then treated in the same manner. The differences in subsequent iteration steps can be expressed by the eigenfunctions and eigenvalues: $\sum C_k u_k$, $\sum C_k \rho_k \vec{u}_k$, $\sum C_k \rho_k^2 \vec{u}_k$. The individual terms of the sums are given by geometric series. If there were a predominant eigenvalue, then one would obtain a behavior of the differences close to that of a geometric series after a number of iteration steps, and one would expect this formula to be effective. For the distribution of eigenvalues obtained under the present circumstances, this is unlikely because the eigenvalues are so closely spaced. An attempt to apply the procedure in the present problem was without success. The convergence with the use of the Aitken-Shanks formula was worse than that of direct iterations.

In addition, we have used an improved version. It is based on the observation that, in the present problem, the eigenvalues occur in complex conjugate pairs. Under favorable circumstances, two eigenvalues will be dominant. The general version of the Aitken-Shanks formula holds if the differences $\phi_k^2 - \phi_k^1, \phi_k^3 - \phi_k^2, \phi_k^4 - \phi_k^3 \dots$ are the sums of the corresponding terms of a finite number of geometric series. This observation can be found in the Section "Heuristic Motivation of the Transform" of Ref. 5.

Following Shanks, we denote A_n ($n = 0, 1, 2, \dots$) a sequence of numbers or functions and set

$$\Delta A_\ell = A_{\ell+1} - A_\ell \quad (11)$$

The starting point is Equation 2 of Reference 5. For the present purpose, we set $n = k$. The extrapolated value (that is the value which one obtains by applying the Aitken-Shanks formula) is then given by

$$B_{k,k} = D_1/D_2 \quad (12)$$

where

$$D_1 = \left| \left(\begin{array}{cccc} A_0 & A_1 & A_2 & \dots & A_k \\ \hline & & & & M \end{array} \right) \right| \quad (13)$$

$$D_2 = \left| \left(\begin{array}{cccc} 1 & 1 & 1 & \dots & 1 \\ \hline & & & & M \end{array} \right) \right| \quad (14)$$

and M is the matrix of dimension k by $k+1$ whose elements are given by

$$M_{i,j} = \Delta A_{i+j} \quad \begin{array}{l} i = 0, 1, 2, \dots, k-1 \\ j = 0, 1, 2, \dots, k \end{array} \quad (15)$$

We express the A_i by the first term of the sequence A_0 and the differences ΔA_ℓ . One has for the row vector occurring in D_1

$$[A_0, A_1, A_2, \dots, A_k] = A_0 [1, 1, 1, \dots, 1] + [0, A_1 - A_0, A_2 - A_0, \dots, A_k - A_0]$$

Hence, from Equation (12),

$$B_{k,k} = A_0 + D_3/D_2$$

where

$$D_3 = \left| \left(\frac{0, A_1 - A_0, A_2 - A_0, \dots, A_k - A_0}{M} \right) \right| \quad (16)$$

Let us evaluate B_{kk} under the assumption that

$$\Delta A_\ell = \sum_{n=1}^k b_n r_n^\ell, \quad \ell = 0, 1, 2, \dots \quad (17)$$

The r_n 's are the ratio of consecutive terms in the individual geometric series. Then one obtains

$$A_m - A_0 = \sum_{\ell=0}^{m-1} \Delta A_\ell = \sum_{n=1}^k b_n \sum_{\ell=0}^{m-1} r_n^\ell = \sum_{n=1}^k b_n \frac{1 - r_n^m}{1 - r_n} \quad (18)$$

Therefore,

$$[0, A_1 - A_0, A_2 - A_0, \dots, A_k - A_0] = \sum_{n=1}^k \frac{b_n}{1 - r_n} \left\{ [1, 1, 1, \dots, 1] - [1, r_n, r_n^2, \dots, r_n^k] \right\}$$

This is substituted into Equation (16). Using Equation (14), one obtains

$$B_{kk} = A_0 + \sum_{n=1}^k \frac{b_n}{1 - r_n} - D_4/D_2 \quad (19)$$

where

$$D_4 = \begin{vmatrix} \sum \frac{b_n}{1-r_n} & \sum \frac{b_n r_n}{1-r_n} & \sum \frac{b_n r_n^2}{1-r_n} & \dots & \sum \frac{b_n r_n^k}{1-r_n} \\ \sum b_n & \sum b_n r_n & \sum b_n r_n^2 & \dots & \sum b_n r_n^k \\ \sum b_n r_n & \sum b_n r_n^2 & \sum b_n r_n^3 & \dots & \sum b_n r_n^{k+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sum b_n r_n^{k-1} & \sum b_n r_n^k & \sum b_n r_n^{k+1} & \dots & \sum b_n r_n^{2k-1} \end{vmatrix} \quad (20)$$

The rows of the $k+1$ by $k+1$ determinant D_4 can be expressed as linear combinations of only k vectors; which appear as the rows of the third matrix in the following equation:

$$D_4 = \begin{pmatrix} \frac{1}{1-r_1} & \frac{1}{1-r_2} & \frac{1}{1-r_3} & \dots & \frac{1}{1-r_k} \\ 1 & 1 & 1 & \dots & 1 \\ r_1 & r_2 & r_3 & \dots & r_k \\ r_1^2 & r_2^2 & r_3^2 & \dots & r_k^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ r_1^{k-1} & r_2^{k-1} & r_3^{k-1} & \dots & r_k^{k-1} \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_k \end{pmatrix} \begin{pmatrix} 1 & r_1 & r_1^2 & \dots & r_1^k \\ \vdots & r_2 & r_2^2 & \dots & r_2^k \\ 1 & r_3 & r_3^2 & \dots & r_3^k \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & r_k & r_k^2 & \dots & r_k^k \end{pmatrix} \quad (21)$$

Therefore,

$$D_4 = 0$$

and

$$B_{kk} = A_0 + \sum_{n=1}^k b_n / (1-r_n)$$

With Equations (17) and (11) one then obtains

$$A_{\infty} = B_{kk}$$

To take the fact into account that the dominant eigenvalues of our problem occur in conjugate complex pairs we have used the Aitken Shanks formula for $k = 2$. Then one deals with 3 by 3 determinants, and the difference between consecutive terms of the sequences are approximately the sum of the respective terms of two geometric series. One has specifically

$$D_2 = \begin{vmatrix} 1 & 1 & 1 \\ \Delta A_0 & \Delta A_1 & \Delta A_2 \\ \Delta A_1 & \Delta A_2 & \Delta A_3 \end{vmatrix} = (\Delta A_1 \Delta A_3 - \Delta A_2^2) - (\Delta A_0 \Delta A_3 - \Delta A_1 \Delta A_2) + (\Delta A_0 \Delta A_2 - \Delta A_1^2) \quad (22)$$

$$D_1 = \begin{vmatrix} 0 & \Delta A_0 & (\Delta A_0 + \Delta A_1) \\ \Delta A_0 & \Delta A_1 & \Delta A_2 \\ \Delta A_1 & \Delta A_2 & \Delta A_3 \end{vmatrix} = -\Delta A_0 (\Delta A_3 \Delta A_2 - \Delta A_1 \Delta A_2) + (\Delta A_0 + \Delta A_1) (\Delta A_0 \Delta A_2 - \Delta A_1^2) \quad (23)$$

$$B_{kk} = A_0 + D_1 / D_2 \quad (24)$$

Under certain conditions, the determinant D_2 , Equation (14) may vanish. Assuming that ΔA_n has the form (16), one has

$$D_2 = \begin{vmatrix} 1 & 1 & 1 & \dots & 1 \\ \sum b_n r_n & \sum b_n r_n & \sum b_n r_n^2 & \dots & \sum b_n r_n^k \\ \sum b_n r_n & \sum b_n r_n^2 & \sum b_n r_n^3 & \dots & \sum b_n r_n^{k+1} \\ \sum b_n r_n^2 & \sum b_n r_n^3 & \sum b_n r_n^4 & \dots & \sum b_n r_n^{k+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sum b_n r_n^{k-1} & \sum b_n r_n^k & \sum b_n r_n^{k+1} & \dots & \sum b_n r_n^{2k-1} \end{vmatrix}$$

The matrix encountered here can be written as the product of three $k+1$ by $k+1$ matrices

$$D_2 = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 1 & \dots & 1 \\ 0 & r_1 & r_2 & \dots & r_k \\ 0 & r_1^2 & r_2^2 & \dots & r_k^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & r_1^{k-1} & r_2^{k-1} & \dots & r_k^{k-1} \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & r_1 & r_1^2 & \dots & r_1^k \\ 1 & r_2 & r_2^2 & \dots & r_2^k \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & r_n & r_n^2 & \dots & r_n^k \end{pmatrix}$$

It is evident that D_2 will vanish if two or more values r_n coincide, or if some of the r_n 's are zero. Incidentally, the first and third of these matrices are closely related to Vandermond's determinant. On this basis, one obtains:

$$D_2 = \{b_1 b_2 b_3 \dots b_n\} \{[(r_2 - r_1)][(r_3 - r_2)(r_3 - r_1)][(r_4 - r_3)(r_4 - r_2)(r_4 - r_1)] \dots \\ \dots [(r_n - r_{n-1})(r_n - r_{n-2})(r_n - r_{n-3}) \dots (r_n - r_1)]\} \times \\ \times \{[(r_1 - 1)][(r_2 - r_1)(r_2 - 1)][(r_3 - r_2)(r_3 - r_1)(r_3 - 1)][(r_4 - r_3)(r_4 - r_2)(r_4 - r_1)(r_4 - 1)] \dots \\ \dots [(r_n - r_{n-1})(r_n - r_{n-2})(r_n - r_{n-3}) \dots (r_n - r_1)(r_n - 1)]\} \quad (25)$$

If one or more of the r_n 's are zero, then the sum of the corresponding geometric series gives infinity. The extrapolation given by Equation (12) or (24) is therefore correct, although one will question whether the formula should be applied under these circumstances.

The following discussions are restricted to the case $k = 2$. For $r_2 = r_1 \neq 1$ one has just one geometric series rather than two. In this case, one obtains 0/0 from Equation (24). One must go

back to the formula for $k = 1$. This case is characterized by the conditions

$$\Delta A_0 \Delta A_2 - \Delta A_1^2 = 0$$

and

$$\Delta A_1 \Delta A_0 - \Delta A_2^2 = 0$$

The result is then given by

$$A_0 + \Delta A_0 / (1 - \Delta A_1 / \Delta A_0)$$

If

$$\Delta A_0 \Delta A_2 - \Delta A_1^2 \neq 0$$

but

$$\Delta A_1 \Delta A_3 - \Delta A_2^2 = 0$$

then one of the values of r is zero and one has

$$\Delta A_0 = b_1 + b_2$$

$$\Delta A_1 = b_2 r_2$$

$$\Delta A_2 = b_2 r_2^2$$

$$\Delta A_3 = b_2 r_2^3$$

In this case, Equation (24) is applicable, but one must decide whether vanishing of one of the r 's is compatible with the nature of the problem.

If

$$\Delta A_0 \Delta A_2 - \Delta A_1^2 = 0$$

but

$$\Delta A_1 \Delta A_3 - \Delta A_2^2 \neq 0$$

then one of the r 's is infinite. One has

$$\Delta A_0 = b_2$$

$$\Delta A_1 = b_2 r_2$$

$$\Delta A_2 = b_2 r_2^2$$

$$\Delta A_3 = b_2 r_2^3 + \bar{b}_1$$

$$(\Delta A_4 = \infty)$$

This case must, of course, be excluded although Equation (24) will assign a limiting value to the sequence.

The case

$$\Delta A_0 = c_1$$

$$\Delta A_1 = c_1 r_1 + c_2$$

$$\Delta A_2 = c_1 r_1^2 + 2 c_2 r_1$$

$$\Delta A_3 = c_1 r_1^3 + 3 c_2 r_1^2$$

arises by a limiting process where $r_2 \rightarrow r_1$ and $b_2 \rightarrow \infty$, $b_1 \rightarrow \infty$. Here Equation (24) is applicable without modifications.

We have experimented with Equation (24) as a means of accelerating the convergence of the iterative procedure whose results are shown in Figures 1 and 2. In this case, one generates five consecutive values of $\phi^{(i)}$ and then uses (24) to extrapolate. The results give initial^k values for a next step of the same kind. It was found that the results are somewhat better than those obtained with Equation (10), but there is no noticeable improvement of the convergence in comparison with straight iterations.

One will remember that the extrapolation procedure is a non-linear process. It is therefore difficult to generalize results obtained by examples.

SECTION VII

CONCLUSIONS

The practical aspects of the Martin-Lomax iterations have been quite thoroughly explored in the work of these authors. To this facet of the work, the present discussions cannot claim to make a contribution. We hope that they are useful as background information in cases where one encounters phenomena that are difficult to explain. In this regard, the data about eigenfunctions and eigenvalues can be rather revealing. The observation that the presence of a shockpoint does not lead to a significant change of the convergence properties is, of course, reassuring. The discussion (carried out in Section I) of the relation between the boundary conditions for a hyperbolic problem and those used in the present iteration scheme is important for the understanding of the working of the procedure. According to the present examples, it seems to be rather difficult to find values of the free parameters α_1 and α_2 which guarantee convergence under all circumstances. Martin's numerical experiments show that these difficulties are less pronounced if the procedure is applied to computations of an actual flow field. The fact that the eigenvalues ρ are clustered closely around 1 (at least in the present examples) is disappointing, it may mean that convergence is somewhat precarious; this may create difficulties if one wants to make procedures of this kind fully automatic.

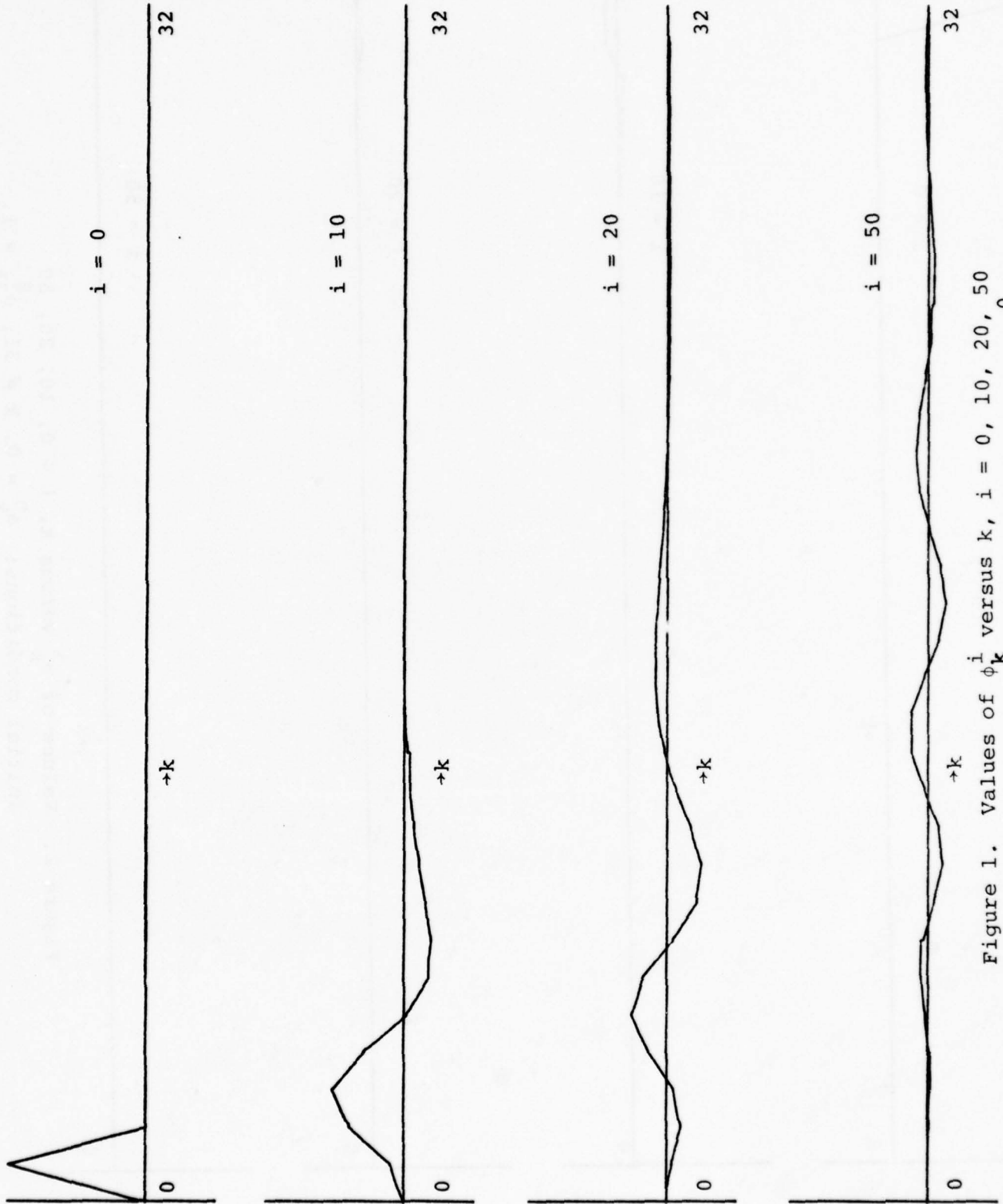


Figure 1. Values of ϕ_k^i versus k , $i = 0, 10, 20, 50$
 Initial conditions: $\phi_k^0 = 0$, $k \neq 1$; $\phi_1^0 = 1$.

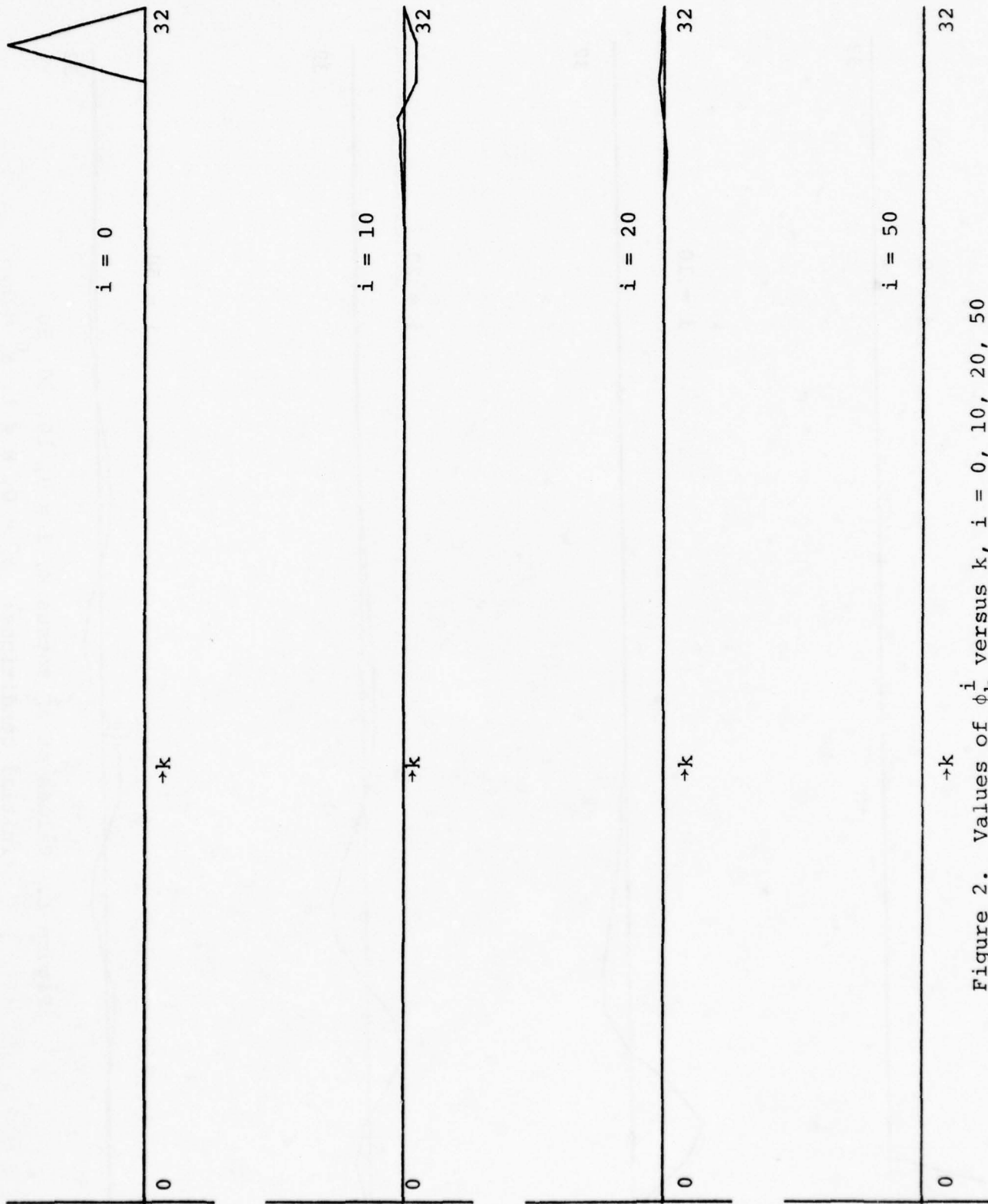


Figure 2. Values of ϕ_k^i versus k , $i = 0, 10, 20, 50$
 Initial conditions: $\phi_k^0 = 0$, $k \neq 31$, $\phi_{31}^0 = 1$.

squares	eigenvalues for a finite region ($K = 32$)
open circles	eigenvalues for periodicity condition
full circles	auxiliary values for the case of an infinite interval.

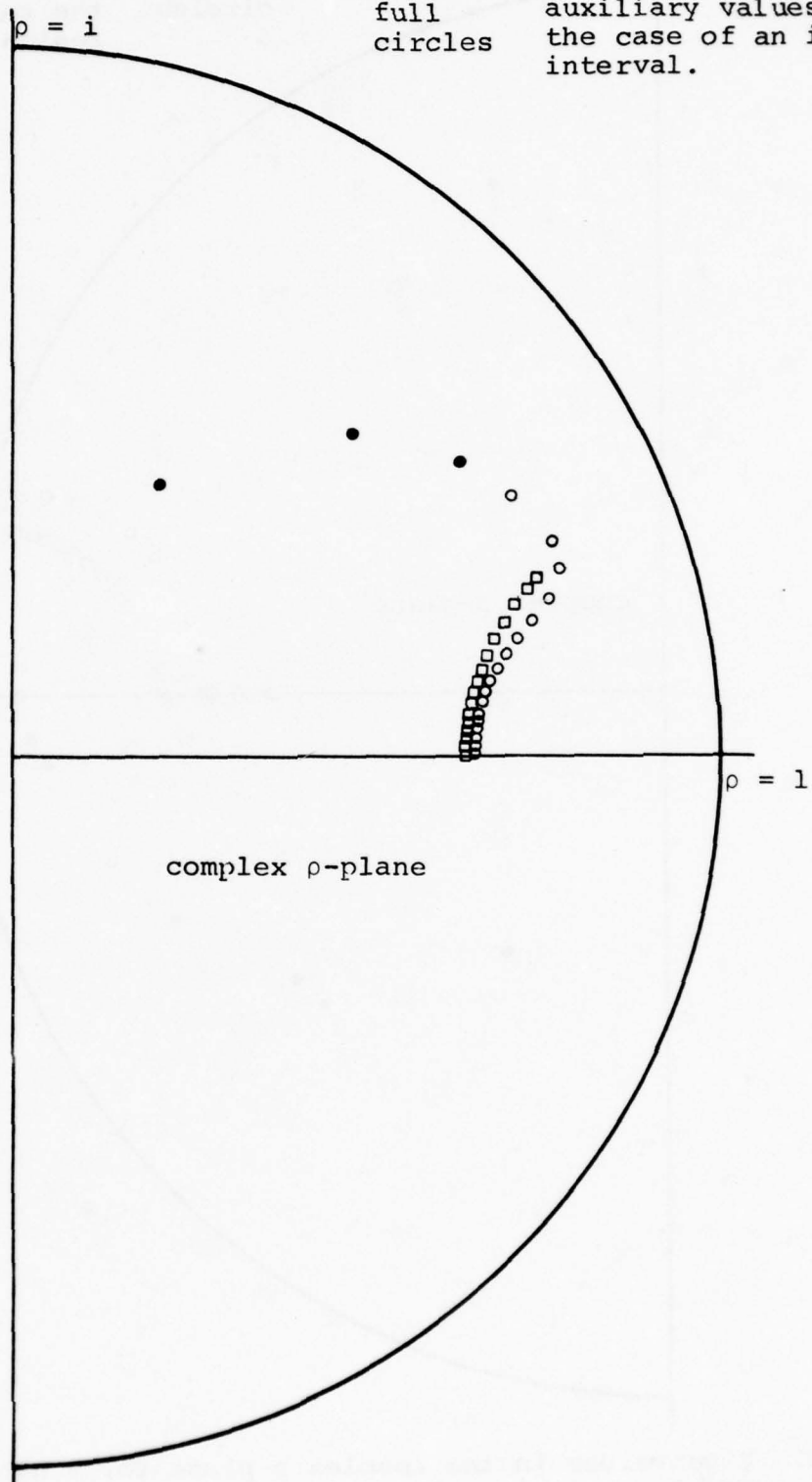


Figure 3. Eigenvalues in the complex ρ plane for an elliptic problem. $|u_\lambda| = .5$, $n/N = .05$, $\alpha_1 = 0_1$, $\alpha_2 = 1$.

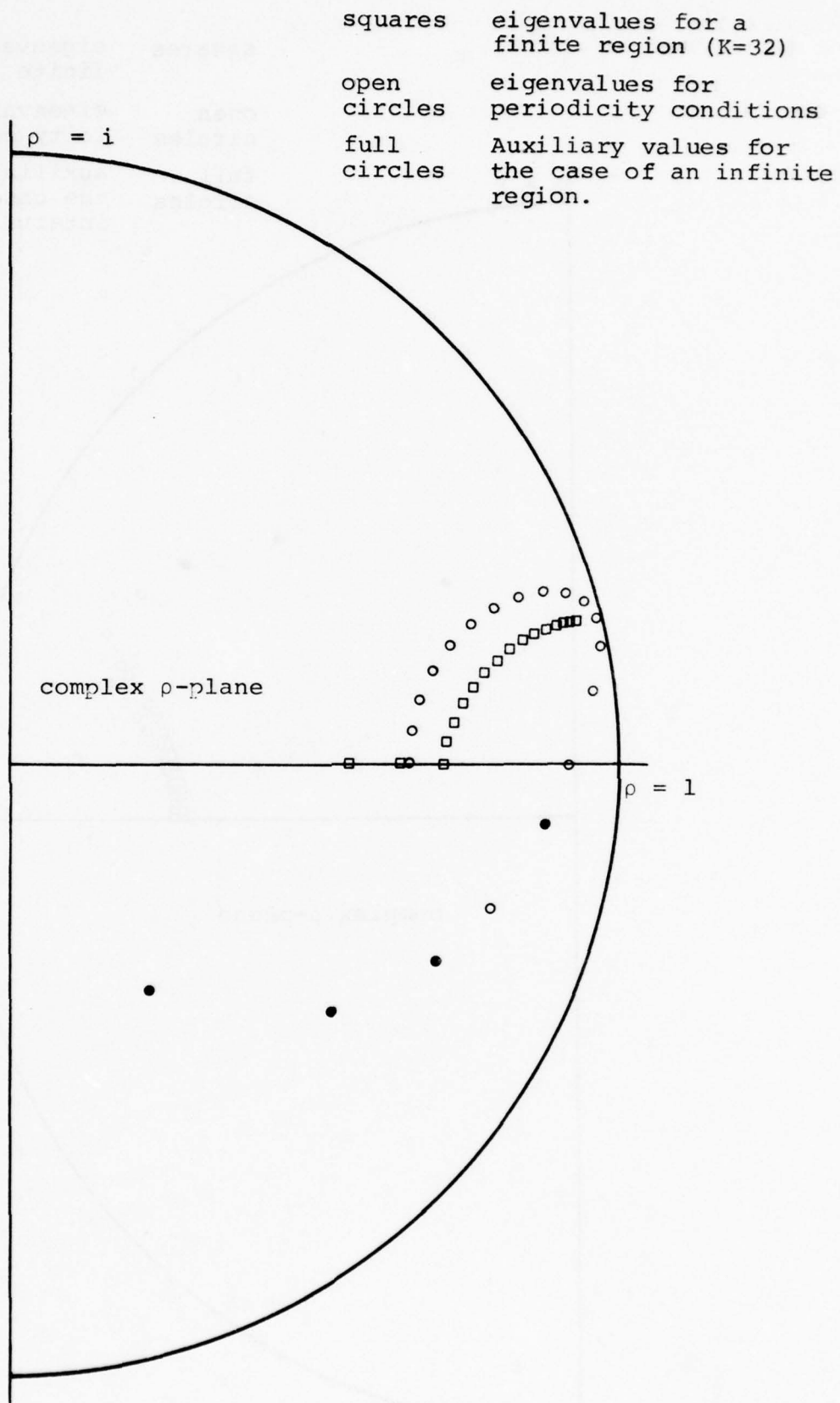


Figure 4. Eigenvalues in the complex ρ plane for a hyperbolic problem. $|u_0| = .5$, $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$.

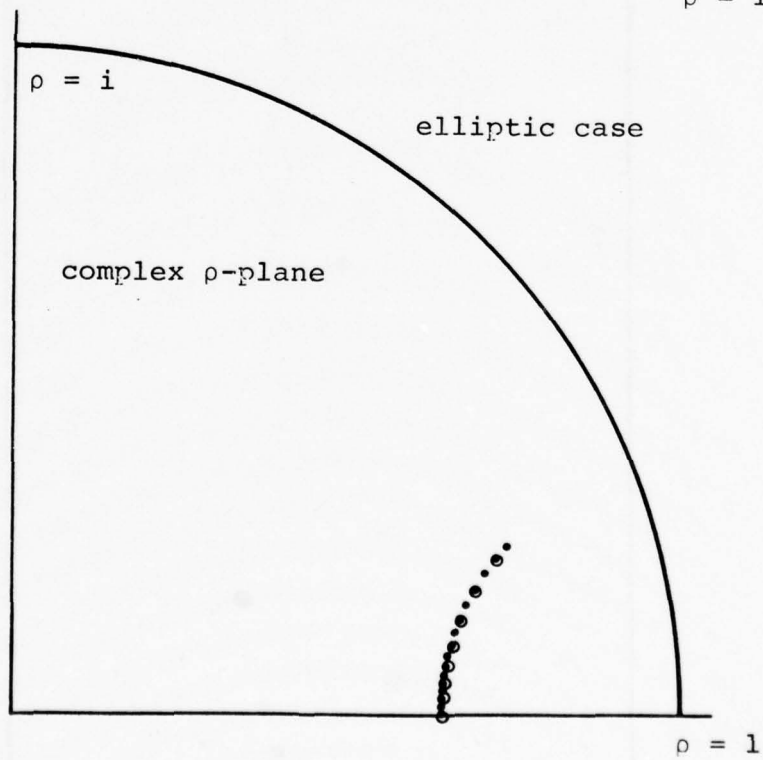
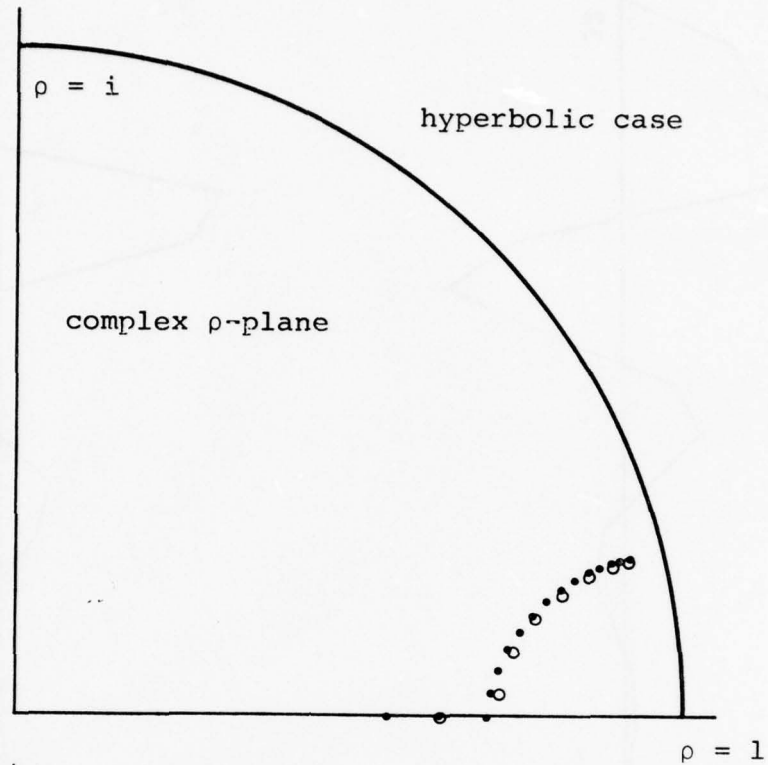


Figure 5. Eigenvalues in the complex ρ plane
 $|u_\ell| = .5, n/N = 0.05, \alpha_1 = 0, \alpha_2 = 1$
 full small circles $K = 32$
 open circles $K = 16$

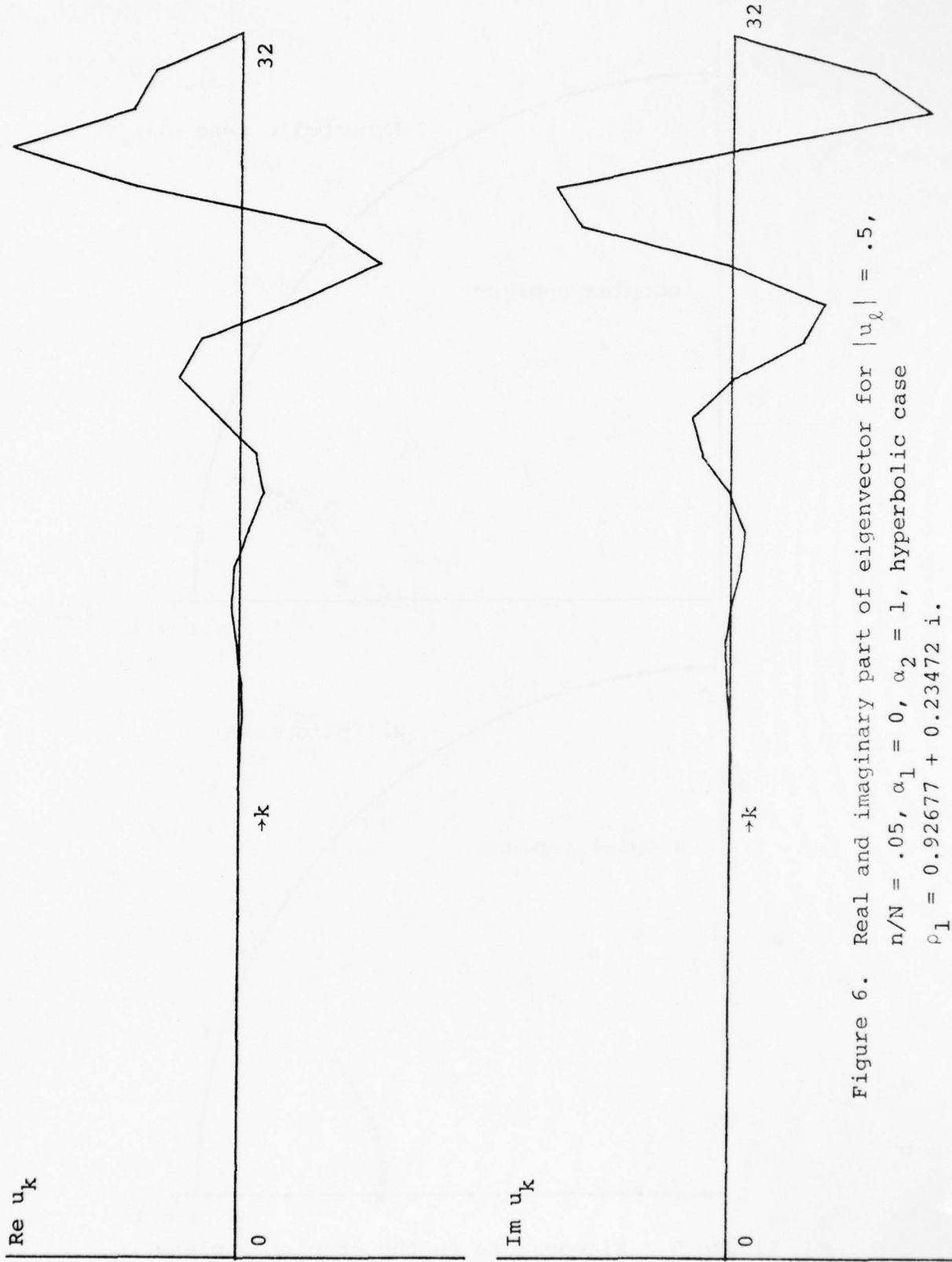


Figure 6. Real and imaginary part of eigenvector for $|u_\ell| = .5$,
 $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, hyperbolic case
 $\rho_1 = 0.92677 + 0.23472 i$.

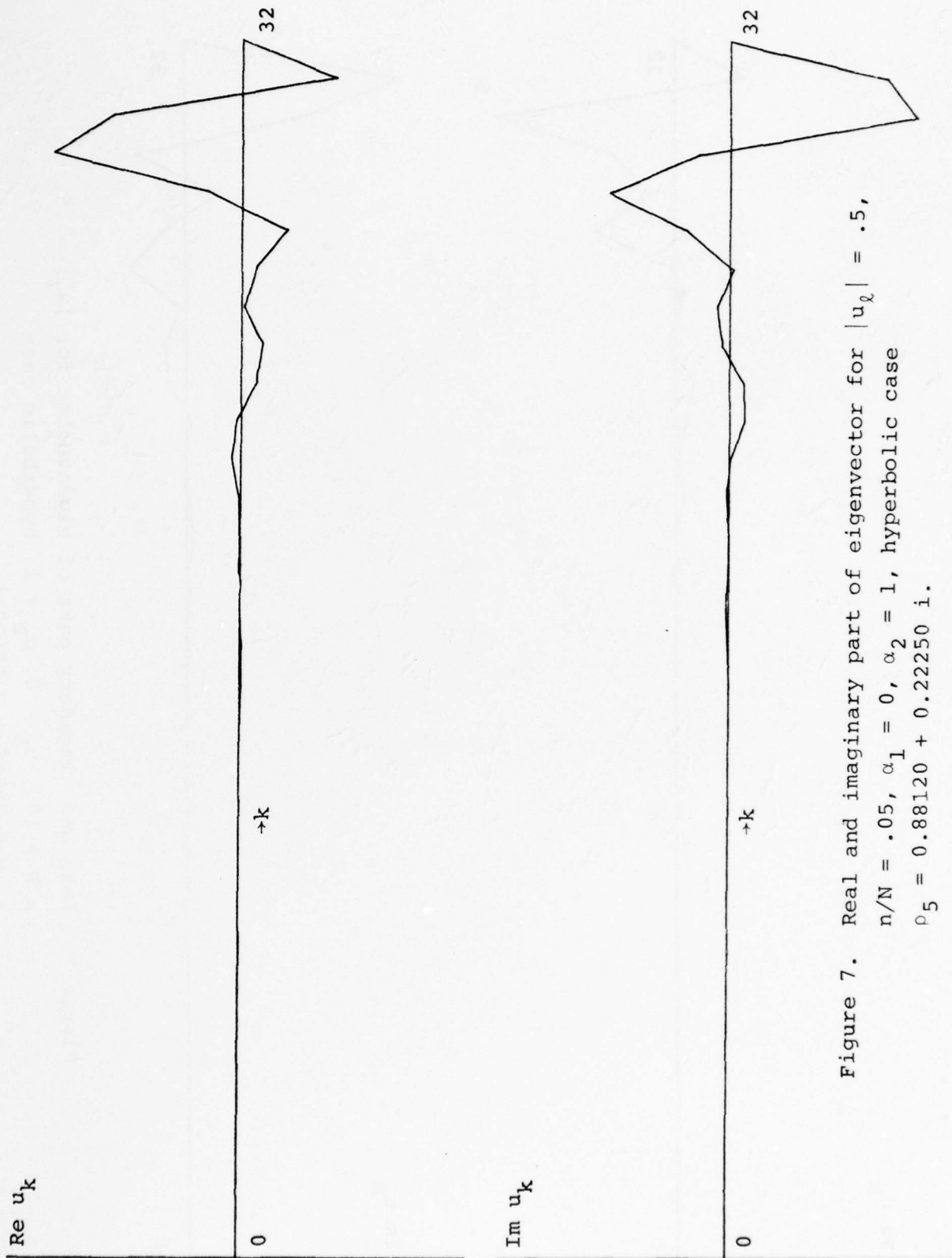


Figure 7. Real and imaginary part of eigenvector for $|u_0| = .5$,
 $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, hyperbolic case
 $\rho_5 = 0.88120 + 0.22250 i$.

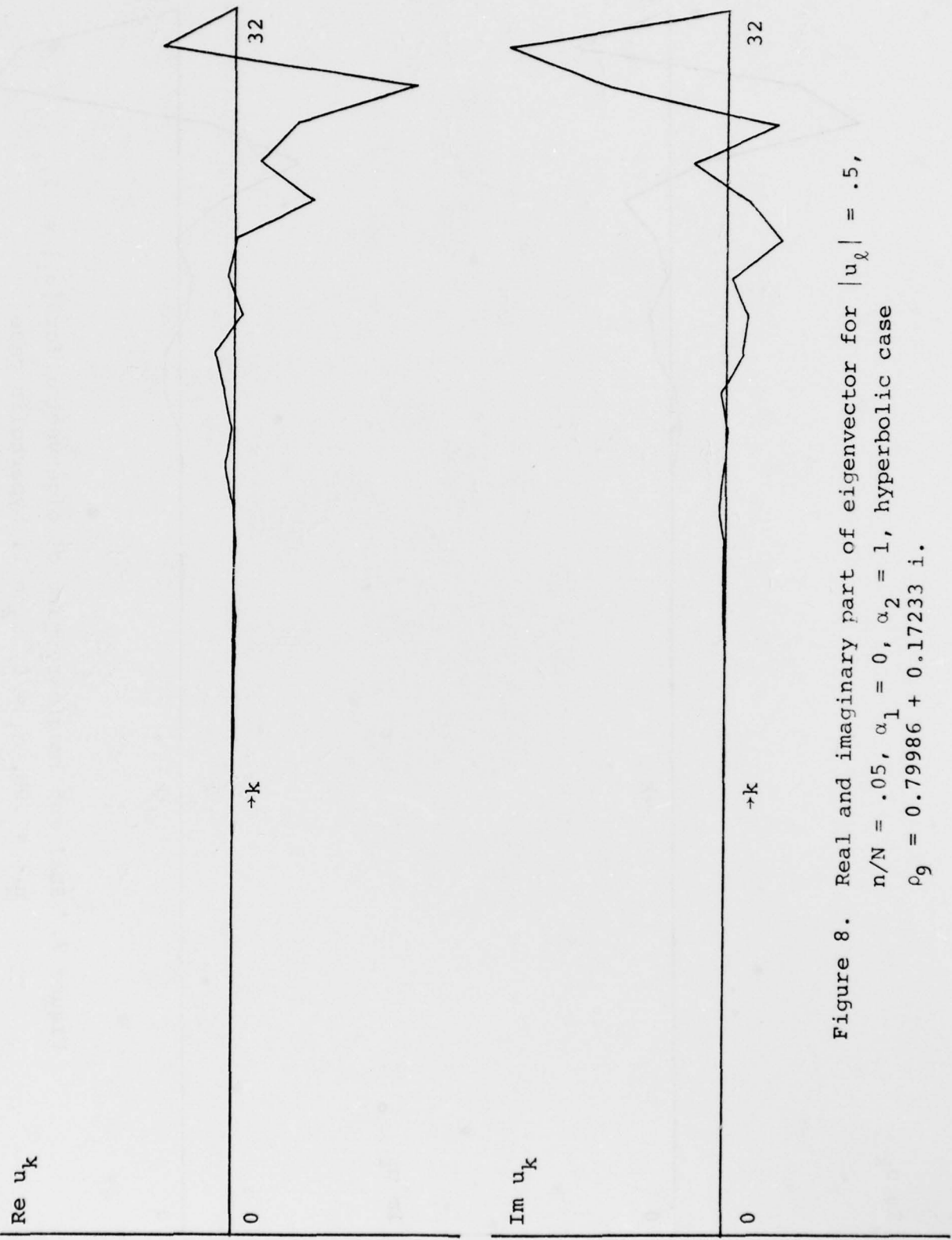


Figure 8. Real and imaginary part of eigenvector for $|u_\xi| = .5$,
 $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, hyperbolic case
 $\rho_9 = 0.79986 + 0.17233 i$.

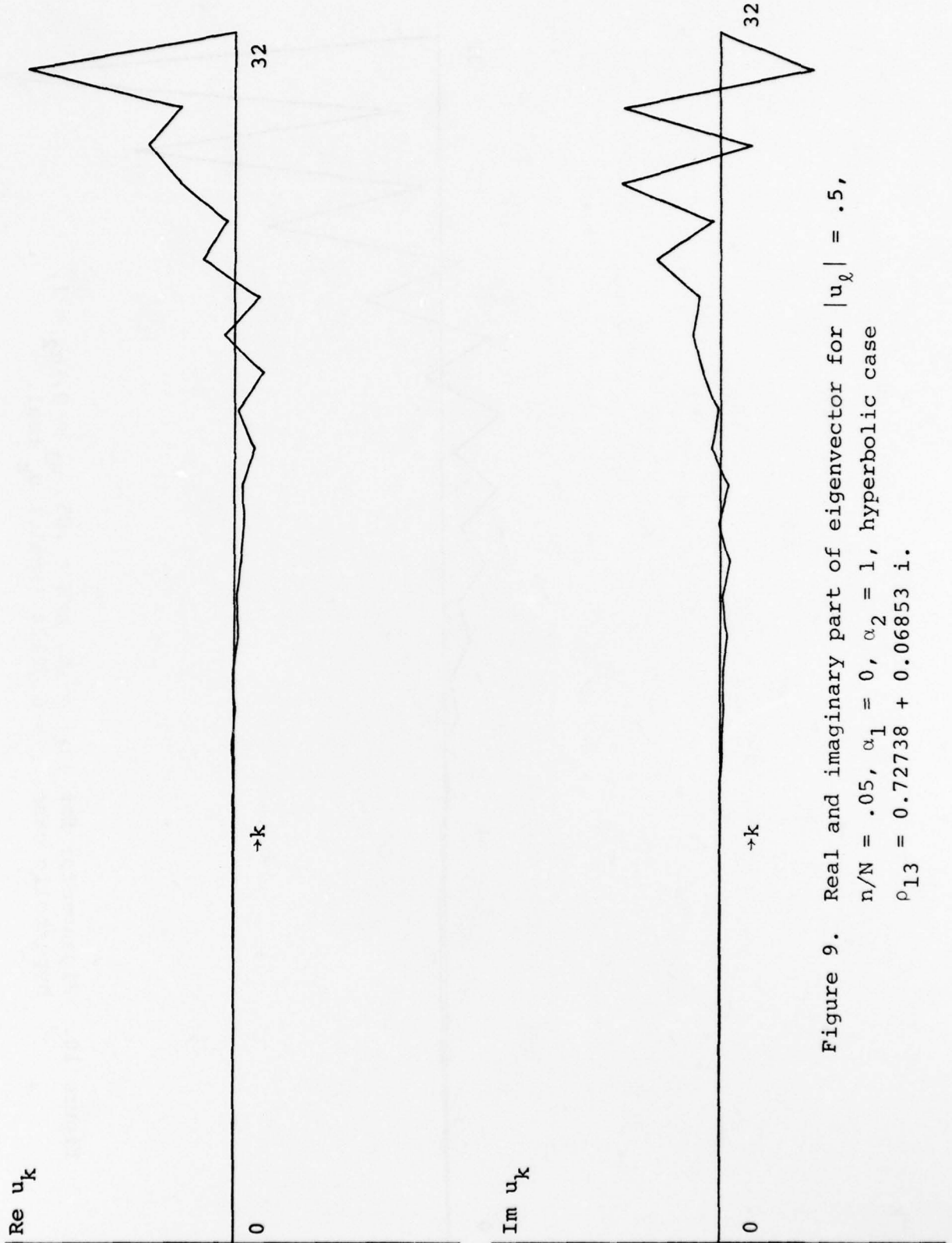


Figure 9. Real and imaginary part of eigenvector for $|u_0| = .5$,
 $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, hyperbolic case
 $\rho_{13} = 0.72738 + 0.06853 i$.

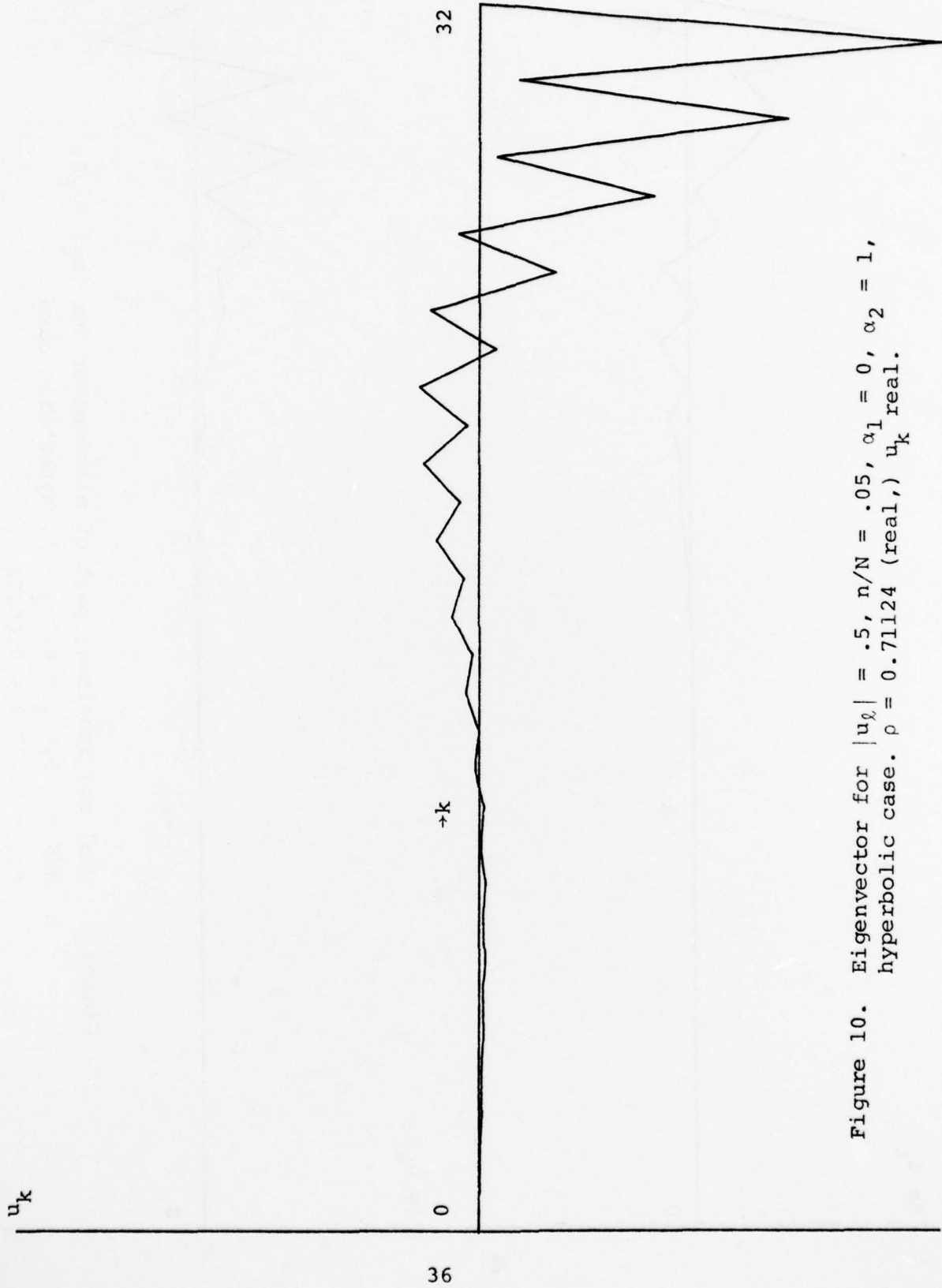


Figure 10. Eigenvector for $|u_k| = .5$, $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, hyperbolic case. $\rho = 0.71124$ (real,) u_k real.

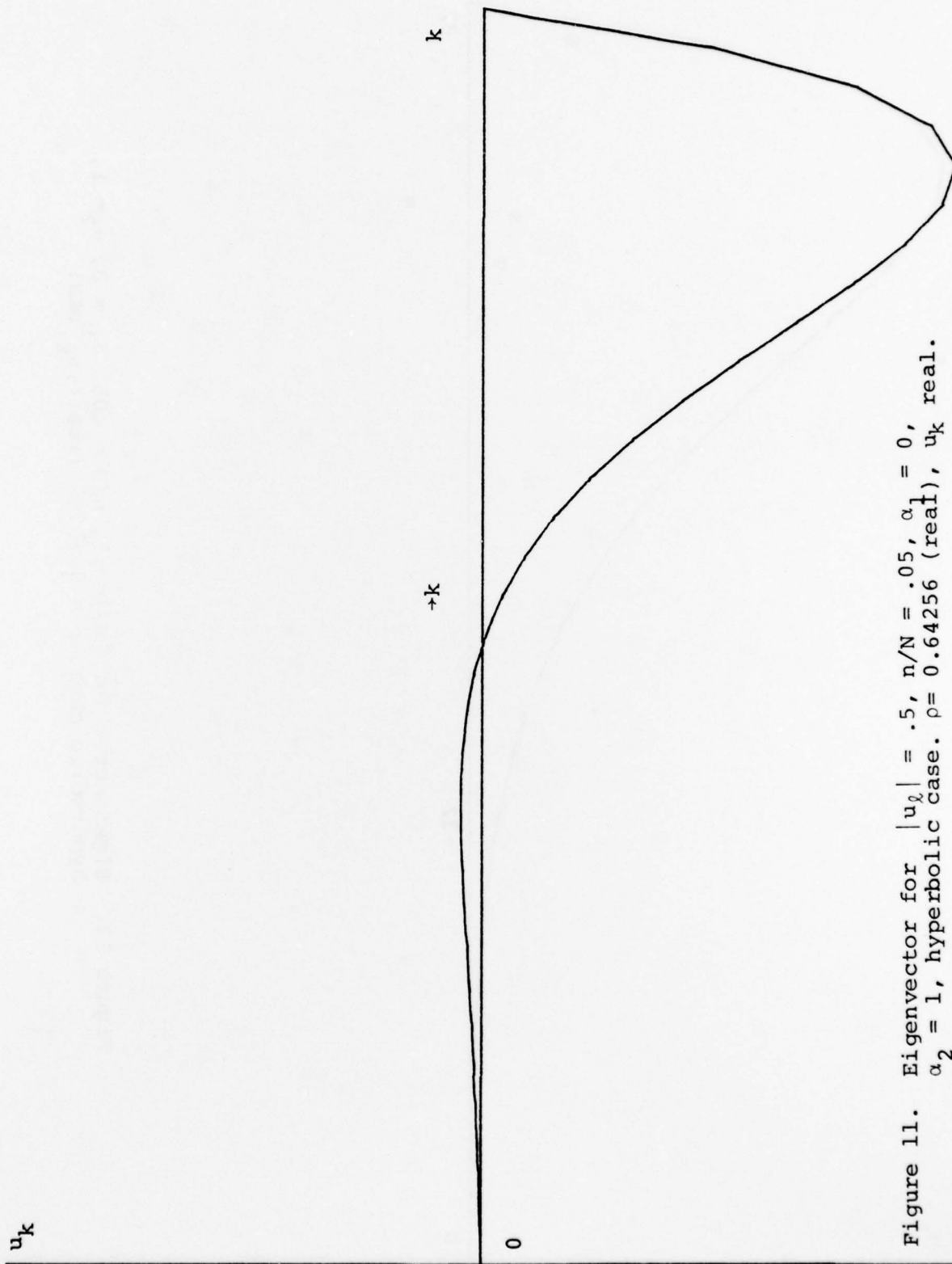


Figure 11. Eigenvector for $|u_k| = .5$, $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, hyperbolic case. $\rho = 0.64256$ (real), u_k real.

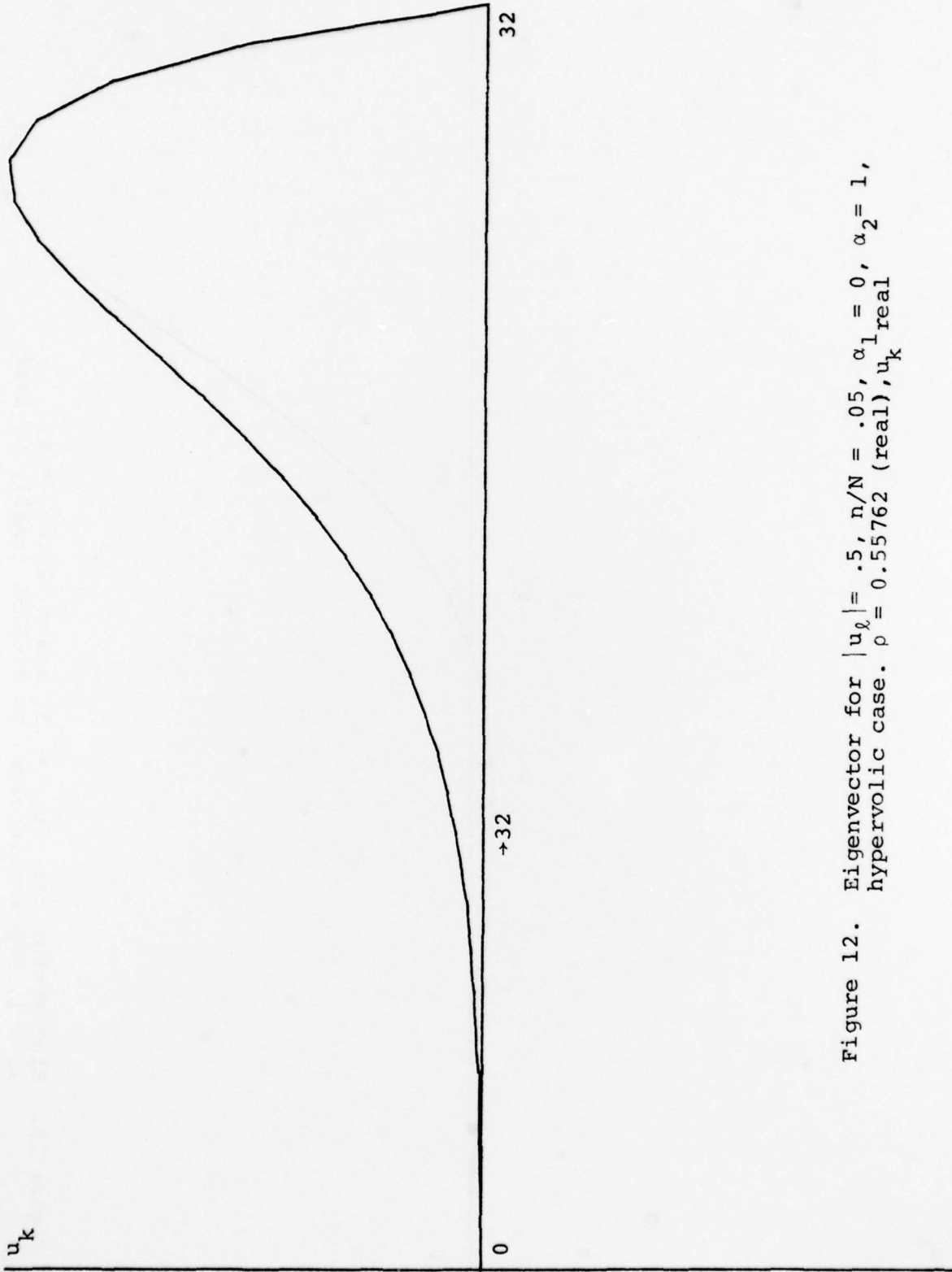


Figure 12. Eigenvector for $|u_k| = .5$, $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$,
 hypervolic case. $\rho = 0.55762$ (real), u_k real

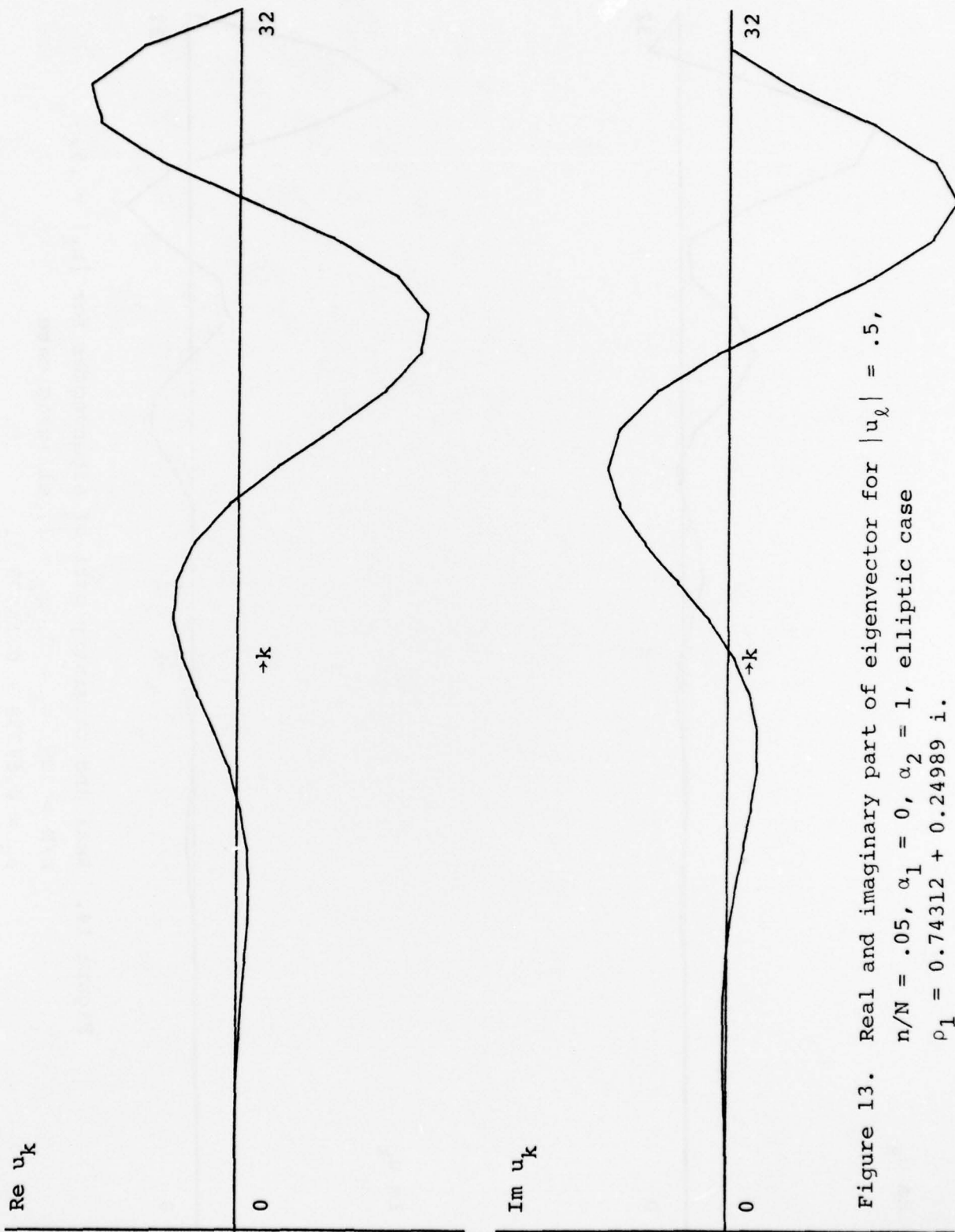


Figure 13. Real and imaginary part of eigenvector for $|u_\ell| = .5$,
 $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, elliptic case
 $\rho_1 = 0.74312 + 0.24989 i$.

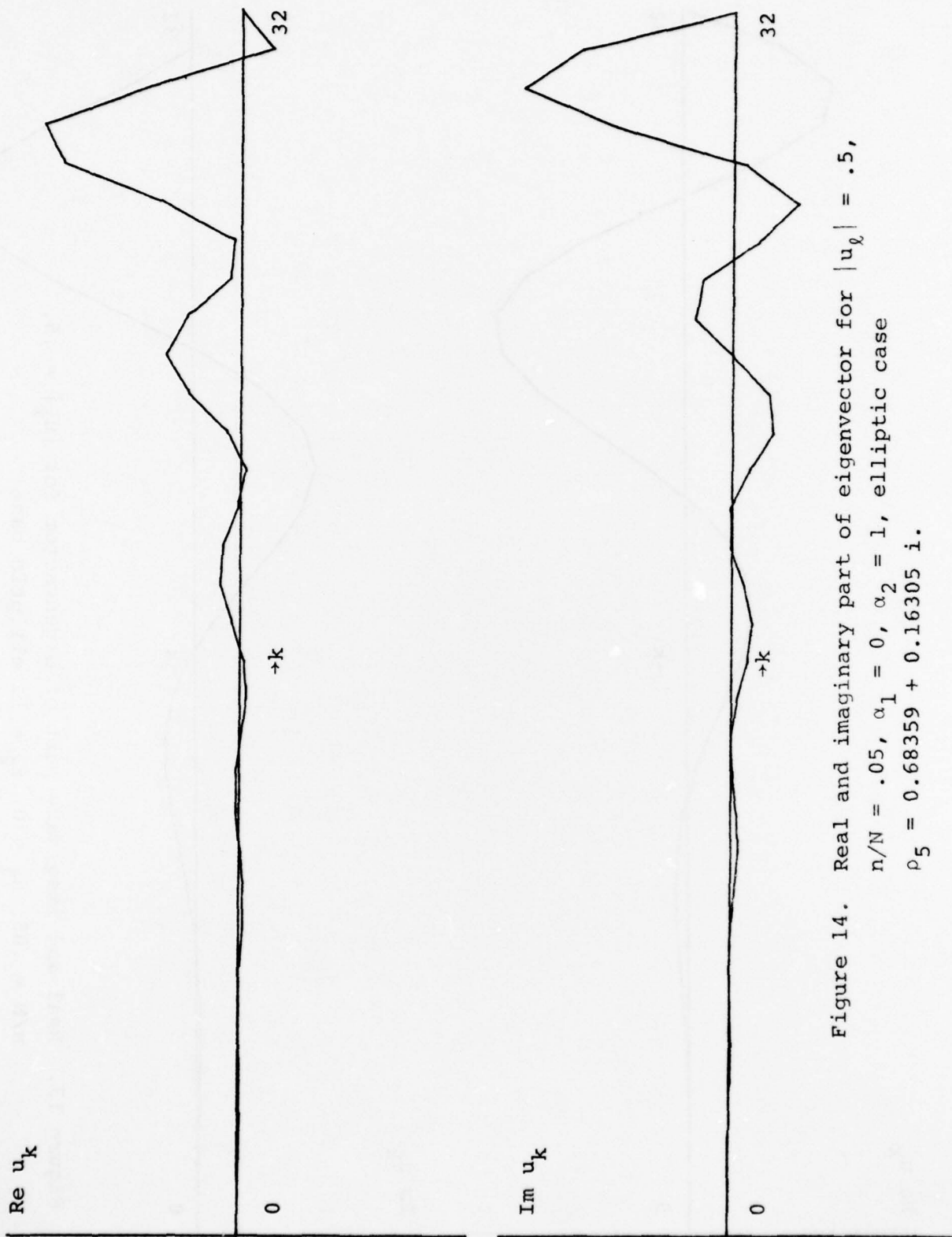


Figure 14. Real and imaginary part of eigenvector for $|u_\ell| = .5$,
 $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, elliptic case
 $\rho_5 = 0.68359 + 0.16305 i$.

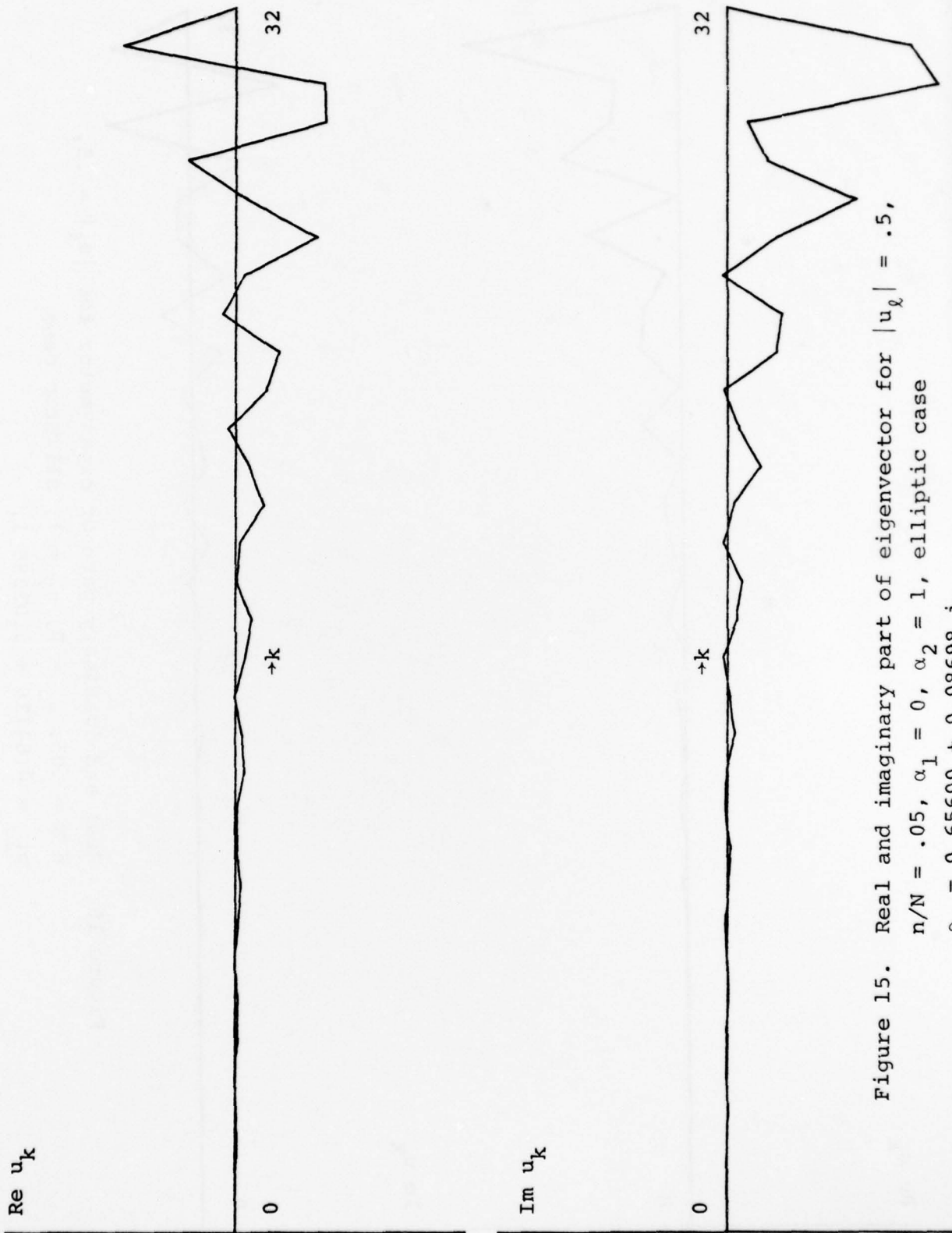


Figure 15. Real and imaginary part of eigenvector for $|u_q| = .5$,
 $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, elliptic case
 $\rho_g = 0.65600 + 0.08698 i$.

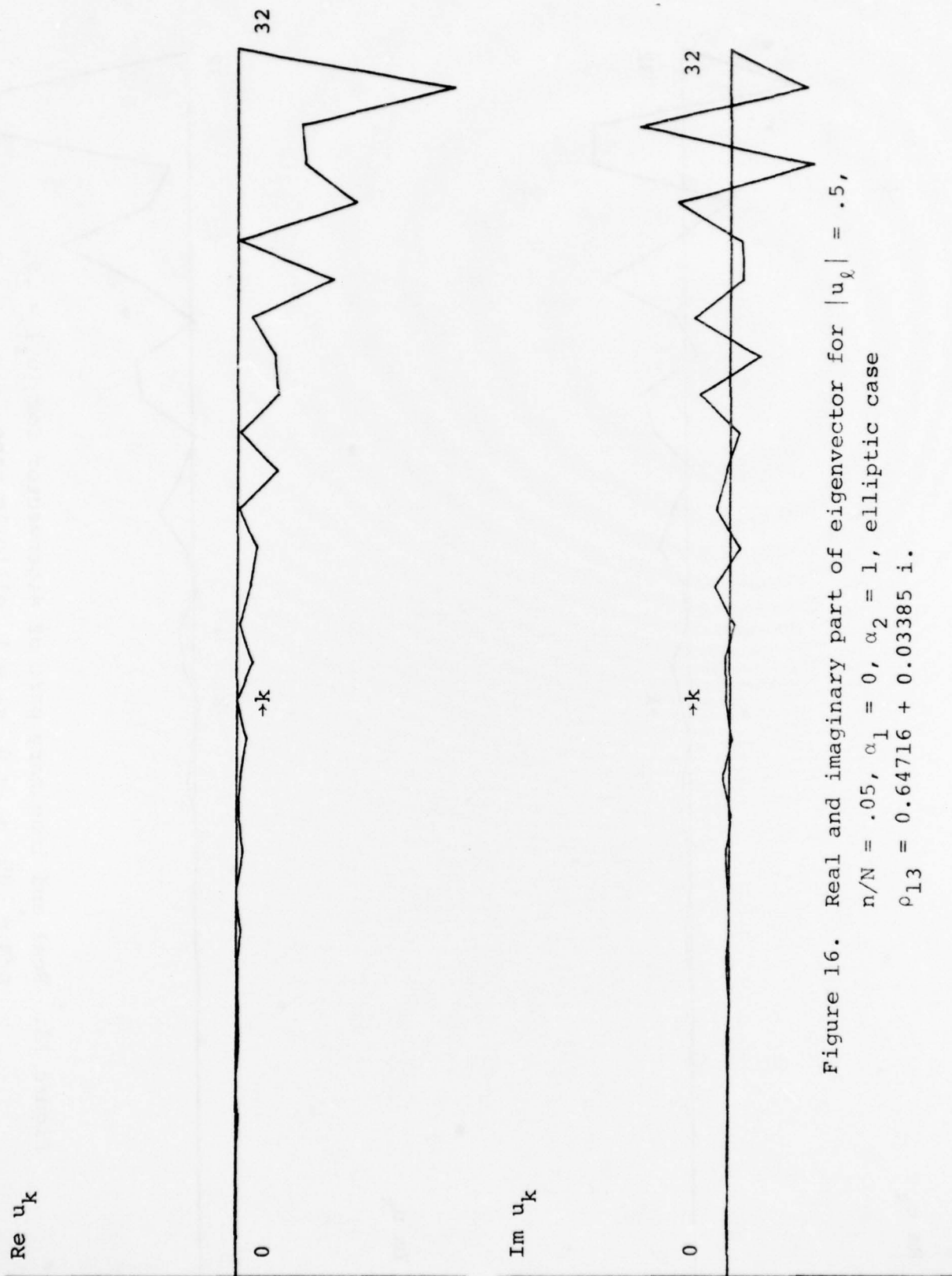


Figure 16. Real and imaginary part of eigenvector for $|u_\varrho| = .5$,
 $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, elliptic case
 $\rho_{13} = 0.64716 + 0.03385 i$.

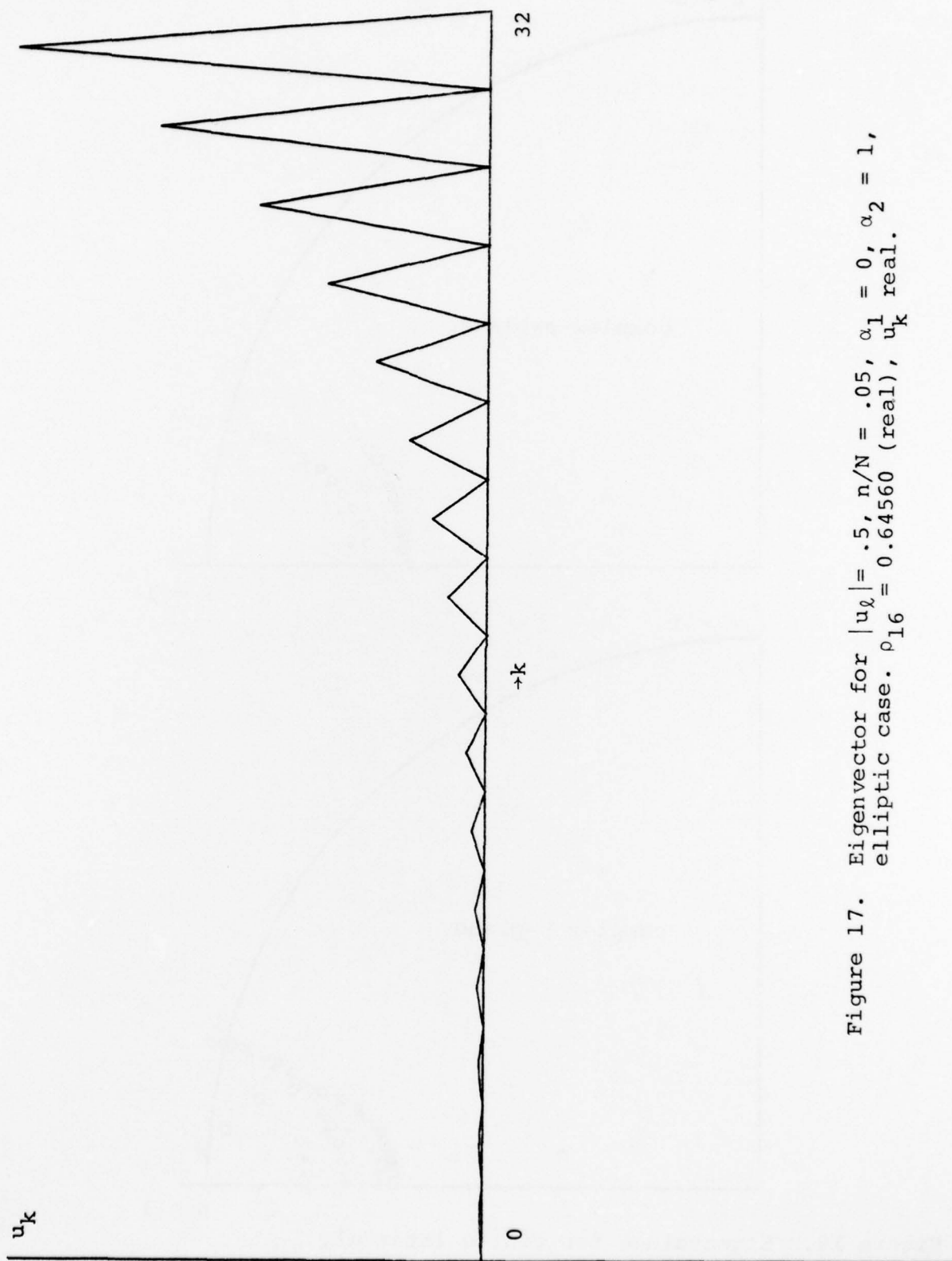


Figure 17. Eigenvector for $|u_k| = .5$, $n/N = .05$, $\alpha_1 = 0$, $\alpha_2 = 1$, elliptic case. $\rho_{16} = 0.64560$ (real), u_k real.

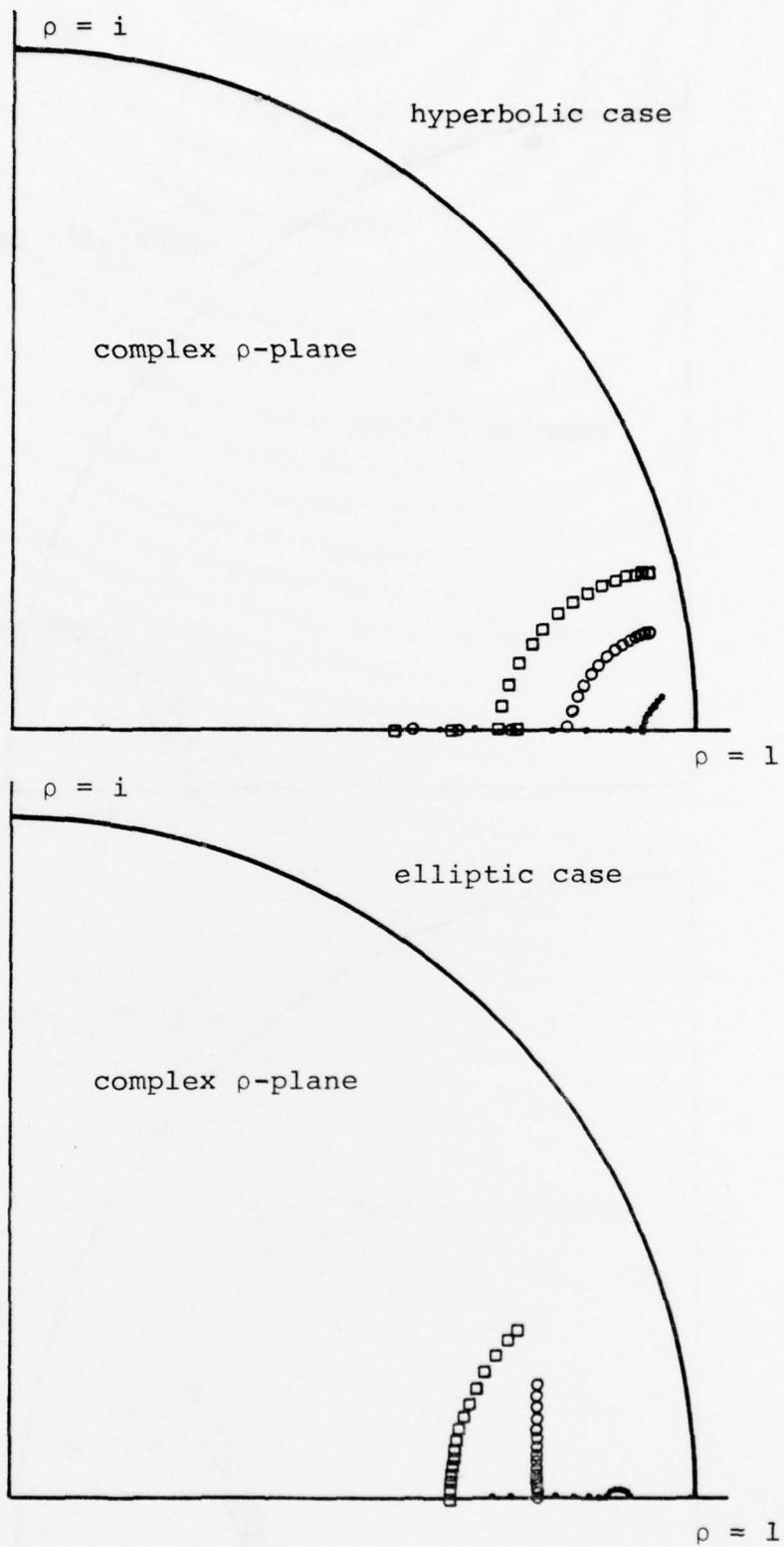


Figure 19. Eigenvalues in the complex ρ plane
 $n/N = 0.05$, $\alpha_1 = 0$, $\alpha_2 = 1$

full small circles	$ u_\ell = .1$
empty circles	$ u_\ell = .3$
empty squares	$ u_\ell = .5$

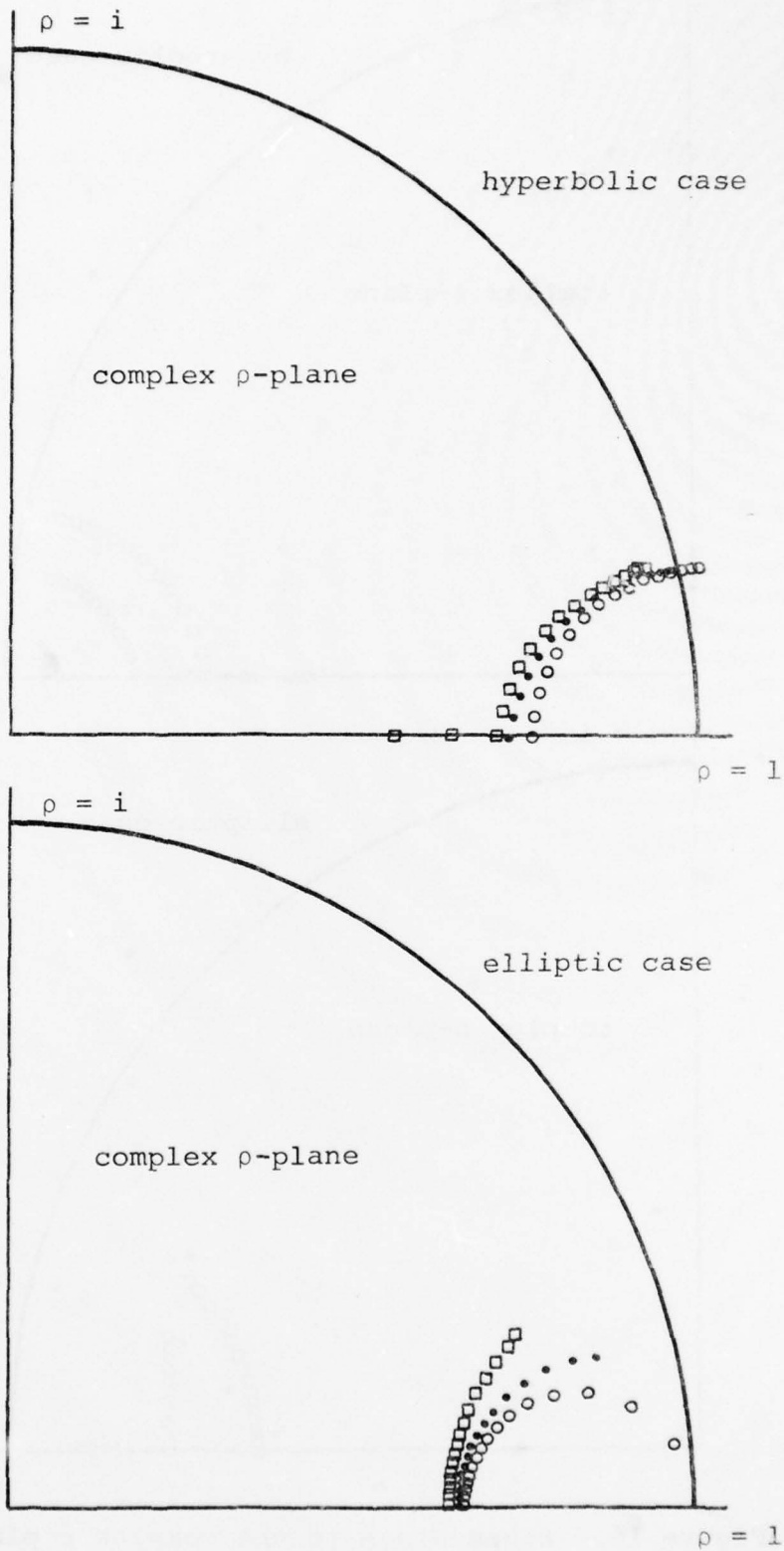


Figure 20. Eigenvalues in the complex ρ plane
 $|u_\ell| = .5, \alpha_1 = 0, \alpha_2 = 1$

empty circles	$n/N = 0$
full small circles	$n/N = 1/32$
empty squares	$n/N = 1/20$

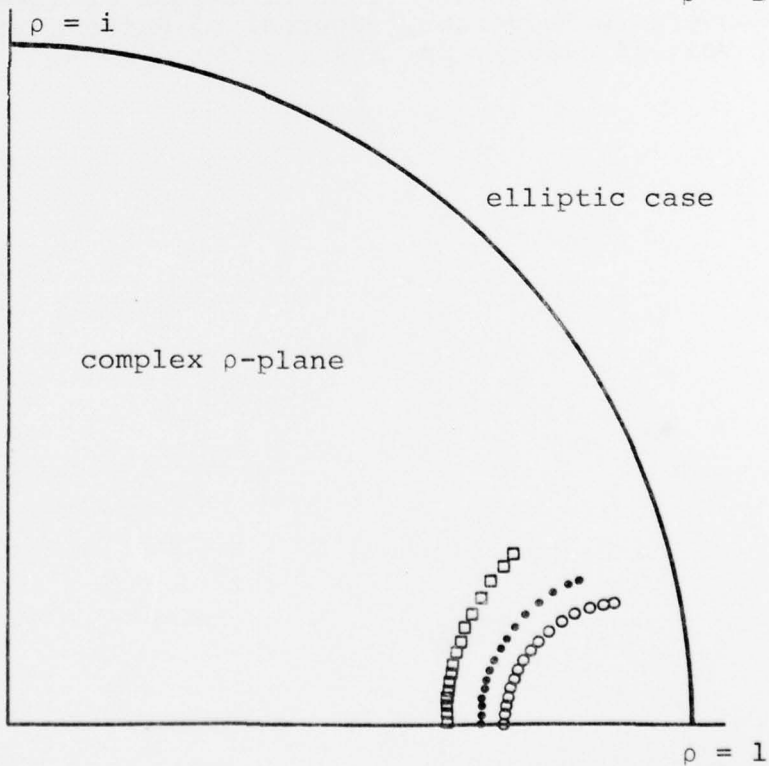
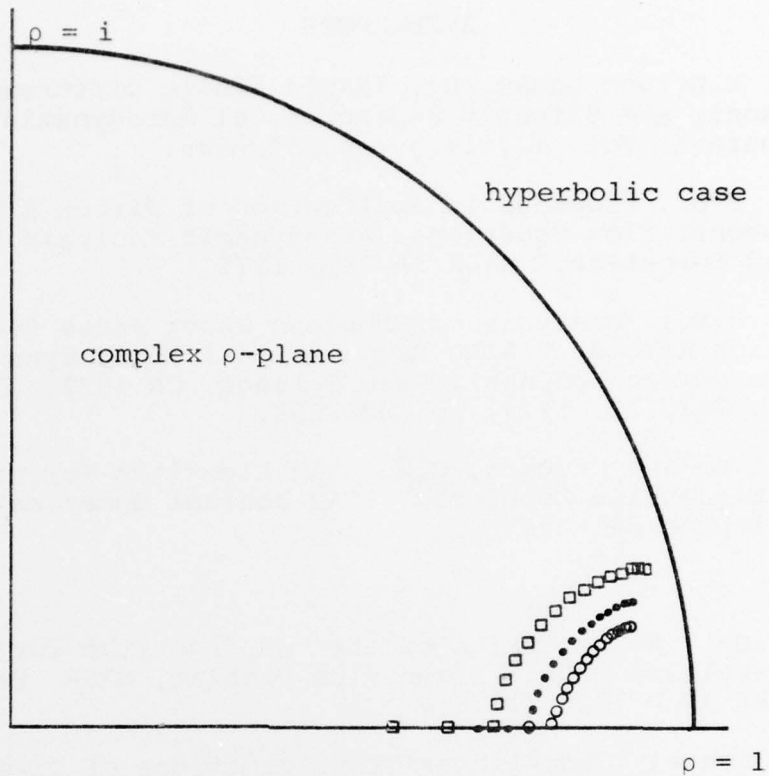


Figure 21. Eigenvalues in the complex ρ plane
 $n/N = 0.05$, $|u_\lambda| = .5$, $\alpha_1 = 0$,
 empty circles $\alpha_2 = 2$
 full small circles $\alpha_2 = 1.5$
 empty squares $\alpha_2 = 1$

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