Correction p42 lines onwards

We will consider the data $y_{-h}, y'_{-h}, y_h, y'_h$, and we will collocate at $x = 0$. These five conditions give the correct degree of over-determination if we choose a cubic interpolation polynomial

$$y = A + Bx + Cx^2 + Dx^3 .$$

We have the equations

$$y_{-h} = A - Bh + Ch^2 - Dh^3 ,$$
$$y'_{-h} = B - 2Ch + 3Dh^2 ,$$
$$y_h = A + Bh + Ch^2 + Dh^3 ,$$
$$y'_h = B + 2Ch + 3Dh^2 ,$$

and

$$g_0 = f_0 A + B .$$

We have $A = (y_h + y_{-h})/2 - h(y'_h - y'_{-h})/4 ,$

$$B = 3(y_h - y_{-h})/4h - (y'_h + y'_{-h})/4 ,$$

and the difference equation is

$$g_0 = f_0 \{ (y_h + y_{-h})/2 - h(y'_h - y'_{-h})/4 \} + 3(y_h - y_{-h})/4h - (y'_h + y'_{-h})/4 .$$

We have compared the solutions given by this equation with those given by the trapezoidal rule difference equation for the differential equation

$$dy/dx - y = 0 , \quad y(0) = 1 .$$

These results are set out in the following table

n	Trapezoidal Rule	Our Equation
1	$y(1) = 3.0$	$y(1) = 2.714285$
2	" $= 2.778$	" $= 2.718040$
4	" $= 2.733$	" $= 2.718274$

Here n gives the number of integration steps .

SUMMARY : This Thesis is concerned with the numerical solution of differential equations : in particular their numerical solution by finite difference methods .

The first two chapters contain introductory material . Chapter (I) gives a survey of two specific problems which require numerical methods for their complete reduction . These problems provide a motivation for much that follows . Chapter (II) contains a discussion of finite difference methods for numerical differentiation .

In chapter (III) we suggest a general method for constructing approximating finite difference equations . This method seems particularly suitable for application on electronic computers . We also discuss some exact difference equations and apply them to obtain expressions for the truncation error in some standard formulae

In chapter (IV) we give a proof of the convergence of the solution of the approximating difference equation to the solution of the differential equation as the mesh spacing h tends to zero . We consider the initial value problem , and a general class of self aadjoint eigenvalue and boundary value problems for second order differential equations in normal form .

In chapter (V) we discuss some problems concerned with the numerical solution of partial differential equations . The main topics of the chapter are the feasibility and convergence of the numerical technique of difference correction . Here we restrict ourselves to the consideration of a class of boundary value problems for elliptic partial differential equations .

INTRODUCTION

That part of the work of the Thesis which falls under the heading 'The Numerical Solution of Differential Equations' is concentrated in the last three chapters . Here the topics considered are as follows .

Chapter (III) . The Construction of Finite Difference Equations . We briefly survey the standard method of setting up the finite difference equations (section A) before suggesting a general method for systematically tackling the problem (section B) . Here the basic approach is of extreme simplicity and must surely have been noted before although I am not aware of this . Certainly its systematic exploitation is new ; and this is of prime importance We are lead to suggest that the computer be used not only to solve the set of linear equations that result from the finite difference approximation , but also to construct the difference approximation itself . In this way we can hope to achieve much greater accuracy in our difference equations . In section C. we consider some exact difference equations and approximations based on them . An application of this work is to the construction of integral forms for the truncation error in some standard finite difference approximations . Our general line of approach is similar to that of reference [5] of chapter (III)

Chapter (IV) . Convergence of Finite Difference Approximations . Here we restrict the class of differential equations considered

to second order equations in normal form ; and we use only the simplest central difference approximations . We hope to counterbalance this specialisation by obtaining results more general than those hitherto available (see references [4] and [5] of chapter (IV)) . The need for such generality is implicit in reference [3] of chapter (IV) .

The result for the initial value problem (section A) is not new . However we obtain a generalisation to the case where the coefficient functions are no more than continuous by using a new form for the truncation error (mostly due to Hersch reference [5] of Chapter (III)) .

In considering two point boundary problems (section B) we restrict the possible types of boundary conditions to a subclass of those which make the differential equation self adjoint . However the only important condition which we do not consider would appear to be that of periodicity . We show the convergence of the eigenvalues and eigenvectors of the difference equation to the corresponding eigenvalues and eigenfunctions of the differential equation . We also show the ultimate convergence of the finite difference approximation as h tends to zero for the case of a boundary value problem provided that the solution to this problem is unique . In all cases the result holds provided only that the coefficients in the differential equation are continuous . We point out that this is perhaps as much as can be expected as additional information about the solution would

appear to be required at a point of discontinuity of one of the coefficient functions . This point is discussed in appendix I to Chapter (IV) .

Chapter (V) . Some Problems in the Numerical Solution of Partial Differential Equations .

In section A of this chapter we discuss the extension of the methods of chapter (III) to partial differential equations . The bulk of the remainder of the chapter is devoted to a critical discussion of the numerical technique of difference correction (which we describe in section B) . In section C we discuss some difficulties which are inherent in the method . The material of this section owes much to Mr Sidney Michaelson and Professor W.G.Bickley - in particular the example of page 19 . In fact both the subject matter and the presentation of the whole chapter owes much to their constructive criticism . In sections D and E we discuss the convergence and the nature of the approximation by difference correction . The results here are my own .

The results of chapter (II) 'Finite Difference Formulae for Numerical Differentiation' are of particular relevance to chapter (V) . Especially the results which relate these differentiation formulae to the cardinal function (section C). Sections A and B contain well known material .

The other introductory chapter - chapter (I) 'On Some Problems Requiring Numerical Solution' - contains in section A a summary

of my paper 'On the Propagation of Sound in a Layered Fluid Medium' which has been accepted for publication in the Quarterly Journal of Mechanics and Applied Mathematics . Here we present an example of an eigenvalue problem that requires numerical methods for its solution ; but this example is to be seen in the wider setting of the reduction of a problem involving a radiation condition into a numerically tractable form .

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Chapter I. On Some Problems Requiring Numerical Solution

We have considered two problems of practical physical interest:

(A) the propagation of sound in a layered fluid medium, and

(B) the solution of Reynold's equation for a finite journal bearing.

We find that (A) requires the solution of an eigenvalue problem for a second order ordinary differential equation, while (B) requires the solution of an elliptic partial differential equation in two independent variables (a special case reduces to a boundary value problem for a second order ordinary differential equation).

We will take these examples as a guide to the types of problem to be studied in the following chapters. In appendices to chapter (IV) and chapter (V) we will give accounts of specific computations associated with these problems.

A. Propagation of sound in a layered fluid medium

Here we assume that the propagation can be adequately described by the wave equation, and that the velocity of propagation C depends only on the depth coordinate Z. Thus the acoustic pressure satisfies the equation

$$\nabla^2 P = \frac{1}{C(Z)^2} \frac{\partial^2 P}{\partial t^2} \qquad (A.1)$$

If we also permit the density ρ of the medium to be a function of Z then equation (1) takes the slightly more general form

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \rho \frac{\partial}{\partial z}\left\{\frac{1}{\rho}\frac{\partial P}{\partial z}\right\} = \frac{1}{C(z)^2}\frac{\partial^2 P}{\partial t^2} .$$

An important case is that when ρ has step discontinuities corresponding to layers of immiscible fluid of different densities. This occurs in practice for instance when studying the acoustic properties of sea water over a mud bottom. For the present we will restrict ourselves to a discussion of equation (A.1) or, rather, the wave equation for a simple harmonic dependence on time (with frequency ω)

$$\nabla^2 P + \frac{\omega^2}{C(z)^2} P = 0 . \qquad (A.2)$$

However, we will have occasion to return to the more general equation (see the appendix).

Our aim is to show that in this case the solution of equation (A.2) with a radiation boundary condition at $Z = \infty$ can be approximated by solutions which have boundary conditions set at finite values of Z . Such an approximation is of obvious importance in numerical working.

We will consider the boundary conditions

(a) radially outgoing wave (or radiation condition) as

$$r = \sqrt{(x^2 + y^2)} \to \infty .$$

For our purposes it will be satisfactory to say that $f(v)$ satisfies a radiation condition at ∞ if

$$f(v) \to Ae^{-iv} + g(v) , \quad \text{and} \quad g(v) \to 0 , \quad v \to \infty .$$

(b) $P(Z=0) = 0$ (pressure release surface).

(c) $\cos\alpha\, P(H) + \sin\alpha \frac{dP(H)}{dZ} = 0 .$

It is natural to separate equation (2) in cylindrical polar coordinates by putting $P = \Theta(r)\phi(Z)$. This gives the pair of equations

$$\frac{d^2\theta}{dr^2} + \frac{1}{r}\frac{d\theta}{dr} + k^2\theta = 0 \qquad (A.3)$$

and $$\frac{d^2\phi}{dz^2} + \left(\frac{\omega^2}{C(z)^2} - k^2\right)\phi = 0 \qquad (A.4)$$

The boundary condition (a) tells us that the appropriate solution of (A.3) is the Hankel function $H_0^{(2)}(kr)$. In this case the radiation condition leads to a solution in terms of a known function. This would in general not be true of (A.4).

Boundary conditions (b) and (c) make (A.4) into a self adjoint eigenvalue problem. It thus has a discrete sequence of real eigenvalues $k_n^2 \to -\infty$ and eigenfunctions ϕ_n as its possible solutions.

It is now not difficult to show (reference [1]) that the Green's function for equation (A.2) with the specified boundary conditions is

$$G(r; z, z_p) = -\frac{i}{4}\sum_{n=0}^{\infty} H_0^{(2)}(k_n r)\phi_n(z)\phi_n(z_p) , \qquad (A.5)$$

the series on the right converging for all values of its argument which lie within the volume considered provided that we interpret $(-k^2)$ as $-i|k|$. The Hankel function $H_0^{(2)}$ then decays exponentially for $r > 0$ as $k_n^2 \to -\infty$.

We will need the limiting form of (A.5) as $H \to \infty$. For this purpose we will assume that $C(z)$ -> positive limit $\leq \infty$. Therefore $\omega^2/C(z)^2 \to \alpha^2 \geq 0$; and we write equation (A.4) as

$$\frac{d^2\phi}{dz^2} + \left\{\frac{\omega^2}{C(z)^2} - a^2 + a^2 - k^2\right\}\phi = 0$$

or $$\frac{d^2\phi}{dz^2} + \left\{q(z) + \lambda\right\}\phi = 0 .$$

We will also assume that $\int_0^\infty |q(z)|dz < \infty$.

This implies that (4) has a fundamental set of solutions

$$N(z) \to e^{i\sqrt{\lambda}z} \quad , \quad z \to \infty$$

and $$N(z) \to e^{-i\sqrt{\lambda}} \quad , \quad z \to \infty \ ;$$

these being the leading terms of asymptotic expansions valid in the neighbourhood of $z = \infty$. In particular $N(z)$ satisfies a radiation condition at ∞ .

The behaviour of the spectrum (values of λ for which a solution exists) of equation (A.4) as $H \to \infty$ is summarised in the following result .

If $-q_{\max} < \lambda < 0$, then $\lambda(H)$ takes discrete values which tend to definite limits independent of α as $H \to \infty$. Values of $\lambda \geq 0$ lie in the continuous spectrum when $H = \infty$.

To put the Green's function in a form which is valid when $H = \infty$ we write it as a Stieltjes integral by introducing the function $\sigma(k^2)$ which is constant except at the eigenvalues $k^2 = k_n^2$ when it jumps by $1\Big/\int_0^H \phi_n^2 \, dz$ (that is, $\sigma(k_n^2 + 0) - \sigma(k_n^2 - 0) = 1/\int_0^H \phi_n^2 \, dz$) .

We now have

$$G(r; z, z_p) = -\frac{i}{4} \int_{k^2=-\infty}^{k^2=\infty} H_0^{(2)}(kr)\phi(z,k)\phi(z_p,k)d\sigma$$

where, as before, the convention $\sqrt{-k^2} = -i|k|$ must be observed.

The limit of $\sigma(k^2)$ as $H \to \infty$ is again a step function for k^2 in the discrete spectrum. However σ is continuous (even differentiable)

for k^2 in the continuous spectrum. For proofs of these results see [2] or [3].

An alternative approach is to construct $G(r, Z, Z_p)$ as the sum of the residues of a contour integral in the complex k plane. This method has been applied to this problem by Pekeris in [4]; and we will indicate his approach

(a) for the problem as we have stated it; and

(b) for an outgoing wave condition at $Z = \infty$.

This latter is the problem solved by Pekeris in a number of special cases.

We begin by attempting to find a solution which has a point source singularity at $(r = 0, Z = Z_p)$.

Thus we seek a solution which behaves like

$$\int_0^\infty J_0(kr) \frac{e^{-i\Omega|Z - Z_p|}}{-i\,\Omega} k\, d\, k$$

as $\sqrt{r^2 + (Z - Z_p)^2} \to 0$,

where $\Omega^2 = (\omega^2/C(Z_p)^2) - k^2$.

We try the solution

$$P = \int_0^\infty J_0(kr)\phi(Z, Z_p)\, k\, d\, k .$$

As ϕ satisfies the second order differential equation (A.4), we see that together with the boundary conditions the conditions

(1) $\phi(Z = Z_p - 0) = \phi(Z = Z_p + 0)$, and

(2) $$\frac{d\phi(Z_p + 0)}{dZ} - \frac{d\phi(Z_p - 0)}{dZ} = 2$$

are sufficient to specify the solution uniquely.

We put $\phi_1(z) = A_1 M(z) + B_1 N(z)$ for $z < z_p$,

and $\phi_2(z) = A_2 M(z) + B_2 N(z)$ for $z > z_p$.

The boundary conditions then give

$$\phi_1(z) = A\left\{N(0)\,M(z) - M(0)\,N(z)\right\},$$

and

$$\phi_2(z) = B\left[\left\{N(H)\cos\alpha + \frac{dN(H)}{dz}\sin\alpha\right\}M(z) - \left\{M(H)\cos\alpha + \frac{dM(H)}{dz}\sin\alpha\right\}N(z)\right].$$

The matching conditions then give

(1) $$A\left\{N(0)\,M(z_p) - M(0)\,N(z_p)\right\} - B\left[\left\{N(H)\cos\alpha + \frac{dN(H)}{dz}\sin\alpha\right\}M(z_p) - \left\{M(H)\cos\alpha + \frac{dM(H)}{dz}\sin\alpha\right\}N(z_p)\right] = 0,$$

and

(2) $$A\left\{N(0)\frac{dM(z_p)}{dz} - M(0)\frac{dN(z_p)}{dz}\right\} - B\left[\left\{N(H)\cos\alpha + \frac{dN(H)}{dz}\sin\alpha\right\}\frac{dM(z_p)}{dz} - \left\{M(H)\cos\alpha + \frac{dM(H)}{dz}\sin\alpha\right\}\frac{dN(z_p)}{dz}\right] = 2.$$

These equations can be written

$$\begin{bmatrix} M(z_p) & N(z_p) \\ \frac{dM(z_p)}{dz} & \frac{dN(z_p)}{dz} \end{bmatrix}\begin{bmatrix} N(0) & N(H)\cos\alpha + \frac{dN(H)}{dz}\sin\alpha \\ -N(0) & -M(H)\cos\alpha - \frac{dM(H)}{dz}\sin\alpha \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \end{bmatrix}.$$

We see that the first matrix is the matrix of the Wronskian of M and N, and hence is non singular as M and N are a fundamental set of solutions, while the second matrix is the matrix of the determinant whose zeros (as functions of k^2) are the eigenvalues of (A.4). Thus we can always solve for A and B unless k^2 is an eigenvalue of (A.4); and in this case our integrand has a pole singularity.

These singularities occur on the real axis and we interpret the integral as a Cauchy principal value by the usual methods of contour integration.

In the case of an outgoing wave at $Z = \infty$ we have

$$\phi_2(Z) = B\, N(Z) ,$$

and the matching condition leads to the matrix equation

$$\begin{bmatrix} M(Z_p) & N(Z_p) \\ \frac{dM(Z_p)}{dZ} & \frac{dN(Z_p)}{dZ} \end{bmatrix} \begin{bmatrix} N(0) & 0 \\ -M(0) & 1 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \end{bmatrix} .$$

We see that the characteristic equation is

$$N(0) = 0$$

which is the limit of the characteristic equation for the boundary conditions (a) as $H \to \infty$ provided that $-q_{max} < \lambda < 0$ (~~in the case~~ here $N(Z) \to 0$, $N(Z) \to \infty$ as $Z \to \infty$).

Thus the discrete spectrum is identical in both cases. The outgoing wave condition is necessarily set on an infinite range so that it is of interest to ask what, in this case, corresponds to the continuous spectrum. Peierls, using the radiation condition, found an integral term which he called the branch line integral. We will reproduce an example solved by Peierls and show that the branch line integral is identical with the contribution of the continuous spectrum (appendix).

The physical interpretation of these results is the following [1] . The terms in the discrete spectrum correspond to signals propagated ~~in the radially direction~~ radially while the continuous spectrum ultimately ($Z \to \infty$) has the character of an outgoing spherical wave.

As, in practice, one is usually interested in signals received for large values of r and moderate values of z the terms in the discrete spectrum (which fall off as $\frac{1}{\sqrt{r}}$) are relatively more important than the terms in the continuous spectrum which fall off as $\frac{1}{r}$.

The propagation of a transient pulse is described by taking the Fourier transform of the Green's function. We have, if $g(\omega)$ is the Fourier transform of the pulse,

$$P(r,z,t) = \frac{1}{\pi} \int_{-\infty}^{\infty} g(\omega)\, G(r:z,z_p,\omega) e^{i\omega t}\, d\omega .$$

We assume that we can replace the Hankel function by its asymptotic representation

$$H_0^{(2)}(k_n r) \sim \sqrt{\frac{2}{\pi k_n r}}\; e^{-i\left\{\frac{\pi}{4} + k_n r\right\}}$$

and that the method of stationary phase can be used to approximately evaluate the Fourier transform integral.

In this case the points of stationary phase are given by

$$\frac{d}{d\omega}(\omega t - k_n r) = 0 ,$$

that is by

$$r = \frac{d\omega}{dk_n}\, t = {}^{n}C_g\, t$$

where ${}^{n}C_g$ is the group velocity of the m^{th} mode; and the solution is

$$P \sim \frac{-i}{4\pi r} \sum_n g(\omega) \left\{ \frac{1}{k_n} \left| \frac{d({}^{n}C_g)}{d\omega} \right| \right\}^{\frac{1}{2}} \phi_n(z)\, \phi_n(z_p)\; e^{-i\left\{\frac{\pi}{4} + \frac{\pi}{4} + k_n r - \omega t\right\}} \qquad (A.6)$$

where the summation is taken over those values of ω such that

$r = {}^{n}C_g\, t$, and $k_n^2 > 0$.

When $\frac{d({}^{n}C_g)}{d\omega} = 0$ the formula breaks down. Peeris has given a formula to evaluate P in this case.

The computation of P from formula (A.6) requires in general the numerical solution of (A.4) for, at any rate, the first few eigenvalues and eigenfunctions for a set of values of ω within the desired frequency range (sufficient for other values to be filled in by interpolation). We also require ${}^{n}C_g$ and $\frac{d}{d\omega}({}^{n}C_g)$; and the latter quantity could be obtained from the former by numerical differentiation. To compute ${}^{n}C_g$ we differentiate equation (A.4) with respect to ω . This gives

$$\frac{d^2}{dz^2}\left(\frac{\partial \phi_n}{\partial \omega}\right) + \left\{\frac{\omega^2}{C(z)^2} - k_n^2\right\}\frac{\partial \phi_n}{\partial \omega} = \left\{2k_n \frac{dk_n}{d\omega} - \frac{2\omega}{C(z)^2}\right\}\phi_n .$$

As the boundary conditions are independent of ω we must have the right hand side orthogonal to ϕ_n over (0, H) for a solution to be possible.

Hence

$$\int_0^H \left\{k_n \frac{dk_n}{d\omega} - \frac{\omega}{C(z)^2}\right\}\phi_n^2\, dz = 0 ,$$

and thus $${}^{n}C_g = \frac{k_n \int_0^H \phi_n^2\, dz}{\int_0^H \left\{\omega/c(z)^2\right\}\phi_n^2\, dz} .$$

This argument could be continued to give $\frac{d}{d\omega}({}^{n}C_g)$ if we are prepared to solve for $\frac{\partial \phi_n}{\partial \omega}$ (possibly numerical differentiation will be more convenient and give sufficient accuracy). Note however that $\frac{\partial \phi_n}{\partial \omega}$ is determinate only up to a multiple of ϕ_n .

As the scale of ϕ_n is arbitrary we can fix one value, i.e. $\phi_n(\bar{z}) = 1$ for all ω . We must then have $\frac{\partial \phi_n(\bar{z})}{\partial \omega} = 0$; and this gives us an additional condition which will enable us to avoid ill conditioned equations in our numerical working.

B. Solution of the Reynold's equation

We have not carried out a detailed analysis of this equation; and we will content ourselves in this section with describing the salient features of the problem that requires numerical solution.

The Reynold's equation for the pressure in the oil film of a journal bearing is

$$\frac{\partial}{\partial x}\left\{h^3 \frac{\partial P}{\partial x}\right\} + \frac{\partial}{\partial y}\left\{h^3 \frac{\partial P}{\partial y}\right\} = 6\eta U \frac{dh}{dx} \qquad \text{(B.1)}$$

where h is the clearance in the bearing, and is assumed to be a function of x (the distance round the bearing from a fixed position) only, η is the coefficient of viscosity assumed constant, and U is the speed of rotation.

In the derivation of (B.1) it is assumed

(a) that the film h is so thin that the pressure can be considered constant throughout its thickness, and

(b) that the viscosity η is independent of the pressure and temperature.

Assumption (a) has been considered by Wannier [5] who derived the Reynold's equation for the constant viscosity case from the Stoke's equations as a first approximation for small h. He also derived an exact solution to the Stoke's equations for the journal bearing of infinite breadth assuming that the pressure is periodic around the bearing and compared this with the corresponding solution to Reynold's equation. Assumption (b) has been tested by Christopherson [6] by integrating numerically the equations for the pressure and temperature dependent case, and comparing the results with numerical solutions of Reynold's equation.

The general conclusion in both these tests is that Reynold's equation constitutes a very useful first approximation provided (case (b)) that the value of the viscosity is chosen appropriately.

The boundary conditions on equation (B.1) have been the subject of some discussion. Perhaps the obvious condition is periodicity in the pressure as one circuits the bearing. However, this condition leads to negative pressures in regions where the fluid streamlines diverge and is thus physically unacceptable. What we get is a region of cavitation where the difference between the actual pressure and atmospheric pressure will be negligible.

Certainly the boundary of the film will be characterised by the condition $P = 0$. It is convenient to describe distance round the circumference of the journal in terms of the angle the radius vector of the point makes with the radius to the point on the circumference where the clearance is greatest. One boundary of the lubricating film will be in the neighbourhood of $\Phi = 0$, and we call this the start position. In practice the pressures in the vicinity of $\Phi = 0$ are small in magnitude, and the solution is comparatively independent of what is happening in this region. We have taken $\Phi = 0$ as an initial approximation to the start boundary. One of our aims is to study the effect on the solution of varying this position.

The most important condition is the 'end' condition which will be in the neighbourhood of $\Phi = \pi$. It turns out that the pressure is quite sensitive to changes in the position of this end of the film. It is suggested by Christopherson [6] that this boundary should be

characterised by the condition that the film blend smoothly with the region of cavitation where $P = 0$. That is, $P = 0$ should be a tangent plane to the film at the end boundary. This condition gives

$$P = \frac{\partial P}{\partial n} = 0 \qquad \text{(B.2)}$$

where n is the ~~interval~~ outward normal to the film.

As $P = 0$, then also $\frac{\partial P}{\partial s} = 0$ where s is the tangential direction. Thus $\frac{\partial P}{\partial x}$ and $\frac{\partial P}{\partial y}$ also vanish on the end line.

Appendix. On a Problem solved by Pekeris

When the density ρ is allowed to vary with Z equation (A.4) becomes

$$\frac{d}{dz}\left(\frac{1}{\rho}\frac{d\phi}{dz}\right) + \frac{1}{\rho}\left\{\frac{\omega^2}{C(z)^2} - k^2\right\}\phi = 0 .$$

Our boundary conditions again lead to a self adjoint eigenvalue problem; and our previous arguments can be applied to it. However, the orthogonality relation becomes

$$\int_0^H \frac{1}{\rho}\phi_i \phi_j \, dz = \delta_{ij} ,$$

and equation (4) becomes

$$G(r : Z, Z_p) = \frac{-i}{4} \sum_n H_0^{(2)}(k_n r) \frac{\phi_n(z)\,\phi_n(z_p)}{\rho\,(z_p)} .$$

Also if ρ is discontinuous at certain depths then we must have the additional conditions (matching conditions)

$$\phi \text{ continuous}, \quad \frac{1}{\rho}\frac{d\phi}{dz} \text{ continuous}$$

satisfied at these points. These correspond to asking that the pressure and the normal velocity at the interface be continuous.

We will consider the special model where both ρ and c have step discontinuities at $Z = D$ and are otherwise constant. Our boundary conditions are $P = 0$ at $Z = 0$ and $Z = H$.

The eigenfunctions are given by

$$\phi = A \sin \sqrt{\frac{\omega^2}{C_1^2} - k^2} Z = A \sin \Omega_1 Z$$

in layer (1), and

$$\phi = B \sin \sqrt{\frac{\omega^2}{c_2^2} - k^2}\,(H-Z) = B \sin \Omega_2 (H-Z)$$

in layer (2).

The condition that the matching conditions be satisfied leads to the characteristic equation

$$\begin{vmatrix} \sin \Omega_1 D & \sin \Omega_2 (H-D) \\ \frac{1}{\rho_1} \Omega_1 \cos \Omega_1 D & -\frac{1}{\rho_2} \Omega_2 \cos \Omega_2 (H-D) \end{vmatrix} = 0$$

For $\frac{\omega^2}{c_1^2} > k^2 > \frac{\omega^2}{c_2^2}$ the spectrum is discrete in the limt $H = \infty$.

The characteristic equation in this case is

$$\tan \Omega_1 D = -\frac{\rho_2 \Omega_1}{\rho_1 |\Omega_2|} \tanh |\Omega_2| (H-D)$$

which tends to

$$\tan \Omega_1 D = -\frac{\rho_2 \Omega_1}{\rho_1 |\Omega_2|} \quad \text{as} \quad h \to \infty .$$

This equation has discrete solutions if it has solutions at all.

The spectrum is continuous in limit $\overset{as}{\wedge} H \to \infty$ if $\omega^2/c_2^2 > k^2$. The characteristic equation is

$$\frac{\tan \Omega_2 H - \tan \Omega_2 D}{1 + \tan \Omega_2 H \tan \Omega_2 D} = -\frac{\rho_1 \Omega_2}{\rho_2 \Omega_1} \tan \Omega_1 D .$$

The spacing between two conse$\overset{cu}{}$rvative zeros of $1+\tan \Omega_2 H \tan \Omega_2 D$ is given by

$$\Delta \Omega = \frac{\pi}{H} + O\left(\frac{1}{H^2}\right) .$$

Now exactly one eigenvalue lies in this range. Thus the number of eigenvalues lying in any finite range $(\Omega_2, \Omega_2 + \Delta\Omega_2)$ tends to infinity with $\Delta \Omega_2 H/\pi$ - that is with H.

We will now construct the spectral function σ for this problem. Our eigenfunction will have the form $\left(\omega^2/c_2^2 > \Omega^2 \right)$

$$\varphi = \frac{\rho_1 \sin \Omega_1 z}{\Omega_1 \cos \Omega_1 D} \qquad \text{in layer (1)},$$

$$= \frac{\rho_1 \Omega_2 \sin \Omega_1 D \cos \Omega_2 (z-D) + \rho_2 \Omega_1 \cos \Omega_1 D \sin \Omega_2 (z-D)}{\Omega_1 \Omega_2 \cos \Omega_1 D}$$

in layer (2).

For large values of H we have

$$\int_0^H \frac{1}{\rho} \varphi^2 dz = \frac{H}{2} \left[\frac{\rho_1^2 \Omega_2^2 \sin^2 \Omega_1 D + \rho_2^2 \Omega_1^2 \cos^2 \Omega_1 D}{\rho_2 \Omega_1^2 \Omega_2^2 \cos^2 \Omega_1 D} \right] + O\left(\frac{D}{H}\right)$$

and, for the distance between adjacent eigenvalues,

$$(\Delta \Omega_2) H = \pi + O(1/H) .$$

Thus we have

$$\frac{\Delta \sigma(\Omega_2)}{\Delta \Omega_2} = \frac{H}{\pi} \left[\frac{H}{2} \left(\frac{\rho_1^2 \Omega_2^2 \sin^2 \Omega_1 D + \rho_2^2 \Omega_1^2 \cos^2 \Omega_1 D}{\rho_2 \Omega_1^2 \Omega_2^2 \cos^2 \Omega_1 D} \right) \right]^{-1} + O\left(\frac{D}{H}\right)$$

and, in the limit $H \to \infty$,

$$\frac{d\sigma(\Omega_2)}{d\Omega_2} = \frac{2}{\pi} \frac{\rho_2^2 \Omega_1^2 \Omega_2^2 \cos^2 \Omega_1 D}{\rho_1^2 \Omega_2^2 \sin^2 \Omega_1 D + \rho_2^2 \Omega_1^2 \cos^2 \Omega_1 D} .$$

For terms in the discrete spectrum we have

$$\int_0^\infty \frac{\varphi^2}{\rho} dz = \int_0^D \frac{1}{\rho_1} \left(\frac{\rho_1^2 \sin^2 \Omega_1 D}{\Omega_1^2 \cos^2 \Omega_1 D} \right) dz + \int_D^\infty \frac{1}{\rho_2} \left(\frac{\rho_2^2 e^{2|\Omega_2|(D-z)}}{|\Omega_2|^2} \right) dz$$

$$= \frac{\rho_1}{\Omega_1^2 \cos^2 \Omega_1 D} \left\{ \frac{D}{2} - \frac{\sin 2\Omega_1 D}{4\Omega_1} \right\} + \frac{\rho_2}{2|\Omega_2|^3}$$

$$= \frac{\rho_1}{2\Omega_1^3 \cos^2 \Omega_1 D} \left\{ \Omega_1 D - \sin \Omega_1 D \cos \Omega_1 D + \frac{\rho_2 \Omega_1^3}{\rho_1 |\Omega_2|^3} \cos^2 \Omega_1 D \right\} .$$

Using $\tan \Omega_1 D = - \dfrac{\rho_2 \Omega_1}{\rho_1 |\Omega_2|}$ we get

$$\int_0^\infty \frac{\varphi^2}{\rho} dz = \frac{\rho_1}{2\Omega_1^3 \cos^2 \Omega_1 D} \left\{ \Omega_1 D - \sin \Omega_1 D \cos \Omega_1 D - \left(\frac{\rho_1}{\rho_2}\right)^3 \sin \Omega_1 D \tan \Omega_1 D \right\}.$$

This gives for the Green's function

$$G(r : z, z_p) =$$

$$- \frac{i}{2} \sum_m H_0^{(2)}(k_m r) \frac{\Omega_1 \sin \Omega_1 z \sin \Omega_1 z_p}{\Omega_1 D - \sin \Omega_1 D \cos \Omega_1 D - \left(\frac{\rho_1}{\rho_2}\right)^3 \sin \Omega_1 D \tan \Omega_1 D}$$

$$+ \frac{i}{2\pi} \int_{-i\infty}^{\omega/c_2} H_0^{(2)}(kr) \frac{\rho_1 \rho_2 \Omega_2 \sin \Omega_1 z \sin \Omega_1 z_p}{\rho_1^2 \Omega_2^2 \sin^2 \Omega_1 D + \rho_2^2 \Omega_1^2 \cos^2 \Omega_1 D} k \, dk$$

which is effectively the form given by Pekeris.

Chapter II. Finite Difference Formulae for Differentiation

The main topic of this thesis is the application of finite difference methods to the numerical solution of differential equations In this section we give a summary of results concerning the use of finite difference formulae for numerical differentiation as a preliminary to our main topic.

(A) Notation and Derivation of Formulae

We concern ourselves with functions specified by their numerical values (tabular values) for a discrete set of equispaced values of their arguments. This distance will be denoted by h. The argument values are then $x_n = x_0 + nh$. The numerical values will be denoted by $f(x_n) = f_n$. It should be noted that f(x) is by no means uniquely specified its tabular values, as any function which vanishes for all x_n (for example $\sin \frac{\pi(x-x_0)}{h}$) can be used to generate a set of such functions.

The aggregate of all functions having the tabular values is usually called a cotabular set.

We define the central difference operator by

$$\delta f_n = f_{n+1/2} - f_{n-1/2}$$

(Note that only even powers of δ operate on the tabular values (f_n) of f), and the differentiation operator by

$$Df_n = \left.\frac{df}{dx}\right|_{x=x_n}$$

These operations can be formally related for, by Taylor's theorem

$$f_{n+1} = \left\{1 + hD + \frac{h^2D^2}{2!} + \cdots\right\} f_n = e^{hD} f_n .$$

Thus

$$\delta f_n = 2 \sinh (\tfrac{1}{2} hD) f_n ,$$

and

$$hD f_n = 2 \sinh^{-1} (\tfrac{1}{2}\delta) f_n .$$

Expanding the right hand side of this last relation in powers of δ we have a finite difference formula for the numerical value of the first derivative of $f(x)$ at the ordinate point $x = x_n$. However this formula involves only odd powers of δ. To obtain a formula acting on tabular values of f we introduce the averaging operator defined by

$$\mu f_n = \tfrac{1}{2}(f_{n+1/2} + f_{n-1/2}) = \cosh \tfrac{1}{2} hD f_n = \sqrt{1 + \frac{\delta^2}{4}}\, f_n .$$

Introducing this operator into the differentiation formula gives

$$hD f_n = \frac{2 \sinh^{-1} \tfrac{1}{2}\delta}{\sqrt{1 + \frac{\delta^2}{4}}}\, \mu f_n .$$

We have no need of this device in deriving formulae for even order derivatives as even powers of $\sinh^{-1} \frac{1}{2}\delta$ involve only even powers of δ.

To set up general finite difference formulae we must expand

(i) $(hD)^{2n}$, & (ii) $(hD)^{2n+1}/\mu$

as functions of δ. This can be done by making use of recurrence relations connecting the differentiation formulae of different orders. We have

$$(hD)^n = \frac{1}{n+1} \frac{d(hD)^{n+1}}{d(hD)} = \frac{1}{n+1} \frac{d(hD)^{n+1}}{d\delta} \frac{d\delta}{d(hD)}$$

$$= \frac{\mu}{n+1} \frac{d(hD)^{n+1}}{d\delta}$$

In particular

$$\frac{(hD)^{2r+1}}{\mu} = \frac{1}{2r+2} \frac{d(hD)^{2r+2}}{d\delta} \qquad (A\cdot 1)$$

and $$(hD)^{2r} = \frac{\mu}{2r+1} \frac{d}{d\delta}\left[\frac{(hD)^{2r+1}}{\mu}\mu\right]$$

$$= \frac{\mu^2}{2r+1} \frac{d}{d\delta}\left[\frac{(hD)^{2r+1}}{\mu}\right] + \frac{\delta}{4(2r+1)}\left[\frac{(hD)^{2r+1}}{\mu}\right].$$

Replacing μ^2 by $I + \frac{1}{4}\delta^2$ gives

$$(hD)^{2r} = \frac{1+\frac{\delta^2}{4}}{2r+1} \frac{d}{d\delta}\left[\frac{(hD)^{2r+1}}{\mu}\right] + \frac{\delta}{4(2r+1)}\left[\frac{(hD)^{2r+1}}{\mu}\right] \qquad (A\cdot 2).$$

We set

$$(hD)^{2r} = \sum_{p=r}^{\infty} a_p^{(r)} \delta^{2p},$$

$$\frac{(hD)^{2r+1}}{\mu} = \sum_{p=r}^{\infty} b_p^{(r)} \delta^{2p+1},$$

and

$$(hD)^{2r+2} = \sum_{p=r}^{\infty} c_p^{(r)} \delta^{2p+2} = \sum_{p=r+1}^{\infty} a_p^{(r+1)} \delta^{2p}.$$

Relations (A.I) and (A.2) then give

$$b_p^{(r)} = -\frac{2p}{4(2p+1)} b_{p-1}^{(r)} + \frac{2r+1}{2p+1} a_p^{(r)},$$

and $$c_p^{(r)} = \frac{2r+2}{2p+2} b_p^{(r)}.$$

In this latter case we have

$$c_{p-1}^{(r)} = \frac{2r+2}{2p} b_{p-1}^{(r)},$$

whence

$$C_p^{(r)} = -\frac{(2p)^2}{4(2p+2)(2p+1)} C_{p-1}^{(r)} + \frac{(2r+2)(2r+1)}{(2p+2)(2p+1)} a_p^{(r)} .$$

To start the recursion we have $(hD)^r = I$ when $r = 0$. This gives

$$b_0^{(0)} = 1 , \; b_p^{(0)} = -\frac{2p}{4(2p+1)} b_{p-1}^{(0)} , \text{ and}$$

$$C_0^{(0)} = 1 , \; C_p^{(0)} = -\frac{(2p)^2}{4(2p+2)(2p+1)} C_{p-1}^{(0)} .$$

Thus we have (writing out explicitly the first few terms of these series)

$$\frac{hD}{\mu} = \delta - \frac{\delta^3}{6} + \frac{\delta^5}{30} - \frac{\delta^7}{140} + \cdots \qquad (A\cdot 3),$$

and

$$(hD)^2 = \delta^2 - \frac{\delta^4}{12} + \frac{\delta^6}{90} - \frac{\delta^8}{560} + \cdots \qquad (A\cdot 4).$$

(B) On the Convergence of these Expansions

For the finite difference series just derived we must distinguish between two different uses of the term convergence. These are (I) convergence of the series in the usual manner when the difference operators are replaced by certain numerical values (for example one might discuss the case $|\delta^n f| \leq \lambda^n |f|$), and (2) convergence of the series to the numerical value of the required derivative of $f(x)$ at the ordinate point in question (assuming convergence in the sense of (I)).

We now consider convergence in the sense of (I).

In the case $r = 0$ we have

$$b_p^{(0)} = (-1)^p \frac{2p\,(2p-2)\cdots 2}{4^p\,(2p+1)\cdots 3} = (-1)^p \frac{(p!)^2}{(2p+1)!},$$

and

$$c_p^{(0)} = (-1)^p \frac{(2p)^2(2p-2)^2\cdots 2^2}{4^p\,(2p+2)(2p+1)\cdots 43} = (-1)^p \frac{(p!)^2}{(p+1)(2p+1)!}.$$

We can estimate the values of these coefficients for large values of p by means of Stirling's formula

$$n! \sim \sqrt{2\pi}\; n^{n+1/2} e^{-n}.$$

We have

$$\frac{(p!)^2}{(2p+1)!} \sim \frac{2\pi\, p^{2p+1} e^{-2p}}{\sqrt{2\pi}\,(2p+1)^{2p+3/2} e^{-2p-1}} = \frac{\sqrt{2\pi}}{2^{2p+1}} \frac{1}{(1+\frac{1}{2p})^{2p+1}} \frac{e}{(2p+1)^{1/2}}.$$

As $\lim_{p\to\infty} (1+1/2p)^{2p+1} = e$, then

$$b_p^{(0)} \to 0 \quad \text{with} \quad \frac{\sqrt{\pi}}{2^{2p+1} p^{1/2}},$$

and

$$c_p^{(0)} \to 0 \quad \text{with} \quad \frac{\sqrt{\pi}}{2^{2p+1} p^{3/2}}.$$

Thus $\sum_0^\infty c_p^{(0)} \delta^{2p+2}$ is convergent provided $|\delta| \leq 2$,

while $\sum_0^\infty b_p^{(0)} \delta^{2p+1}$ is convergent for $|\delta| < 2$.

We can show that $c_p^{(r)}$ and $b_p^{(r)}$ tend to zero in the same manner as $c_p^{(0)}$ and $b_p^{(0)}$. This follows readily by induction for then

$$b_p^{(r)} = -\frac{2p}{4(2p+1)}\, b_{p-1}^{(r)} + O\left(1/p^{3/2}\right),$$

and

$$c_p^{(r)} = -\frac{2p}{4(2p+2)(2p+1)}\, c_{p-1}^{(r)} + O\left(1/p^{3/2}\right).$$

As $\delta^2 e^x = 4 \sinh^2 \frac{h}{2}\, e^x$, and $\delta^2 e^{ix} = -4 \sin^2 \frac{h}{2}\, e^{ix}$ we see that the even order difference expansions converge for the elementary trigonometric and hyperbolic functions (provided that $\sinh^2 h/2 \leq I$ in the hyperbolic case). For the odd order operators there is an exceptional case $f(x) = e^{ix}$ and $h = \pi$ when the series for $(hD)^{2r+1}/\mu$ diverges. As $\mu\, e^{ix} = \cos \frac{h}{2}\, e^{ix}$ vanishes when $h = \pi$ the differentiation formulae are indeterminate.

The even order difference expansions converge for every real valued function bounded on $(-\infty, \infty)$ for then we have

$|f(x)| \leq K$ and, therefore,

$$|\delta^2 f(x)| = |f(x+h) - 2f(x) + f(x-h)| \leq 4K.$$

There is equality only if f_r is cotabular with $(-I)^r K$; and this is the only exceptional case for the odd order operators.

(C) On the Second Problem of Convergence

From the examples in section (B) we see that a function need not be bounded on $(-\infty, \infty)$ for the difference expansion of its derivatives to converge (although it must of course be bounded on every finite sub interval), nor need it tend to zero at $\pm\infty$.

We now turn to the problem of determinating that function (if any) of the cotabular set which has its derivatives represented exactly.

Certainly the expansions are valid for polynomials (as differences of order greater than the degree of the polynomial must vanish, the formulae can be readily verified either directly or by induction). It then follows that the expansions must give asymptotic (as $h \to 0$) representations of the derivatives of an arbitary function regular at the point in question.

We now show that the difference expansions are exact for the elementary trigonometric functions (we will consider $\sin \lambda x$). As the even order differences of $\sin \lambda x$ are proportional to $\sin \lambda x$ we have to show that (considering $(hD)^2$)

$$h^2\lambda^2 = 4 \sin^2 \frac{\lambda h}{2} + \frac{1}{12}\left[4 \sin^2 \frac{\lambda h}{2}\right]^2 + \cdots$$

However we have already shown that

$$4\left[\sinh^{-1} \tfrac{1}{2} x\right]^2 = x^2 - \frac{x^4}{12} + \frac{x^6}{90} - \cdots$$

and that this series is convergent for $|x| \leq 2$. Our result now follows on putting $x = 2i \sin \lambda h/2$. The result for derivatives of arbitary order can now be verified in similar fashion by using the recurrence relations(I.I) and (I.2). We note that the series for the even order derivatives are valid for $h \leq \pi/|\lambda|$, while those for the odd order derivatives hold only for $h < \pi/|\lambda|$. This is because of the singularities of $\frac{1}{\sqrt{1 + \frac{\delta^2}{4}}}$ at $\delta = \pm 2i$.

We now extend these results to functions bounded on the real axis.

It has been shown by E.T. Whittaker that the limit of any central difference interpolation formula approximating to some function f(x) bounded on $(-\infty, \infty)$ as more and more function values are taken into account (with h fixed) is the function

$$F(x) = \sum_{-\infty}^{\infty} f_r \frac{\sin \pi (x-rh)/h}{\pi (x-rh)/h},$$

$$= \sum_{-\infty}^{\infty} f_r \int_{-\pi/h}^{\pi/h} \frac{h}{2\pi} e^{i\lambda(x-rh)} d\lambda$$

which he called the cardinal function of the cotabular set [I, p62].

We will show that the finite difference formulae produce exactly the numerical values of the derivatives of the cardinal function at the ordinate point in question. We consider first the case when the cardinal function can be represented in the form

$$F(x) = \int_{-\pi/h}^{\pi/h} g(\lambda) e^{i\lambda x} d\lambda$$

where $g(\lambda) = \frac{h}{2\pi} \sum_r f_r e^{-i\lambda rh}$ (for example if $\sum_r |f_r|$ is convergent).

The result is immediate for the finite difference formulae associated with even order derivatives for these are valid everywhere within the range of integration (that is for $\lambda \leq \pi/h$).

In the case of the odd order formulae, we have $\sum b_p^{(r)} \delta^{2p+1}$ divergent at the ends of the range of integration. However the differentiation formula is given by the operator

$B_r = \mu \sum b_p^{(r)} \delta^{2p+1}$; and we have

$\lim_{\lambda \to \frac{\pi}{h} - 0} B_r e^{i\lambda x} = (-1)^r \left(\frac{\pi}{h}\right)^{2r+1} e^{i\lambda x}$ - the zero of $\mu e^{i\lambda x}$

compensating for the divergence of $\sum b_p^{(r)} \delta^{2p+1}$

In the case when $F(x)$ is bounded on $(-\infty, \infty)$ we require a theorem of Wiener and Paley and some related results [2, pp. I30-I40].

As $F(x)$ is bounded on $(-\infty, \infty)$ then

$\int_{-\infty}^{\infty} \left\{ \frac{|F(x) - F(0)|}{x} \right\}^2 dx$ is convergent. Now $F(x)$ is an integral function of exponential type with exponent π/h,

hence so also is $\frac{F(x) - F(0)}{x}$. Thus, by the Wiener-Paley theorem,

$$\frac{F(x) - F(0)}{x} = \int_{-\pi/h}^{\pi/h} g(\lambda) e^{i\lambda x} d\lambda$$

where $g(\lambda) \in L^2(-\pi/h, \pi/h)$.

$$\therefore \quad F(x) = F(0) + x \int_{-\pi/h}^{\pi/h} g(\lambda) e^{i\lambda x} d\lambda .$$

We will demonstrate the result for the particular case $(hD)^2$ which is typical. We have to show that

$$(hD)^2 \left[x e^{i\lambda x} \right] = \left(\delta^2 - \tfrac{1}{12}\delta^4 + \tfrac{1}{90}\delta^6 - \dots \right) \left[x e^{i\lambda x} \right].$$

We have

$$\delta\left[x e^{i\lambda x}\right] = x\delta e^{i\lambda x} + \delta x \cos\frac{\lambda h}{2} e^{i\lambda x},$$

$$\delta^2\left[x e^{i\lambda x}\right] = x\delta^2 e^{i\lambda x} + 2\delta x \cos\frac{\lambda h}{2} \delta e^{i\lambda x},$$

$$\delta^3\left[x e^{i\lambda x}\right] = x\delta^3 e^{i\lambda x} + 3\delta x \cos\frac{\lambda h}{2} \delta^2 e^{i\lambda x},$$

... and so on. The general term is

$$\delta^n\left[x e^{i\lambda x}\right] = x\delta^n e^{i\lambda x} + n\delta x \cos\frac{\lambda h}{2} \delta^{n-1} e^{i\lambda x}.$$

Substituting these expressions in the right hand side above we get

$$x\left[\delta^2 - \tfrac{1}{12}\delta^4 + \tfrac{1}{90}\delta^6 - \cdots\right] e^{i\lambda x}$$
$$+ \delta x\left[2\delta - \tfrac{4}{12}\delta^3 + \tfrac{6}{90}\delta^5 - \cdots\right] e^{i\lambda x}\cos\frac{\lambda h}{2}$$

$$= x\left[\delta^2 - \tfrac{1}{12}\delta^4 + \tfrac{1}{90}\delta^6 - \cdots\right] e^{i\lambda x}$$
$$+ 2\delta x\left[\delta - \tfrac{1}{6}\delta^3 + \tfrac{1}{30}\delta^5 - \cdots\right] \mu e^{i\lambda x}$$

$$= x(hD)^2 e^{i\lambda x} + 2(hD)x(hD)e^{i\lambda x}$$

by the equivalence of our formula with differentiation for the elementary trigonometric functions with $|h| < \pi/\lambda$. The result now follows as in the previous case.

Chapter III. Finite difference approximations to ordinary differential equations.

The problems discussed in chapter I all require for their complete solution the numerical solution of certain differential equations. The procedure we will adopt will be to replace the differential equation by an approximate difference equation whose solution can be obtained by solving a finite set of linear algebraic equations. In this chapter we will consider three methods for the construction of these approximating difference equations. These are

(a) by approximation to the derivative with truncated finite difference formulae for numerical differentiation (chapter 2),

(b) by polynomial interpolation of the solution, and

(c) by approximation to the exact difference equation.

It will be convenient to consider each of these methods in separate sections; and the chapter will be broken up accordingly. Each section will be indicated by a capital letter. Where necessary it will be divided into subsections which will be denoted in the usual way.

(A) The basic approach of method (a) has been very fully documented and would appear to require little comment here. Perhaps [1] is the best reference. However, we must point out that the difference expansions cannot be truncated at terms of arbitrary order. For example, a second order differential equation has its solution (in general) uniquely specified by two additional conditions; and this is true also of a second order difference equation (three term recurrence relation). In this case the appropriate approximation is

$$h^2 D^2 \cong \delta^2$$

as higher order differences would require values at more than three consecutive points, and the resulting difference equation would not then have its solution uniquely specified by the imposed conditions. However, it has been suggested [2] that equations involving higher order differences (more accurate equations) be used away from boundary points.

It is possible to increase the order of the differences ignored in the approximation to the differential equation without increasing the order of the difference equation by means of the following device which is best illustrated by an example. Let the differential equation be

$$y'' + f(x)\, y = g(x)$$

The full finite difference equation is

$$\delta^2 y_i + h^2 f_i y_i = h^2 g_i + \left\{ \frac{\delta^4}{12} - \frac{\delta^6}{90} + \cdots \right\} y_i$$

If we operate on both sides of this equation with $(1 + \delta^2/12)$ we get

$$\delta^2 y_i + h^2 (1 + \delta^2/12) f_i y_i = h^2 (1 + \delta^2/12) g_i + \left\{ -\delta^6/240 + {}^{13}/_{15120}\, \delta^8 - \cdots \right\} y_i .$$

Thus the second order difference equation

$$\delta^2 y_i + h^2 (1 + \delta^2/12) f_i y_i = h^2 (1 + \delta^2/12) g_i \qquad \text{(A·1)}$$

ignores only quantities which are at least $O(\delta^6)$.

This device can be further exploited. For example, if a term involving

a first derivative appears in the differential equation with a constant coefficient p then the operator

$$1 + \mu\delta \frac{hp}{12 - \frac{5h^2p^2}{2}} + \delta^2 \frac{1 - \frac{5h^2p^2}{12}}{12 - \frac{5h^2p^2}{2}}$$

can be used.

Another method which takes account of the high order differences is that of difference correction [3] . We will refer our discussion of the method to a later chapter.

(B.1) We now outline the manner in which the usual methods of polynomial interpolation can be used to construct the approximating finite difference equations. We will assume a fixed mesh length h in our discussion although this is not necessary.

The idea of the method is the following. Let us assume that we know the values of the solution $y(x)$ at $(n+1)$ successive points, and that we wish to interpolate y between these points. In constructing our interpolation polynomial we can also use the fact that y satisfies the differential equation at each of these points. This gives $(2n+1)$ conditions, and these will determine (in general) a polynomial of degree $(2n+1)$. If, however, we ask for an interpolation polynomial of degree $2n$ then we have $(2n+2)$ equations for the $(2n+1)$ unknown coefficients; and a solution is only possible if these equations are linearly dependent. The condition expressing this linear dependence is the desired difference equation.

We will illustrate the method with the following examples.

(1) First order equation

$$\frac{dy}{dx} + f(x)\,y = g(x).$$

(a) two point equation.

As we know, y_0 , y_0', y_n , and y_n' we try the quadratic interpolating polynomial

$$y = A + Bx + Cx^2.$$

We get

$$y_0 = A \quad , \qquad y_n = A + Bh + Ch^2,$$
$$y_0' = B \quad , \qquad y_n' = B + 2Ch .$$

The difference equation is then clearly

$$\Delta y_0 - h y_0' = \frac{h}{2}\,\Delta y_n'$$

which can be written (using the differential equation)

$$y_n\left(1 + \tfrac{h}{2} f_n\right) = y_0\left(1 - \tfrac{h}{2} f_0\right) + \frac{h}{2}(g_n + g_0).$$

This equation can also be obtained by integrating the differential equation with the trapezoidal rule.

(b) three point equation.

We try

$$y = A + Bx + Cx^2 + Dx^3 + Ex^4.$$

We get the equations

$$y_{-n} = A - Bh + Ch^2 - Dh^3 + Eh^4,$$
$$hy_{-n}' = \quad Bh - 2Ch^2 + 3Dh^3 - 4Eh^4,$$

$$y_0 = A ,$$
$$hy_0' = \quad Bh ,$$

$$y_n = A + Bh + Ch^2 + Dh^3 + Eh^4,$$
$$hy_n' = \quad Bh + 2Ch^2 + 3Dh^3 + 4Eh^4.$$

from which we have

$$\mu\delta y_0 = \Box h + \Box h^3,$$

and

$$h\delta^2 y_0' = \qquad 6\Box h^3.$$

Thus the difference equation is

$$\mu\delta y_0 - h y_0' = h/2\ \delta^2 y_0', \text{ or}$$

$$\tfrac{1}{2} y_h \left(1 + \frac{h f_h}{3}\right) + 2\,\frac{f_0 y_0}{3} + \tfrac{1}{2} y_{-h}\left(-1 + \frac{h f_{-h}}{3}\right) = \frac{h}{6}\left(g_h + 4 g_0 + g_{-h}\right).$$

This equation can also be obtained by integrating the differential equation by Simpson's rule.

(2) Second order equation (no first derivative)

$$y'' + f(x)\, y = g(x).$$

three point equation.

We take $y = A + Bx + Cx^2 + Dx^3 + Ex^4$

We have

$$y_{-h} = A - Bh + Ch^2 - Dh^3 + Eh^4,$$

$$h^2 y''_{-h} = \qquad 2Ch^2 - 6Dh^3 + 12Eh^4,$$

$$y_0 = A,$$

$$h^2 y_0'' = \qquad 2Ch^2,$$

$$y_h = A + Bh + Ch^2 + Dh^3 + Eh^4,$$

$$h^2 y_h'' = \qquad 2Ch^2 + 6Dh^3 + 12Eh^4.$$

Thus the difference equation is

$$\delta^2 y_0 - h^2 y_0'' = \frac{h^2}{12}\delta^2 y_0'',$$

or

$$y_h\left(1 + \frac{h^2 f_h}{12}\right) - y_0\left(2 - \frac{5h^2 f_0}{6}\right) + y_{-h}\left(1 + \frac{h^2 f_{-h}}{12}\right) = h^2\left(\frac{g_h}{12} + \frac{5 g_0}{6} + \frac{g_{-h}}{12}\right).$$

This is the equation derived in section (A). Note that it is not possible to obtain an interpolation polynomial of degree 5 from this data, and that the difference equation expresses a relation between differences and derivatives which is satisfied identically by polynomials of degree ≤ 5. The interpolating polynomial is

$$y = y_0 + x h^{-1}\mu\delta\left(y_0 - \frac{h^2}{6} y_0''\right) + \frac{x^2}{2} y_0'' + \frac{x^3}{6} h^{-1}\mu\delta y_0'' + \frac{x^4}{24} h^{-2}\delta^2 y_0'' \qquad \text{(B.1.1)}$$

(3) Calculation of the usual finite difference equations.

Let the differential equation be

$$y'' + p(x)y' + q(x)y = r(x).$$

We will assume a quadratic interpolating polynomial

$$y = A + Bx + Cx^2$$

We get the correct degree of overspecification by taking the values of y at $x = -h, 0, h$ and using the differential equation at $x = 0$. The equations are

$$y_{-h} = y_0 - Bh + Ch^2,$$

$$y_h = y_0 + Bh + Ch^2,$$

and $$r_0 = q_0 y_0 + p_0 B + 2C.$$

We have $B = h^{-1}\mu\delta y_0$, $C = \frac{1}{2} h^{-2}\delta^2 y_0$,

and the difference equation is

$$\left[\delta^2 + p_0 h\mu\delta + h^2 q_0\right] y_0 = h^2 r_0 \qquad \text{(B.1.2)}$$

In general we get the standard finite difference formulae by assuming an interpolating polynomial having the same order as the differential equation. We get the correct degree of overdetermination by using the values

of y at the ordinate points plus the differential equation at the point on which the interpolation is centred.

(4) We can use the following approach to increase the accuracy of the difference equation without increasing its order. The simplest case is the first order equation

$$y' + f y = g .$$

Let us consider the conditions

$$\begin{cases} y \text{ \& } y' & \text{at} \quad x = 0 \\ y \text{ \& } y' & \text{at} \quad x = h \\ \text{differential equation} & \text{at} \quad x = h/2 \end{cases}$$

These five conditions give the correct degree of overdetermination if we choose a cubic interpolating polynomial, and it is convenient to centre this polynomial on $h/2$.

Thus $y = A + B(x-h/2) + C(x-h/2)^2 + D(x-h/2)^3$.

We have

$$y_0 = A - Bh/2 + Ch^2/4 - Dh^3/8,$$

$$y_h = A + Bh/2 + Ch^2/4 + Dh^3/8,$$

$$y_0' = B - 2Ch/2 + 3Dh^2/4,$$

$$y_h' = B + 2Ch/2 + 3Dh^2/4,$$

$$g_{h/2} = f_{h/2} A + B .$$

Solving the first four equations for A and B gives

$$A = \frac{y_0 + y_h}{2} - h/8 (y_h' - y_0'),$$

$$B = 3h^{-1}(y_h - y_0) - (y_0' + y_h').$$

Thus the desired difference equation is

$$3h^{-1}(y_n - y_0) - (y_0' + y_n')$$
$$+ \tfrac{1}{2} f_{h/2} \{(y_0 + y_n) - h/4 (y_n' - y_0')\} = g_{h/2}.$$

Eliminating the first derivatives using the differential equation and grouping terms gives

$$y_n \{3h^{-1} + f_n + \tfrac{1}{2} f_{h/2} + h/8 f_{h/2} f_n\}$$
$$+ y_0 \{-3h^{-1} + f_0 + \tfrac{1}{2} f_{h/2} - h/8 f_{h/2} f_0\}$$
$$= g_0 + g_{h/2} + g_n + h/8 f_{h/2} (g_n - g_0).$$

We can compare this with the usual equation given by tropezoidal rule integration for the equation

$$y' - y = 0, \quad y(0) = 1.$$

	T.R.	Our equation
$h=1$	$y(1) = 3.0$	$y(1) = 2.85$
$h=1/2$	$y(1) = 2.77^*$	$y(1) = 2.749$
$h=1/4$	$y(1) = 2.733$	$y(1) = 2.727$

(B.2) General procedures.

In all the previous examples the form of the differential equation was such as to permit the elimination to be carried out readily. In each case our procedure lead to a familiar difference equation. In the general case of an n^{th} order equation it would not be practical to attempt to calculate explicitly the form of the difference equation (for the general second order equation a tedious calculation leads to a result which is both clumsy and difficult to apply); but it is precisely in the general case that our approach is likely to prove most useful. Let us assume that the values $y_1, y_2, \cdots y_n$ are known, and that it is required to calculate y_{n+1}. The equations for the interpolating polynomial can be broken into two sets. The first $2n$ equations in each set are the conditions that the polynomial

takes the values $y_1, \cdots y_n$ and satisfy the differential equation at the ordinate points $x_1, \cdots x_n$. The last equation in one set expresses the condition that the differential equation be satisfied for $x = x_{n+1}$ while the last equation in the other set expresses the condition $y = y_{n+1}$, $x = x_{n+1}$. If we now triangularise the sets of equations we can apply the condition that the final row in each set must be equivalent up to a factor of proportionality. This condition allows us to calculate y_{n+1} .

In matrix notation we may write the sets of equations as

$$A_1 \underset{\sim}{x} = \underset{\sim}{v}^1,$$

$$\text{and } A_2 \underset{\sim}{x} = \underset{\sim}{v}^2.$$

From their manner of construction they must permit a decomposition of the form

$$A_1 \underset{\sim}{x} = \begin{bmatrix} L & 0 \\ \underset{\sim}{\theta}' & 1 \end{bmatrix} \begin{bmatrix} U & \underset{\sim}{\phi} \\ 0 & a_1 \end{bmatrix} \underset{\sim}{x} = \begin{bmatrix} \underset{\sim}{v} \\ b_1 \end{bmatrix},$$

$$\text{and } A_2 \underset{\sim}{x} = \begin{bmatrix} L & 0 \\ \underset{\sim}{\theta}' & 1 \end{bmatrix} \begin{bmatrix} U & \underset{\sim}{\phi} \\ 0 & a_2 \end{bmatrix} \underset{\sim}{x} = \begin{bmatrix} \underset{\sim}{v} \\ b_2 \end{bmatrix}.$$

Here L is a lower triangular matrix, U an upper triangular matrix - both of side $2n$. The vectors in the partition have length $2n$.

Carrying out the first stage of the usual procedure for solution we have

$$\begin{bmatrix} U & \underset{\sim}{\phi} \\ 0 & a_1 \end{bmatrix} \underset{\sim}{x} = \begin{bmatrix} L^{-1} \underset{\sim}{v} \\ b_1 - \underset{\sim}{\theta}' L^{-1} \underset{\sim}{v} \end{bmatrix},$$

and $$\begin{bmatrix} U & \underset{\sim}{\theta} \\ 0 & a_2 \end{bmatrix} \underset{\sim}{x} = \begin{bmatrix} \lambda^{-1} \underset{\sim}{V} \\ b_2 - \underset{\sim}{\theta}_2' \lambda^{-1} \underset{\sim}{V} \end{bmatrix}.$$

Using the equivalence of the final rows we must have

$$\frac{1}{a_1} \{ b_1 - \underset{\sim}{\theta}_1' \lambda^{-1} \underset{\sim}{V} \} = \frac{1}{a_2} \{ b_2 - \underset{\sim}{\theta}_2' \lambda^{-1} \underset{\sim}{V} \}.$$

If the equations have been arranged so that y_{n+1} corresponds to b_1 then the difference equation is

$$y_{n+1} = \frac{a_1}{a_2} \{ b_2 - \underset{\sim}{\theta}_2' \lambda^{-1} \underset{\sim}{V} \} + \underset{\sim}{\theta}_1' \lambda^{-1} \underset{\sim}{V} \qquad \text{(B.2.1)}$$

The computation can also be modified without difficulty to compute the difference equation explicitly. To do this we arrange that the first elements of $\underset{\sim}{V}$ are $y_1, y_2, \cdots y_n$ and then calculate

$$\left(\underset{\sim}{\theta}_1 - \frac{a_1}{a_2} \underset{\sim}{\theta}_2 \right)' \lambda^{-1} = \underset{\sim}{\psi}'.$$

We now have, from (B.2.1), that

$$y_{n+1} - \psi_n y_n - \cdots - \psi_1 y_1 = \frac{a_1}{a_2} b_2 + \sum_{r=n+1}^{2n} \psi_r V_r \qquad (B.2.2).$$

It would seem that (B.2.1) is most suitable for the solution of initial value problems. If it is desired to use direct methods (non iterative methods) in solving boundary value problems then equation (B.2.2) is appropriate.

We can carry through the above calculations very easily in the case of the first order equation

$$\frac{dy}{dx} + f(x) y = g(x).$$

The sets of equations are (compare §8.1 example 1.a)

$$y_0 = A,$$
$$g_0 = f_0 A + B,$$
$$y_n = A + Bh + Ch^2,$$

$$\Phi \quad y_0 = A,$$
$$g_0 = f_0 A + B,$$
$$g_n = f_n A + B(hf_n + 1) + C(h^2 f_n + 2h).$$

We have

$$L = \begin{bmatrix} 1 & 0 \\ f_0 & 1 \end{bmatrix}, \quad L^{-1} = \begin{bmatrix} 1 & 0 \\ -f_0 & 1 \end{bmatrix},$$

$$\underset{\sim}{Q}_1 = \begin{bmatrix} 1 \\ h \end{bmatrix}, \quad \underset{\sim}{Q}_2 = \begin{bmatrix} f_n \\ hf_n + 1 \end{bmatrix}, \quad a_1 = h^2, \quad a_2 = h^2 f_n + 2h,$$

$$b_2 = g_n,$$

$$\Phi \quad \underset{\sim}{Q}_1 - a_1/a_2 \, \underset{\sim}{Q}_2 = \begin{bmatrix} 1 \\ h \end{bmatrix} - \frac{h^2}{h^2 f_n + 2h} \begin{bmatrix} f_n \\ hf_n + 1 \end{bmatrix},$$

$$= \frac{1}{h^2 f_n + 2h} \begin{bmatrix} 2h \\ h^2 \end{bmatrix}.$$

Thus $\Psi_1 = \dfrac{2h - h^2 f_0}{h^2 f_n + 2h}$, $\Psi_2 = \dfrac{h^2}{h^2 f_n + 2h}$,

and the difference equation is

$$y_n \left(1 + \frac{h f_n}{2}\right) = y_0 \left(1 - \frac{h f_0}{2}\right) + \frac{h}{2}(g_n + g_0)$$

The feature of our method which would seem to make it superior to that discussed for example by Kopal [2] and by Collatz [4] (there are very close similarities between the two approaches) is that we are lead <u>even in the most general case</u> to a straightforward and easily programmed procedure for computing the difference equation. However, we do not get an expression for the truncation error in our equation although we can be reasonably sure of its order of magnitude.

Obviously it is easier to use the standard finite difference equations than to apply our method. However, the additional complexity is counterbalanced by the greater accuracy of our equations; and the accuracy can be expected to increase with the order of the differential equation. This is not difficult to see for the standard equations can be deduced using a polynomial of degree equal to the order of the differential equation, while our method employs a polynomial of degree twice the order of the differential equation. Thus we would expect in general that the error in our equation would be $O(h^n)$ times smaller than the error in the standard equation when approximating to an n^{th} order differential equation.

We may note that the methods of this section are not restricted to differential equations and would certainly be applicable to the numerical solution of integral equations. In this case the same set of data must not be applied to determine the difference equations associated with two distinct ordinate points. This would seem to be achieved most easily by dropping systematically one of the conditions for each ordinate point. This method should work for kernels which are integrable although singular (in contrast to the Gaussian quadrature method which it should at least approach in accuracy).

(B.3) Boundary conditions.

To fit the boundary conditions on a particular problem we will in general need expressions containing derivatives. These can be readily derived using the general approach of this section.

For example, consider the equation

$$y'' + f(x)\,y = g(x)$$

We can use the conditions y, y' and the differential equation at the boundary point, and y, and the differential equation at the adjacent point. To these five conditions we fit a cubic polynomial. We get

$$y_h = y_0 + y_0' h + \tfrac{1}{2} y_0'' h^2 + \Delta h^3,$$

and $$y_h'' = y_0'' + 6\Delta h.$$

Thus the condition is

$$(y_h - y_0) - y_0' h - \tfrac{1}{2} y_0'' h^2 = \frac{h^2}{6}(y_h'' - y_0'')$$

that is

$$h y_0' = \Delta y_0 - \frac{h^2}{2} y_0'' - \frac{h^2}{6}\Delta y_0'' \qquad \text{(B.3.1)}.$$

A more symmetric procedure is to proceed as for the usual three point difference equation (example (2), (B.1)) but using the first derivative rather than the function value as one condition at the mid point. We get

$$y_{-h} = A - y_0' h + \tfrac{1}{2} y_0'' h^2 - \Delta h^3 + E h^4,$$

$$y_{-h}'' = y_0'' - 6\Delta h + 12 E h^2,$$

$$y_h = A + y_0' h + \tfrac{1}{2} y_0'' h^2 + \Delta h^3 + E h^4,$$

and $$y_h'' = y_0'' + 6\Delta h + 12 E h^2.$$

Thus we have

$$\mu\delta y_0 = \Delta h^3 + h^* y_0',$$

and $$\mu\delta y_0'' = 6\Delta h,$$

whence the difference equation is

$$h y_0' = \mu\delta y_0 - \frac{h^2}{6}\mu\delta y_0'' \qquad \text{(B.3.2)}$$

This expression contains the unknown pivotal value y_{-h} ; but this can be eliminated by combining this equation with the difference equation

$$\delta^2 y_0 - h^2 y_0'' = \frac{h^2}{12} \delta^2 y_0''$$

which also holds for these points.

As another example, consider the differential equation

$$\frac{d^2y}{dx^2} + \frac{1}{x}\frac{dy}{dx} + k^2 y = 0$$

which has a singular point at $x=0$. If we impose the conditions that y be finite at $x=0$, and $y=0$ at $x=1$ then the values of k for which a solution is possible are the zeros of the J_0 Bessel function. Instead of the condition y finite we can impose the condition $y'=0$ at $x=0$.

The boundary condition at the singular point can be conveniently dealt with by fitting a quadratic to the conditions y_0', y_h, y_{2h} and the differential equation at $x=h$. We get the equations

$$y_0' = B - 2Ch,$$
$$0 = k^2 y_h + \frac{1}{h} B + 2C,$$
$$y_{2h} = y_h + Bh + Ch^2.$$

Some simplification gives

$$y_0' - h k^2 y_h = 2B,$$

and $$2(y_{2h} - y_h) + h^2 k^2 y_h = Bh.$$

Thus

$$h(y_0' + h k^2 y_h) = 4(y_{2h} - y_h) + 2h^2 k^2 y_h,$$

or

$$h y_0' = 4(y_{2h} - y_h) + 3h^2 k^2 y_h.$$

We have used this condition in conjunction with the standard finite difference equation

$$\left[\delta^2 + \frac{h}{x_i} \mu\delta + h^2 k^2 \right] y_i = 0$$

to calculate the first few approximations to the first root of J_0 (exact value $k = 2{\cdot}405$). These are

h =	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$
k =	$2{\cdot}315$	$2{\cdot}345$	$2{\cdot}382$

(C.1) The third of our methods of constructing the approximate difference equation is based on the fact that every solution of a linear ordinary differential equation is also the solution of a certain linear difference equation of the same order. There are two stages to the argument which we will carry through for second order differential equations. These are

(a) construction of the exact difference equation

and (b) approximation to this exact equation.

Let $u(x)$ and $v(x)$ form a fundamental set of solutions for the equation

$$L_2(y) = \frac{d^2y}{dx^2} + a(x)\frac{dy}{dx} + b(x)y = 0 .$$

If the difference equation is

$$A_{i-1} y_{i-1} + A_i y_i + A_{i+1} y_{i+1} = 0$$

then, in particular, it must hold for $y = u$, and $y = v$.

We have

$$A_{i-1}\,U_{i-1} + A_i U_i + A_{i+1} U_{i+1} = 0,$$

and

$$A_{i-1}\,v_{i-1} + A_i v_i + A_{i+1} v_{i+1} = 0.$$

Thus the difference equation is

$$\begin{vmatrix} U_i & U_{i+1} \\ v_i & v_{i+1} \end{vmatrix} y_{i-1} - \begin{vmatrix} U_{i-1} & U_{i+1} \\ v_{i-1} & v_{i+1} \end{vmatrix} y_i + \begin{vmatrix} U_{i-1} & U_i \\ v_{i-1} & v_i \end{vmatrix} y_{i+1} = 0$$

In particular if we choose U and v such that

$$\begin{aligned} U_{i-1} &= v_{i+1} = 0, \\ U_i &= v_i = 1 \end{aligned} \qquad \text{(C.1.1)}$$

then the difference equation becomes

$$U_{i+1}\,y_{i-1} - U_{i+1} v_{i-1} y_{i-1} + v_{i-1} y_{i+1} = 0 \qquad \text{(C.1.2)}$$

In the case of the inhomogeneous equation $L_2(y) = f(x)$ we may write down a particular integral using the method of variation of parameters. This is

$$y(x) = -\int^{x} f(t)\, \frac{U(x)\,v(t) - U(t)\,v(x)}{W(t)}\, dt$$

where $W(t)$ denotes the Wronskian of U and v.

Substituting in the difference expression we have

$$A_{i-1}\,y_{i-1} + A_i y_i + A_{i+1} y_{i+1} = -A_{i-1} \int_{x_{i-1}}^{x_i} f\, \frac{U_{i-1} v - U v_{i-1}}{W}\, dt$$

$$- A_i \int_{x_i}^{x_{i+1}} f\, \frac{U_i v - U v_i}{W}\, dt - A_{i+1} \int_{x_{i+1}}^{x} f\, \frac{U_{i+1} v - U v_{i+1}}{W}\, dt.$$

If we now use the fact that $U(x)$ and $v(x)$ satisfy (C.1.1) and (C.1.2) we see that the right hand side vanishes for $t \le x_{i-1}$, and we may write it as

$$- \int_{x_{i-1}}^{x_i} f \left[\frac{v(t)}{w} (A_i + v_{i+1} A_{i+1}) - A_i \frac{v(t)}{w} \right] dt$$

$$- \int_{x_i}^{x_{i+1}} f \, A_{i+1} v_{i+1} \frac{v(t)}{w} \, dt .$$

We have $A_i = - v_{i+1} v_{i-1}$, and $A_{i+1} = v_{i-1}$ so that the difference equation finally becomes

$$v_{i+1} y_{i-1} - v_{i+1} v_{i-1} y_i + v_{i-1} y_{i+1}$$

$$= v_{i+1} v_{i-1} \left\{ \int_{x_{i-1}}^{x_i} f(t) \frac{v(t)}{w} dt + \int_{x_i}^{x_{i+1}} f(t) \frac{v(t)}{w} dt \right\} \qquad \text{(C.1.3)} .$$

We have based this derivation on elementary considerations. An alternative approach using distributions has been given by Joseph Hersch [5]. He defines the distribution $\overline{T}(x)$ as

$$\overline{T} = 0 \qquad |x - x_i| \geq h ,$$

$$\overline{T} = \overline{v}(x) \qquad x_{i-1} \leq x \leq x_i ,$$

$$\overline{T} = \overline{w}(x) \qquad x_i \leq x \leq x_{i+1} ,$$

where $\overline{v}$ and $\overline{w}$ are solutions of the adjoint equation satisfying the conditions (C.1.1).

Green's theorem now gives us

$$(L_2(y), T) = (\overline{L_2}(T), y) = (T, f) .$$

As T has discontinuous first derivatives $\overline{L_2}(T)$ ($\overline{L_2}$ is the adjoint operator to L_2) involves δ functions, and the integral then gives us a difference equation.

The adjoint operator is

$$\overline{L}_2 = \frac{d^2}{dx^2} - \frac{d}{dx}(a\cdot) + b .$$

We have

$$\frac{dT}{dx} = \bar{v}'(x)\, H(x-x_i)\, H(x_i - x) + \bar{v}'(x)\, H(x-x_i)\, H(x_{i+1} - x)$$

where $H(x)$ is the Heavyside unit step function.

Thus
$$\frac{d^2T}{dx^2} = \bar{v}''(x)\, H(x-x_{i-1})\, H(x_i - x) + \bar{v}''\, H(x-x_i)\, H(x_{i+1}-x) + \bar{v}'(x)\left[\delta(x-x_{i-1}) - \delta(x_i - x)\right] + \bar{v}'(x)\left[\delta(x-x_i) - \delta(x_{i+1}-x)\right],$$

and the difference equation is

$$\bar{v}'_{i-1}\, y_{i-1} + (\bar{v}'_i - \bar{v}'_i)\, y_i - \bar{v}'_{i+1}\, y_{i+1} = \int_{x_{i-1}}^{x_{i+1}} T f \, dx .$$

It is not difficult to show that this equation is equivalent to (C.1.3). We have

$$\overline{v(t)} = w_i \frac{v(t)}{w(t)},$$

and
$$\overline{w(t)} = w_i \frac{w(t)}{w(t)} .$$

From (C.1.1)

Thus
$$\bar{v}'_{i-1} = -\frac{\overline{w}_{i-1}}{\overline{v}_{i-1}} = -\frac{\overline{w}_{i-1}}{w_i}\,\frac{w_{i-1}}{v_{i-1}},$$

and
$$\bar{v}'_{i+1} = \frac{\overline{w}_{i+1}}{\overline{v}_{i+1}} = \frac{\overline{w}_{i+1}}{w_i}\,\frac{w_{i+1}}{v_{i+1}} .$$

Now $$\overline{w} = \begin{vmatrix} \overline{v} & \overline{v} \\ \overline{v}' & \overline{v}' \end{vmatrix} = w_i^2 \begin{vmatrix} \frac{v}{w} & \frac{v}{w} \\ \frac{v'}{w} - \frac{vw'}{w^2} & \frac{v'}{w} - \frac{vw'}{w^2} \end{vmatrix}$$

$$= \frac{w_i^2}{w^2} w = \frac{w_i^2}{w},$$

and $$\overline{v}_i - \overline{v}'_i = \overline{w}_i = w_i .$$

Thus the difference equation becomes

$$- \frac{y_{i-1}}{v_{i-1}} + y_i - \frac{y_{i+1}}{v_{i+1}} = \frac{1}{w_i} \int_{x_{i-1}}^{x_{i+1}} T f \, dt$$

which is (C.1.3).

(C.2) Boundary conditions.

In order to satisfy the boundary conditions it is necessary to have equations involving derivatives of the unknown function. In the homogeneous case such a relation is most easily derived by considering the Wronskian of the differential equation. We set

$$W = \begin{vmatrix} y(x) & v(x) \\ y'(x) & v'(x) \end{vmatrix}$$

then

$$W_{i+1} = e^{-\int_{x_i}^{x_{i+1}} a(t)\,dt} W_i ,$$

and we have (setting $v_i = 1$, $v_{i+1} = 0$)

$$y_i v_i' - y_i' = y_{i+1} v_{i+1}' e^{\int_{x_i}^{x_{i+1}} a(t)\,dt}$$

By considering a particular integral of the inhomogeneous equation we get on the right hand side

$$\int_{x_i}^{x_{i+1}} f(t)\, v'_{i+1}\, e^{\int_{x_i}^{x_{i+1}} a(s)\,ds}\, \frac{v_{i+1}\, v(t)}{W(t)}\, dt$$

where $v(x)$ can be any solution of the homogeneous equation independent of v and W refers to the Wronskian of v and v .

Introducing $\bar{v}$ as in (C.1) this reduces to

$$\int_{x_i}^{x_{i+1}} f(t)\, \bar{v}(t)\, dt$$

The left hand side can also be written in terms of $\bar{v}$. We consider the relation governing the Wronskian of the homogeneous equation. This is

$$\begin{vmatrix} y_{i+1} & 0 \\ y'_{i+1} & \dfrac{W_i\, \bar{v}'_{i+1}}{W_{i+1}} \end{vmatrix} = \begin{vmatrix} y_i & 1 \\ \bar{y}'_i & \bar{v}'_i - a_i \end{vmatrix} e^{-\int_{x_i}^{x_{i+1}} a(t)\,dt} .$$

It is easily seen to reduce to

$$y_{i+1}\, \bar{v}'_{i+1} = y_i (\bar{v}'_i - a_i) - y'_i .$$

The boundary conditions can also be obtained by using $T = \bar{v}(x) H(x - x_i)$ as a distribution ($T = 0,\ x \geq x_{i+1}$) in Green's theorem.

We have

$$\frac{dT}{dx} = \bar{v}'(x) H(x - x_i) H(x_{i+1} - x) + \bar{v}(x) \delta(x - x_i),$$

and

$$\frac{d^2T}{dx^2} = \bar{v}''(x) H(x - x_i) H(x_{i+1} - x) + 2\bar{v}'(x) \delta(x - x_i) - \bar{v}'(x) \delta(x_{i+1} - x) + v(x) \delta'(x - x_i)$$

Thus we have

$$\overline{L_2(T)} = \bar{v}(x)\,\delta'(x-x_i) + \bar{v}'(x)\,(2\delta(x-x_i) - \delta(x_{i+1}-x)) - a\,\bar{v}(x)\,\delta(x-x_i)\,;\ \text{or}$$

$$(\overline{L_2(T)}, y) = 0 \quad (\text{or } (T, t))$$

$$= -\bar{v}_i y_i' - \bar{v}_i' y_i + 2\bar{v}_i' y_i - \bar{v}_{i+1} y_{i+1} - a_i \bar{v}_i y_i,$$

$$= y_i(\bar{v}_i' - a_i) - y_i' - \bar{v}_{i+1} y_{i+1} \qquad \text{(C.2.1)}$$

as before.

(C.3) Approximations based on the exact equations.

We will now consider some approximations based on exact difference equations to the differential equation

$$\frac{d^2y}{dx^2} + g(x)\,y = 0$$

If we take U and V as fundamental solutions associated with the operator $\frac{d^2}{dx^2}$ then

$$\left.\begin{aligned} U(x) &= \frac{h+x}{h}, \\ V(x) &= \frac{h-x}{h}, \end{aligned}\right\} \text{ & } W = -\frac{2}{h}.$$

Using (C.1.3) we are lead to the equation

$$2y_{-1} - 4y_0 + 2y_1 = -2h \int_{-h}^{h} T\,g(x)\,y\,dx$$

whence $$\delta^2 y_0 = -h \int_{-h}^{h} T\,g(x)\,y\,dx\,. \qquad \text{(C.3.1)}$$

By Taylor's theorem with integral form of remainder

$$gy = (gy)_{x=0} + x\frac{d(gy)_0}{dx} + \int_0^x (x-t)\,\frac{d^2(gy)}{dt^2}\,dt.$$

The result of inserting this expression for (gy) in (C.3.1) is

$$\delta^2 y_0 = -h^2 (gy)_0 - h\int_{-h}^{h} T\left[\int_0^x (x-t)\frac{d^2(gy)}{dt^2}\,dt\right]dx \qquad (C.3.2)$$

The term $$-h\int_{-h}^{h} T\left[\int_0^x (x-t)\frac{d^2(gy)}{dt^2}\,dt\right]dx$$

provides an expression for the truncation error in the standard finite difference approximation.

The best possible difference equation we can obtain (the one using the maximum amount of information available) is found by substituting for y the interpolation polynomial (B.1.1) and then carrying out the integrations involved in $$\int_{-h}^{h} T\, g(x)\, y\, dx$$

The truncation error in this process is $O(h)$ smaller than the truncation error which results when $gy = -y''$ is replaced by the interpolating polynomial

$$y'' = y_0'' + x h^{-1}\mu\delta y_0'' + \frac{x^2}{2} h^{-2}\delta^2 y_0''.$$

This replacement leads to the familiar equation (A.1).

The reason for the $O(h)$ difference is that, because T is an even function, odd powers of x when integrated with T vanish in the second case but not, in general, in the first.

An important application of these ideas is to the construction of an integral expression for the truncation error in equation (A.1).

We begin by noting that this equation can be deduced by the methods of section B (see example 2), and that the resulting interpolation polynomial

(B.1.1) satisfies the difference equation identically. If $Y(x)$ is this polynomial then, by differentiating it twice, we have

$$Y'' = -g_0 Y_0 - x h^{-1} \mu\delta(g_0 Y_0) - \frac{x^2}{2} h^{-2} \delta^2 (g_0 Y_0) .$$

To compare this with

$$\frac{d^2 y}{dx^2} = -g(x) y$$

we expand gy in the form

$$gy = (gy)_0 + x h^{-1} \mu\delta(gy)_0 + \frac{x^2}{2} h^{-2} \delta^2 (gy)_0 + r(x).$$

We have, using Taylor's theorem with integral remainder,

$$y_1 - y_{-1} = 2h y_0' + \frac{1}{2!} \int_{-h}^{h} T_3 y^{3'} dt$$

where $T_3 = \begin{cases} (h+t)^2, & t<0, \\ (h-t)^2, & t>0, \end{cases}$;

and $$y_1 - 2y_0 + y_{-1} = h^2 y_0'' + \frac{1}{3!} \int_{-h}^{h} T_4 y^{4'} dt$$

where $T_4 = \begin{cases} (h+t)^3, & t<0, \\ (h-t)^3, & t>0, \end{cases}$.

Thus the differential equation may be written

$$y'' = -(gy)_0 - x h^{-1} \mu\delta(gy)_0 - \frac{x^2}{2} h^{-2} \delta^2 (gy)_0$$
$$- \frac{x^3}{6} (gy)_0^{3'} - \frac{1}{6} \int_0^x (x-t)^3 (gy)^{4'} dt$$
$$+ \int_{-h}^{h} \left(\frac{x h^{-1}}{4} T_3 (gy)^{3'} + \frac{x^2 h^{-2}}{12} T_4 (gy)^{4'} \right) dt .$$

The exact difference equation can now be written down using (C.1.3). It is

$$\delta^2 y_0 = -h^2 (gy)_0 - \frac{h^2}{12}\delta^2 (gy)_0$$

$$- \frac{h}{6}\int_{-h}^{h} T\left\{\int_0^x (x-t)^3 (gy)^{4'} dt - \frac{x^2 h^{-2}}{2}\int_{-h}^{h} T_4 (gy)^{4'} dt\right\} dx \qquad (C.3.3)$$

as terms involving odd powers of x vanish when multiplied by T and integrated from $-h$ to h.

The desired expression for the truncation error is thus

$$R = -\frac{h}{6}\int_{-h}^{h} T\left\{\int_0^x (x-t)^3 (gy)^{4'} dt - \frac{x^2 h^{-2}}{2}\int_{-h}^{h} T_4 (gy)^{4'} dt\right\} dx \qquad (C.3.4)$$

Expanding $(gy)^{4'}$ by Taylor's theorem we readily derive the estimate

$R = \frac{h^6 (gy)^{4'}_0}{240} + O(h^8)$ and, by a simple extension of this argument, we get $R = \frac{h^6 (gy)^{4'}_M}{240}$ where the subscript M refers to the fact that there is some value of x in $(-h, h)$ for which equality holds.

We can also reduce the differential equation to a difference equation by writing it as

$$\frac{d^2 y}{dx^2} + g_i y = (g_i - g) y$$

whence

$$U_{i+1} y_{i-1} - U_{i+1} v_{i-1} y_i + v_{i-1} y_{i+1}$$
$$= -\frac{U_{i+1} v_{i-1}}{W_i}\int_{x_{i-1}}^{x_{i+1}} T (g_i - g) y \, dx$$

where

$$U(x) = \frac{\sin \sqrt{g_i}\,(x - x_{i-1})}{\sin \sqrt{g_i}\,(x_i - x_{i-1})},$$

and

$$v(x) = \frac{\sin \sqrt{g_i}\,(x_{i+1} - x)}{\sin \sqrt{g_i}\,(x_{i+1} - x_i)}.$$

If $x_r = r h$ then $\quad v_{i+1} = v_{i-1} = 2 \cos \sqrt{g_i}\, h$

$$w_i = \begin{vmatrix} v_{i-1} & 1 \\ \sqrt{g_i} \cot \sqrt{g_i}\, h & -\sqrt{g_i} \cot \sqrt{g_i}\, h \end{vmatrix} = -2 \sqrt{g_i} \cot \sqrt{g_i}\, h ,$$

and the equation becomes (Hersch [5])

$$y_{i-1} - 2 \cos \sqrt{g_i}\, h \; y_i + y_{i+1} = \frac{\sin \sqrt{g_i}\, h}{\sqrt{g_i}} \int_{x_{i-1}}^{x_{i+1}} T (g_i - g)\, y \, dx \qquad \text{(C.3.5)}.$$

Setting

$$\cos \sqrt{g_i}\, h = 1 - \frac{h^2 g_i}{2} + \frac{1}{6} \int_0^{h\sqrt{g_i}} (h\sqrt{g_i} - t)^3 \cos t \, dt$$

we get

$$\delta^2 y_i + h^2 g_i y_i = \frac{\sin \sqrt{g_i}\, h}{\sqrt{g_i}} \int_{x_{i-1}}^{x_{i+1}} T (g_i - g)\, y \, dx + \frac{1}{3!} \int_0^{h\sqrt{g_i}} (h\sqrt{g_i} - t)^3 \cos t \, dt \qquad \text{(C.3.6)}.$$

The right hand side provides an interesting expression for the truncation error. The important feature being the absence of derivatives in the integrals. Similar methods can be used to derive formulae for fitting the boundary conditions.

Thus, from the formula (C.2.1)

$$y_0' = y_0 (\bar{v}_0' - a_0) - \bar{v}_1' y_1 - (\bar{v}, f),$$

we have, setting

$$\frac{d^2 y}{dx^2} = - g(x)\, y ,$$

and

$$\bar{v}(x) = \frac{h - x}{h} ,$$

$$y_0' = \frac{1}{h} (y_1 - y_0) + \int_0^h \frac{h - x}{h} g\, y \, dx \qquad \text{(C.3.7)}.$$

Now, if $\bar{v}(x)$ makes with $\bar{v}(\bar{x})$ a pair of functions satisfying (C.1.1) then we must have

$$-y_0' = \bar{v}_{-1}' y_{-1} - y_0(\bar{v}_0' - a_0) - (\bar{v}, t)$$

as the result of adding this equation to (C.2.1) must be the difference equation for y.

Setting $\bar{v}(x) = \frac{h+x}{h}$ we have

$$y_0' = \frac{1}{h}(y_0 - y_{-1}) - \int_{-h}^{0} \frac{h+x}{h} g y \, dx \qquad \text{(C.3.8)}.$$

Adding equations (C.3.7) and (C.3.8) we have

$$y_0' = \frac{1}{2h}(y_{+1} - y_{-1}) + \int_{-h}^{h} V g y \, dx$$

where
$$\left.\begin{aligned} V &= \frac{h-x}{h} \quad , x > 0, \\ &= -\frac{h+x}{h} \quad , x < 0, \end{aligned}\right\} \qquad \text{(C.3.9)}.$$

Setting

$$\frac{d^2 y}{dx^2} + g_0 y = (g_0 - g) y,$$

$$\bar{v}(x) = \frac{\sin \sqrt{g_0}(h-x)}{\sin h \sqrt{g_0}},$$

& $\bar{v}(x) = \frac{\sin \sqrt{g_0}(h+x)}{\sin h \sqrt{g_0}}$,

we have

$$y_0' = \frac{\sqrt{g_0}}{\sin h \sqrt{g_0}} (y_1 - y_0 \cosh \sqrt{g_0})$$

$$- \int_0^h \frac{\sin \sqrt{g_0}(h-x)}{\sin h \sqrt{g_0}} (g_0 - g) \, dx,$$

$$y_0' = \frac{\sqrt{g_0}}{\sinh h\sqrt{g_0}}\,(y_0 \cosh h\sqrt{g_0} - y_{-1})$$

$$+ \int_{-h}^{0} \frac{\sinh \sqrt{g_0}\,(h+x)}{\sinh h\sqrt{g_0}}\,(g_0 - g)\,y\,dx,$$

and $$y_0' = \frac{\sqrt{g_0}}{2\sinh h\sqrt{g_0}}\,(y_1 - y_{-1}) - \int_{-h}^{h} V\,(g_0 - g)\,y\,dx$$

where $$\left.\begin{aligned} V &= \bar{v} \quad x \geq 0, \\ &= -\bar{U} \quad x < 0, \end{aligned}\right\}$$ (C.3.10).

Appendix: Some numerical applications.

Consider first the differential equation

$$y'' - xy = 1, \quad y(0) = y(1) = 0.$$

The solution of this using the standard approximation has been given by Kantorovich and Krylov [6] and is summarised in the following table.

	$-y$	
x	$h = \cdot 2$	exact
$\cdot 2$	0·0768	0·0768
$\cdot 4$	0·1143	0·1144
$\cdot 5$		0·1148
$\cdot 6$	0·1136	0·1138
$\cdot 8$	0·0756	0·0757

The exact values were obtained by summing the power series for y.

We have obtained approximate solutions to this differential equation using (A.1) with $h = 1/2$ and $h = 1/3$, and in both cases we used the interpolation polynomial (B.1.1) to fill in the values of y at $x = 0.2$ and $x = 0.8$, and in the second case also at $x = 0.5$.

The results are set out in the following table.

	$-y$	
x	$h = 1/2$	$h = 1/3$
0.2	0.07632	0.076812
1/3	——	0.106218
0.5	0.11851	0.118590 0.118769
2/3	——	0.105232
0.8	0.07632	0.075502

It is interesting to compare the approximation given by (A.1) with the approximation given by substituting (B.1.1) on the right hand side of (C.3.5) and then carrying out the required integrations.

We have applied both methods to the equation

$$\frac{d^2y}{dx^2} + 2\alpha y = 1 \; ; \quad y(0) = 0, \; y(1) = 1.$$

Using (A.1) we have

$h = 1/2$ $\qquad y_{1/2} = .441\ 860,$

$h = 1/4$ $\qquad \begin{cases} y_{1/4} = .193\ 706, \\ y_{1/2} = .442\ 561, \\ y_{3/4} = .724\ 699, \end{cases}$

h^4-extrapolation* $\qquad y_{1/2} = .442\ 608.$

Using the approximation based on (C.3.5) we have

$h = 1/2$ $\qquad y_{1/2} = .442\ 612.$

Compared with these approximations the standard difference formula is not nearly so satisfactory. In this case we have

$h = 1/2$ $\qquad y_{1/2} = .428\ 571,$

$h = 1/4$ $\qquad \begin{cases} y_{1/4} = .191\ 396, \\ y_{1/2} = .439\ 305, \\ y_{3/4} = .722\ 258, \end{cases}$

h^2-extrapolation* $\qquad y_{1/2} = .442\ 883.$

Approximations based on (C.3.5) and similar expressions are rather tedious to construct and, except for certain special cases, other methods are generally to be preferred even though this means working with smaller values of h to achieve comparable accuracy (the truncation error in using (C.3.5) and (B.1.1) is $O(h^2)$ smaller than that in using (A.1)).

However, it is not always true that (A.1) produces less accurate approximations. Consider the eigenvalue problem

$$\frac{d^2y}{dx^2} + \lambda^2 y = 0, \quad y(0) = y(1) = 0.$$

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* See Chapter (4) appendix (2)

The first few eigenvalues for this problem are Kopal [2]

$\lambda_1 = 18.956\ 265,$

$\lambda_2 = 81.886\ 585,$

$\lambda_3 = 189.240\ 936.$

Equation (A.1) gives us the approximations

$h = 1/2 \qquad \lambda_1 = 19.2,$

$h = 1/3 \qquad \begin{cases} \lambda_1 = 18.890, \\ \lambda_2 = 84.210. \end{cases}$

Equation (C.3.5) gives

$h = 1/2 \qquad \begin{cases} \lambda_1 = 19.704, \\ \lambda_2 = \text{———}, \\ \lambda_3 = 177.6. \end{cases}$

$h = 1/3 \qquad \begin{cases} \lambda_1 = 18.979, \\ \lambda_2 = 93.4, \\ \lambda_3 = \text{———}. \end{cases}$

We may note that (C.3.5) leads in the case of the eigenvalue problems, to a trancendental equation for the eigenvalues (hence the approximation to λ_3 in the case $h = 1/2$ above).

Chapter IV. Convergence of finite difference approximations

In this chapter we further analyse approximations based on the standard finite difference equation to second order differential equations in normal form.

We will write the ~~difference~~ differential equation as

$$\frac{d^2 y}{dx^2} + q(x)\, y = f(x) \qquad (1),$$

and the finite difference approximation as

$$\delta^2 y_i + h^2 q_i y_i = f_i \qquad (2).$$

We will approximate to the boundary conditions on equation (1) by making the substitution $h^{-1}\mu\delta$ for $\frac{d}{dx}$; and we will take $h = 1/n$.

A. Initial value (marching) problems

In an initial value problem all the data necessary to specify the solution is given at one point. We begin by considering some properties of the solutions of initial value problems for equation (2). As the equations are linear we see that the solution of any such problem can be readily obtained when we know the solutions to the problems

(a) $y_0 = 0$

$h^{-1}\mu\delta y_0 = 1 \quad (y_{-1} = y_1 - 2h)$, and

(b) $y_0 = 1$

$h^{-1}\mu\delta y_0 = 0 \quad (y_{-1} = y_1)$.

We will consider only problem (b) explicitly as the other case is similar, and the results and restrictions are identical in both cases.

Running the solution forward we have

$$y_1 = 1 - \frac{h^2}{2} q_0 + \frac{h^2}{2} f_0 ,$$

$$y_2 = 1 - h^2 q_0 - h^2 q_1 y_1 + h^2 f_0 + h^2 f_1 ,$$

$$y_3 = 1 - \frac{3h^2}{2} q_0 - 2h^2 q_1 y_1 - h^2 q_2 y_2 + \frac{3}{2} h^2 f_0 + 2h^2 f_1 + f_2 ,$$

. . . . . .

$$y_n = 1 - h^2 \left(\frac{n}{2} q_0 y_0 + (n-1) q_1 y_1 + \cdots + q_{n-1} y_{n-1} \right) + h^2 \left(\frac{n}{2} f_0 + (n-1) f_1 + \cdots + f_{n-1} \right) .$$

Putting $Q = \max |q(x)| , \quad 0 \le x \le 1 ,$

$F = \max |f(x)| , \quad 0 \le x \le 1 ,$

we have, using

$$\frac{n^2}{2} = \frac{n}{2} + (n-1) + \cdots + 2 + 1 ,$$

that

$$\max |y| \le 1 + \frac{Q}{2} \max |y| + \frac{F}{2} ,$$

and this inequality can be solved for $\max |y|$ provided $Q < 2$.

It gives

$$\max |y| \le \frac{1 + F/2}{1 - Q/2} \qquad (A.1) .$$

Thus the solution is bounded on $(0 \le x \le 1)$ provided $Q < 2$; and this condition can be relaxed if we are interested in the solution only on part of the interval $(0, 1)$. For example, if we consider $(0 \le x \le \frac{1}{2})$ then we have

$$y_{n/2} = 1 - h^2 \left(\frac{n}{4} q_0 y_0 + \left(\frac{n}{2} - 1 \right) q_1 y_1 + \cdots + q_{\frac{n}{2}-1} y_{\frac{n}{2}-1} \right) + h^2 \left(\frac{n}{4} f_0 + \left(\frac{n}{2} - 1 \right) f_1 + \cdots + f_{n/2-1} \right) ,$$

and $\max|y| \leq 1 + \frac{Q}{8}\max|y| + \frac{F}{8}$.

$\therefore \max|y| \leq \frac{1 + F/8}{1 - Q/8}$ provided $Q<8$.

The general case for finite Q is similar. We can obtain bounds on some finite interval $(0,a)$ where a depends on Q only; and we can then obtain bounds for the whole of $(0 \leq x \leq 1)$ in a finite number of steps by bounding an initial value problem at each step (as this problem can be reduced to the sum of a problem of type (a) and a problem of type (b)).

Finally, we see that the solution of (2) can be extended to any finite piece of the x axis and is there bounded independent of h provided only that $q(x)$ is bounded for this range of x .

We now show that if $q(x)$ and $f(x)$ are continuous then the solution of equation (2) tends to a definite limit function defined on all the rational points $(0 \leq x \leq 1)$ as we let $h \to 0$ by continually refining the mesh. We will assume $Q < 2$

We will let $\bar{y}(x)$ be the solution to (2) at the ordinate point x with $h = 1/n$, and let $\bar{\bar{y}}(x)$ be the value of the solution at this ordinate point with $h = 1/pn$. With this notation we have (considering the homogeneous equation)

$$\bar{y}(1) = 1 - h^2\left(\tfrac{n}{2}q_0\bar{y}(0) + (n-1)q_1\bar{y}(h) + \cdots + q_{n-1}\bar{y}(1-h)\right) \text{ and}$$

$$\bar{\bar{y}}(1) = 1 - \frac{h^2}{p^2}\left(\tfrac{pn}{2}q_0\bar{\bar{y}}(0) + (pn-1)q_{1/p}\bar{\bar{y}}\left(\tfrac{h}{p}\right) + \cdots + (pn-p)q_1\bar{\bar{y}}(h) + \cdots\cdots + 2q_{n-\frac{2}{p}}\bar{\bar{y}}\left(1-\tfrac{2h}{p}\right) + q_{n-\frac{1}{p}}\bar{\bar{y}}\left(1-\tfrac{h}{p}\right)\right)$$

$$= 1 - \frac{h^2}{p^2}\Big(\frac{p n}{2} q_0 + (p-1) n\, q_{1/p}\, \bar{\bar{y}}\left(\tfrac{h}{p}\right) + \cdots + n\, q_{1-\frac{1}{p}}\, \bar{\bar{y}}\left(h - \tfrac{h}{p}\right)$$

$$+ (n-1)\, q_{\frac{1}{p}}\, \bar{\bar{y}}\left(\tfrac{h}{p}\right) + 2(n-1)\, q_{\frac{2}{p}}\, \bar{\bar{y}}\left(\tfrac{2h}{p}\right) + \cdots + p(n-1)\, q_1\, \bar{\bar{y}}(h)$$

$$+ \cdots + (n-1)\, q_{2-\frac{1}{p}}\, \bar{\bar{y}}\left(2h - \tfrac{h}{p}\right)$$

$$+ \cdots\cdots +$$

$$q_{n-2+\frac{1}{p}}\, \bar{\bar{y}}\left(1 - 2h + \tfrac{h}{p}\right) + \cdots + p\, q_{n-1}\, \bar{\bar{y}}(1-h) + \cdots + q_{n-\frac{1}{p}}\, \bar{\bar{y}}\left(1 - \tfrac{h}{p}\right)\Big).$$

Now $p^2 = 1 + 2 + \cdots + (p-1) + p + (p-1) + \cdots + 2 + 1$

so that a typical term in $\bar{\bar{y}}(1) - \bar{y}(1)$ is (writing $n - j - \frac{p+i}{p}$

$= \alpha_{j,j+i}$)

$$\frac{n-j}{p^2}\Big\{ \left(q_{\alpha_{j,j-1}}\, \bar{\bar{y}}(\alpha_{j,j-1} h) - q_{n-j}\, \bar{y}((n-j)h) \right)$$

$$+ 2\left(q_{\alpha_{j,j-2}}\, \bar{\bar{y}}(\alpha_{j,j-2} h) - q_{n-j}\, \bar{y}((n-j)h) \right) + \cdots \Big\}$$

and the magnitude of this term is

$$\leq (n-j) \max_i \left| q_{\alpha_{j,j+i}}\, \bar{\bar{y}}(\alpha_{j,j+i} h) - q_{n-j}\, \bar{y}((n-j)h) \right|$$

$$\leq (n-j)\Big\{ Q \left| \bar{\bar{y}}((n-j)h) - \bar{y}((n-j)h) \right|$$

$$+ Q \max \left| \bar{\bar{y}}(\alpha_{j,j+i} h) - \bar{\bar{y}}((n-j)h) \right|$$

$$+ \max\left(|\bar{y}|\, |q_{\alpha_{j,j+i}} - q_{n-j}| \right)\Big\}.$$

We may note that the case of the inhomogeneous equation can also be dealt with if we add a term $(n-j) \max |f_{\alpha_{j,j+i}} - f_{n-j}|$ to this expression.

Now

$$\bar{\bar{y}}(1) - \bar{\bar{y}}(1-h) = -\frac{h^2}{p^2}\Big(\frac{p}{2} q_0\, \bar{\bar{y}}(0) + p\, q_{\frac{1}{p}}\, \bar{\bar{y}}\left(\tfrac{h}{p}\right) + \cdots$$

$$+ p\, q_{n-1-1/p}\, \bar{\bar{y}}\left(1 - h - \tfrac{h}{p}\right) + \cdots + q_{n-1/p}\, \bar{\bar{y}}(1 - h/p)$$

$$- \frac{p}{2} f_0 - p f_{1/p} - \cdots - p f_{n-1-1/p} - \overset{(p-1)}{\wedge} f_{n-1} \cdots - f_{n-1/p} \Big)$$

so that

$$|\bar{\bar{\eta}}(1) - \bar{\bar{\eta}}(1-h)| \leq \frac{h^2}{p^2}\left(n p^2 (Q \max|\bar{\bar{\eta}}| + F)\right),$$
$$\leq K/n \qquad (A.2)$$

where $K = Q\left(\frac{1+F/2}{1-Q/2}\right) + F = \frac{Q+F}{1-Q/2}$;

and this provides an upper bound for the magnitude of

$|\bar{\bar{\eta}}(\alpha h) - \bar{\bar{\eta}}((n-j)h)|$ whenever $|n-j-\alpha| \leq 1$.

Using this inequality we have (inhomogeneous equation)

$$\max|\bar{\eta} - \bar{\bar{\eta}}| \leq \tfrac{1}{2}\left\{Q \max|\bar{\eta} - \bar{\bar{\eta}}| + Q K/n + \varepsilon\left(\frac{1+F/2}{1-Q/2} + 1\right)\right\}$$

where we have chosen h such that

$$|q(x \pm h) - q(x)| < \varepsilon \quad , 0 \leq x \leq 1,$$

and $$|f(x \pm h) - f(x)| < \varepsilon \quad , 0 \leq x \leq 1 .$$

Thus $$\max|\bar{\eta} - \bar{\bar{\eta}}| \leq \frac{1}{n}\frac{QK}{1-Q/2} + \varepsilon\frac{2 + \frac{F}{2} - \frac{Q}{2}}{(1-Q/2)^2} \qquad (A.3)$$

(this inequality applying at the ordinate points of the $h = 1/n$ mesh). As ε is arbitrary, and as n can have any value greater than a certain minimum depending on ε we see that the right hand side of the above inequality can be made as small as we wish. This demonstrates the convergence of the solutions obtained by refining the original $(h = 1/n)$ mesh.

To show that the limiting solution is unique we have to show that it is independent of the mesh on which the subdivisions are based. To do this we consider a second mesh $(h = 1/m \; , \; m > n)$ which cannot be obtained by subdividing the original mesh. The solution for these two meshes cannot

be directly compared. However, they have the common mesh $h = 1/mn$ so that we can apply (A.3) twice and we have (at the common mesh points which always include $x = 1$) that

$$\max |y_m - y_n| \leq \frac{QK}{1-Q/2}\left(\frac{1}{n}+\frac{1}{m}\right) + 2\varepsilon\,\frac{2+\frac{F}{2}-\frac{Q}{2}}{(1-Q/2)^2},$$

$$< 2\left[\frac{QK}{1-Q/2}\,\frac{1}{n} + \varepsilon\,\frac{2+F/2-Q/2}{(1-Q/2)^2}\right],$$

where y_m denotes the solution for the mesh $h = 1/m$ and y_n that for the mesh $1/n$. Thus we see that the solution values form Cauchy sequences at their common ordinate points and this guarantees the uniqueness of the limit solution.

We now note two further results which will be useful in what follows. The proof in each case is straightforward and will be omitted.

(1) The limiting solution to equation (2) corresponding to $h = 0$ can be defined at every point of the interval $(0 \leq x \leq 1)$ as a continuous function.

(2) If we replace the 1 on the right hand side of the boundary conditions (a) and (b) by λ then equation (1) becomes

$$\max |y| \leq \frac{|\lambda| + F/2}{1 - Q/2} \qquad \text{(A.1*)}$$

We have indicated that it is unnecessary to impose any condition on other than finiteness to ensure a bounded solution to (2) at $x = 1$ as $h \to 0$. We will now indicate this result by a method which does not require knowledge of bounds for Q .

From the equation

$$y_{i+1} = 2y_i - y_{i-1} - h^2 q_i y_i + h^2 f_i$$

we have

$$|\Delta y_i| \le |\Delta y_{i-1}| + h^2 Q |y_i| + h^2 F .$$

As $y_{n+1} = y_0 + \sum_{i=0}^{n} \Delta y_i$ we see that $|y_i| \le Y_i$

where Y_i satisfies the equation

$$\Delta Y_i = \Delta Y_{i-1} + h^2 Q Y_i + h^2 F$$

with the initial conditions $\begin{cases} Y_0 = |y_0| , \\ \Delta Y_0 = |\Delta y_0| . \end{cases}$

The equation

$$Y_{i+1} - (2 + h^2 Q) Y_i + Y_{i-1} = 0$$

has the general solution

$$Y_i = A \cosh i\beta + B \sinh i\beta$$

where $2 \cosh \beta = 2 + h^2 Q ,$

so the required solution to the inhomogeneous equation above is

$$Y_i = A \cosh i\beta + B \sinh i\beta - F/Q .$$

The initial conditions give

$$A = |y_0| + F/Q ,$$

$$Y_1 = |y_0| + |\Delta y_0| = (|y_0| + F/Q) \cosh \beta + B \sinh \beta - F/Q .$$

Thus $B = (|y_0| + F/Q) \dfrac{1 - \cosh \beta}{\sinh \beta} + \dfrac{|\Delta y_0|}{\sinh \beta} .$

Now $e^{\beta} = 1 + \dfrac{h^2 Q}{2} + \sqrt{h^2 Q + \dfrac{h^4 Q^2}{4}}$ so that

$$\beta = h\sqrt{Q} + O(h^3) \quad \text{for small values of } h .$$

Thus, for large values of n , we have

$$|y_n| \le (|y_0| + F/Q)\cosh(\sqrt{Q} + O(h^2))$$

$$+ \sinh(\sqrt{Q} + O(h^2))\left\{(|y_0| + \frac{F}{Q})\frac{-\frac{h^2Q}{2} + O(h^3)}{h\sqrt{Q} + O(h^2)} + \frac{|\Delta y_0|}{h\sqrt{Q} + O(h^2)}\right\},$$

and the limiting value of this inequality is as $n \to \infty$ and is

$$|y(1)| \le |y_0|\cosh\sqrt{Q} + |y_0'|\frac{\sinh\sqrt{Q}}{\sqrt{Q}} + \frac{F}{Q}(\cosh\sqrt{Q} - 1).$$

Let us now consider the solution of the problem

$$\begin{cases} \varphi(0) = A, \\ \frac{d\varphi(0)}{dx} = B, \\ d^2\varphi/dx^2 + q(x)\varphi = f(x). \end{cases}$$

This problem can be replaced by the exact difference expression (chapter (III))

$$\varphi_0 = A,$$

$$h^{-1}\mu\delta\varphi_0 = B + \int_{-h}^{h} V\varphi''\,dx$$

using (C.3.9), and

$$\delta^2\varphi_i + h^2 q_i\varphi_i = h^2 f_i + h\int_{x_i-h}^{x_i+h} T\left[\int_0^{x-x_i}(x-x_i-t)\frac{d^4\varphi}{dt^4}\,dt\right]dx$$

using (C.3.2).

The standard finite difference equation is

$$\begin{cases} y_0 = A, \\ h^{-1}\mu\delta y_0 = B, \\ \delta^2 y_i + h^2 q_i y_i = h^2 f_i. \end{cases}$$

Thus the difference $\varphi_i - y_i$ satisfies the difference equation

$$\varphi_0 - y_0 = \Delta y_0 = 0 ,$$

$$h^{-1}\mu\delta(\Delta y_0) = \int_{-h}^{h} V\varphi''\,dx ,$$

$$\delta^2(\Delta y_i) + h^2 q_i(\Delta y_i) = h\int_{x_i-h}^{x_i+h} T\Big[\int_0^{x-x_i}(x-x_i-t)\varphi^{IV}\,dt\Big]dx .$$

We have

$$|\lambda| = \Big|\int_{-h}^{h} V\varphi''\,dx\Big| \le h \max|\varphi''| ,$$

$$h^{-1}\int_{x_i-h}^{x_i+h} T\Big[\int_0^{x-x_i}(x-x_i-t)\varphi^{IV}\,dt\Big]dx \le \frac{h^2}{12}\max|\varphi^{IV}| = F .$$

Thus $|\Delta y_i| \le h\left[\max|\varphi''| + \frac{h}{24}\max|\varphi^{IV}|\right]B$

where B is some bound independent of h depending only on φ and the region in which the solution is desired.

$$\therefore \quad \lim_{(h\to 0)} |\Delta y_i| = 0 .$$

Thus the solution of the approximate difference equation tends pointwise to the solution of the differential equation (i.e. to point values) as $h \to 0$. We require $\varphi(x)$ to have a bounded fourth derivative.

Remark: If we integrate by parts $\int_{-h}^{h} V\varphi''dx$ we can derive the estimate $|\lambda| \le \frac{h^2}{6}\max|\varphi'''|$. Thus

$$|\Delta y_i| \le \frac{h^2}{6}\left[\max|\varphi'''| + \frac{1}{4}\max|\varphi^{IV}|\right]B ;$$

and the error tends to zero at least with h^2.

We can get a second bound for $|\Delta y_i|$ if we use equation (C.3.6) of chapter (III) to determine F which will here be of the form $M\varepsilon + Nh^2$

provided only that f and q are continuous. In this case we have

$$|\Delta y_i| \leq \{ h \max|\phi''| + \tfrac{1}{2}(M\varepsilon + Nh^2)\Phi \} B,$$

and the right hand side can be made arbitrarily small by choosing ε small enough.

To conclude this section we note that the results obtained here for the finite difference equation can be extended without difficulty to equation (A.1) of chapter (III). This equation is

$$\delta^2 y_i = h^2 y_0'' + \frac{h^2}{12}\delta^2 y_i''$$

which we can write

$$y_{i+1} = 2y_i - y_{i-1} + h^2 K_i(y)$$

Thus, proceeding as before, we have

$$\max|y| \leq 1 + \tfrac{1}{2}\max|K_i(y)|.$$

Now

$$K_i(y) = \tfrac{1}{12}(-q_{i-1}y_{i-1} - 10q_iy_i - q_{i+1}y_{i+1} + f_{i-1} + 10f_i + f_{i+1})$$

so that

$$\max|K_i(y)| \leq Q\max|y| + F.$$

Thus the bound (A.1) is valid for y in this case, and we can use expressions for the truncation error in this approximation to the differential equation to show its convergence as $h \to 0$ following the same line of argument as used for the standard difference equation. By this method we can show that provided equation (B.3.2) of chapter (III) is used in approximating to the derivatives in the boundary conditions then the error in the solution of (A.1) is at most $O(h^4)$ provided φ has bounded sixth derivatives.

B. Boundary value problems

In this section we will study approximations to the equation

$$\frac{d^2\varphi}{dx^2} - q(x)\,\varphi = f(x) \tag{B.1}$$

with the boundary conditions

$$\left.\begin{aligned} A_0\,\varphi(0) + B_0\,\frac{d\varphi(0)}{dx} &= C_0 \quad , \text{ or} \\ A_1\,\varphi(1) + B_1\,\frac{d\varphi(1)}{dx} &= C_1 \end{aligned}\right\} \tag{B.2}$$

by means of the finite difference equation

$$\delta^2 y_i - h^2 q(ih)\, y_i = h^2 f(ih), \quad i = 0, 1, \cdots, n, \tag{B.3}$$

with the boundary conditions

$$\left.\begin{aligned} A_0 h y_0 + B_0 \mu\delta y_0 &= h C_0 \quad , \text{ or} \\ A_1 h y_n + B_1 \mu\delta y_n &= h C_1 \end{aligned}\right\} \tag{B.4}$$

The finite difference system can be written as the matrix equation

$$A\,\underset{\sim}{y} = \underset{\sim}{f} \tag{B.5}$$

where

$$A = \begin{bmatrix} -2 - h^2 q_0 + 2h A_0/B_0 & 2 & & & \\ 1 & -2 - h^2 q_1 & 1 & & \\ & \cdots & \cdots & \cdots & \\ & & 2 & -2 - h^2 q_n - 2h A_1/B_1 \end{bmatrix}$$

and $\underset{\sim}{f}$ is the vector with components

$$f_0 = f(0) + 2h\,C_0/B_0,$$

$$f_i = f(ih), \quad i = 1, 2, \cdots, n-1,$$

and

$$f_n = f(nh) - 2h\,C_1/B_1.$$

(B.1) We now note some properties of the matrix A .

As it is tridiagonal, and as the off diagonal elements are all positive the principal minors of A form a Sturm sequence. Thus we have

Lemma 1. The eigenvalues of A are distinct. If the eigenvalues are placed in order from the least positive then the corresponding eigenvectors have $0, 1, 2, \cdots, n$ changes of sign respectively.

The first part is a consequence of the Sturm property, see for example reference [1] . To demonstrate the second part we show that the components (y_i) of the eigenvectors are proportional to the corresponding Sturm polynomials (P_i) . We can fix the scale by setting $y_0 = P_0 = 1$ (assuming the boundary condition is not $y_0 = 0$ - this case needs slightly different treatment). We then have

$$\begin{cases} y_0 = 1 \\ P_0 = 1 \end{cases},$$

$$\begin{cases} y_1 = \frac{1}{2}\left[2 + h^2 q_0 - h^2\mu - 2h A_0/B_0\right] y_0 \\ P_1 = \left[2 + h^2 q_0 - h^2\mu - 2h A_0/B_0\right] P_0 \end{cases},$$

$$\begin{cases} y_2 = \left[2 + h^2(q_1 - \mu)\right] y_1 - y_0 \\ P_2 = \left[2 + h^2(q_1 - \mu)\right] P_1 - 2P_0 \end{cases},$$

. . . . . .

$$\begin{cases} y_{i+1} = \left[2 + h^2(q_i - \mu)\right] y_i - y_{i-1} \\ P_{i+1} = \left[2 + h^2(q_i - \mu)\right] P_i - P_{i-1} \end{cases}.$$

Thus $P_i = 2 y_i$, $i > 0$ and the components of the eigenvector are strictly proportional to the corresponding Sturm polynomials $(i > 0)$.

We have

$$\text{Det}\,(A + h^2 \mu \underline{I}) = \left[2 + h^2 (q_n - \mu) + 2h \frac{A_1}{B_1} \right] P_n - 2 P_{n-1},$$

$$= - \{ P_{n-1} - 2P_n + P_{n+1} + h^2 (\mu - q_n) P_n - P_{n+1} + P_{n-1} - 2h A_1/B_1 P_n \},$$

$$\therefore \quad \text{Det}\,(A + h^2 \mu \underline{I}) = 2 B(y_n)$$

where $B(y_n) = (y_{n+1} - y_{n-1}) + 2h A_1/B_1 y_n$

is the difference representation of the terminal boundary condition. Thus we see that μ is an eigenvalue of A if and only if the solution of the initial value problem

$$y_0 = 1,$$

$$h A_0 y_0 + B_0 \mu \delta y_0 = 0,$$

$$\delta^2 y_i + h^2 (\mu - q_i) y_i = 0$$

satisfies the terminal boundary condition

$$h A_1 y_n + B_1 \mu \delta y_n = 0.$$

We will not here consider the boundary condition $y_0 = 0$ (it is actually simpler than the general case); and we note that in all other cases the matrix A is not symmetric. Thus A will have distinct right and left eigenvectors and these will be biorthogonal (we denote the right eigenvector by $\underset{\sim}{y}$ and the left by $\underset{\sim}{y}^*$). However, there is a particularly simple relation between y and y^*.

Lemma 2.

$$\underset{\sim}{y}^{*} = B\,\underset{\sim}{y}$$

where B is the diagonal matrix

$$\begin{bmatrix} 1/2 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1/2 \end{bmatrix}$$

This is readily shown by writing the eigenvalue problem as

$$\left[\bar{A} - Q + h^2 \mu B \right] \underset{\sim}{y} = 0$$

where

$$\bar{A} = \begin{bmatrix} -1 + hA_0/B_0 & 1 & & \\ 1 & -2 & 1 & \\ \cdots & \cdots & \cdots & \cdots \\ & & 1 & -1 - hA_1/B_1 \end{bmatrix}$$

is symmetric, and

$$Q = \begin{bmatrix} h^2 q_0/2 & & & \\ & h^2 q_1 & & \\ & & \ddots & \\ & & & h^2 q_{n/2} \end{bmatrix}$$

is diagonal. In this form the right and left eigenvectors are identical, and the orthogonality relation becomes (because of the weighting matrix B)

$$\underset{\sim}{y}_j' B \underset{\sim}{y}_i = 0 \,, \quad j \neq i \,.$$

Also $\bar{A} - Q = B A$

so that $y'(\bar{A} - Q) y = y' B A y = -h^2 \mu\, y' B y$.

$\therefore \quad y^* = B y$.

The case $Q = 0$ provides a useful comparison problem because here explicit answers can readily be obtained. We will write it as

$$\left[\bar{A} + h^2 \bar{\mu} B \right] \bar{y} = 0 .$$

We now prove the following results:

Lemma 3. $\bar{\mu}_p \leq \mu_p \leq \bar{\mu}_p + \max q_i \,, \; p = 0, 1, \cdots, n$

provided that $\min q_i \geq 0$ (this can always be arranged by altering μ by a constant).

In the proof of this result we will make use of the Rayleigh quotient formulae

(a) $$\mu_p = \min - h^{-2} \frac{y' [\bar{A} - Q] y}{y' B y}$$

subject to the constraints $y' B y_i = 0 \,, \; i = 0, 1, \cdots, p-1,$

and (b) $$\bar{\mu}_p = \min - h^{-2} \frac{y' \bar{A} y}{y' B y}$$

subject to the constraints $y' B \bar{y}_i = 0 \,, \; i = 0, 1, \cdots, p-1.$

We will also need the alternative characterisation of the eigenvalues in terms of the Rayleigh quotients (as for example in [2]). This states that

μ_p = maximum value { minimum values of the Rayleigh quotients subject to any p additional constraints } .

We will prove each half of the inequality separately.

(1) $\bar{\mu}_p \leq \mu_p$

We have

$$\mu_p \geq \min \; h^{-2} \; \frac{-\underset{\sim}{y}'[\bar{A}]\underset{\sim}{y} + \underset{\sim}{y}'[Q]\underset{\sim}{y}}{\underset{\sim}{y}'[B]\underset{\sim}{y}}$$

subject to the constraints $\underset{\sim}{y}'[B]\underset{\sim}{y}_i = 0 \;, \; i = 0, 1, \cdots, p-1 \;,$

$$\geq \min \; -h^{-2} \; \frac{\underset{\sim}{y}'[\bar{A}]\underset{\sim}{y}}{\underset{\sim}{y}'[B]\underset{\sim}{y}} \;,$$

as $$h^{-2} \; \frac{\underset{\sim}{y}'[Q]\underset{\sim}{y}}{\underset{\sim}{y}'[B]\underset{\sim}{y}} \geq 0 \;,$$

$\therefore \mu_p \geq \bar{\mu}_p.$

(2) $\mu_p \leq \bar{\mu}_p + \max q_i$

We have

$$\bar{\mu}_p \geq \min \; -h^{-2} \; \frac{\underset{\sim}{y}'\bar{A}\underset{\sim}{y}}{\underset{\sim}{y}'[B]\underset{\sim}{y}}$$

subject to the constraints $\underset{\sim}{y}'[B]\underset{\sim}{y}_i = 0 \;, \; i = 0, 1, \cdots, p-1.$

$$\therefore \bar{\mu}_p + \max q_i \geq \min \left\{ -h^{-2} \frac{\underset{\sim}{y}'\bar{A}\underset{\sim}{y}}{\underset{\sim}{y}'[B]\underset{\sim}{y}} \right\} + h^{-2} \frac{\underset{\sim}{y}'Q\underset{\sim}{y}}{\underset{\sim}{y}'[B]\underset{\sim}{y}} \;,$$

$$\geq \min \left\{ -h^{-2} \frac{\underset{\sim}{y}'[\bar{A} - Q]\underset{\sim}{y}}{\underset{\sim}{y}'[B]\underset{\sim}{y}} \right\} \;,$$

$$\geq \mu_p \;.$$

Lemma 4. $$4h^{-2}\sin^2\left(\frac{(p-1)\pi}{2n}\right) \leq \bar{\mu}_p \leq 4h^{-2}\sin^2\left(\frac{(p+1)\pi}{2n}\right)$$

provided that $\bar{\mu}_p \geq 0 \;.$

Here we make use of the fact that the difference equation

$$\{\delta^2 + h^2\mu\}\, y = 0$$

has the general solution

$$y = A \sin (kx + \varepsilon) ,$$

where

$$\mu = 4h^{-2} \sin^2 \frac{kh}{2} , \quad \text{and} \quad 0 \leq \varepsilon < \pi .$$

To prove the lemma we have only to establish the limits on k which permit $\bar{y}_p$ to have exactly P changes of sign on $0 \leq x \leq 1$.

Now the argument of y changes by exactly k on $[0,1]$. Therefore for y to change sign P times we must have

$$(P + 1)\pi \geq k + \varepsilon > P\pi$$

thus

$$(P + 1)\pi \geq k > (P - 1)\pi .$$

Provided $(P + 1) \leq n$, $\sin (\frac{P+1}{2n} \pi)$ is an increasing function of P so that the stated result now follows. Using this result and lemma 3 we have (provided $\mu_p \geq 0$)

$$(P + 1)^2 \pi^2 + \max q_i \geq \mu_p \geq 4(P - 1)^2 \pi^2 \qquad \text{(B.1.1).}$$

The methods adopted previously for bounding the solutions of initial value problems are not suitable for application to eigenvectors of arbitrarily large order as they depend on the maximum moduli of the coefficients in the difference equation and these tend to infinity as the eigenvalues tend to infinity. In this case it is again convenient to use the eigenvectors and eigenvalues of $\bar{A}$ to estimate those of A.

We can normalise both eigenvalue problems so that their difference equations satisfy initial conditions of the form

$$y_0 = 1 \ , \ \mu\delta y_0 = \lambda \ .$$

We will now have the difference between their solutions satisfying the difference equation

$$\{\delta^2 + h^2\bar{\mu}\}(y-\bar{y})_i = h^2(\bar{\mu}-\mu)y_i + h^2 q_i y_i \qquad (B\cdot I\cdot 2)$$

with the initial conditions

$$(y-\bar{y})_0 = 0 \ , \ \mu\delta(y-\bar{y})_0 = 0 \ .$$

Provided that $q(x)$ has been adjusted so that $\min(q(x)) \geq 0$, then lemma (3) tells us that the right hand side of (B . I . 2) has modulus $\leq h^2 q \max |y_i|$.

We first consider the solution of the equation

$$\{\delta^2 + h^2\bar{\mu}\}\varphi_i = h^2 F_i$$

by the method of variation of parameters . Thus we try a solution of the form $\varphi_i = a_i u_i + b_i v_i$ where u_i and v_i are independent solutions of the difference equation . We have

$$\Delta\varphi_i = a_{i+1}u_{i+1} - a_i u_i + b_{i+1}v_{i+1} - b_i v_i$$

$$= a_i \Delta u_i + b_i \Delta v_i + u_{i+1}\Delta a_i + v_{i+1}\Delta b_i \ .$$

We adjoin the condition

$$u_{i+1}\Delta a_i + v_{i+1}\Delta b_i = 0 \ .$$

Thus

$$\nabla\Delta\varphi_i = \delta^2\varphi_i = a_i\delta^2 u_i + b_i\delta^2 v_i + \nabla u_i \nabla a_i + \nabla v_i \nabla b_i \ ;$$

and

$$\{\delta^2 + h^2\bar{\mu}\}\varphi_i = h^2 F_i = \nabla u_i \nabla a_i + \nabla v_i \nabla b_i .$$

Thus we have the equations

$$u_i \nabla a_i + v_i \nabla b_i = 0 ,$$

$$\nabla u_i \nabla a_i + \nabla v_i \nabla b_i = h^2 F_i .$$

whence

$$\nabla a_i = \frac{\begin{vmatrix} 0 & v_i \\ h^2 F_i & \nabla v_i \end{vmatrix}}{\begin{vmatrix} u_i & v_i \\ \nabla u_i & \nabla v_i \end{vmatrix}} = - \frac{v_i h^2 F_i}{w_i} ,$$

$$\nabla b_i = \frac{\begin{vmatrix} u_i & 0 \\ \nabla u_i & h^2 F_i \end{vmatrix}}{\begin{vmatrix} u_i & v_i \\ \nabla u_i & \nabla v_i \end{vmatrix}} = \frac{u_i h^2 F_i}{w_i} ,$$

where

$$w_i = \begin{vmatrix} u_i & v_i \\ \nabla u_i & \nabla v_i \end{vmatrix} .$$

As $a_i = a_0 + \sum_{j=1}^{i} \nabla a_j$, and $b_i = b_0 + \sum_{j=1}^{i} \nabla b_j$, we see that the inhomogeneous difference equation has the general solution

$$\varphi_i = Au_i + Bv_i + \sum_{j=1}^{i} h^2 F_j \frac{v_i u_j - v_j u_i}{W_j} .$$

If we put

$$u_i = \sin kih , \text{ and } v_i = \cos kih ,$$

where $\bar{\mu} = 4h^{-2} \sin^2 \frac{kh}{2}$, then $W_i = - \sin kh$.

The solution of the difference equation satisfying the initial conditions $\varphi_0 = \mu\delta\varphi_0 = 0$ is

$$\varphi_i = -\frac{h^2 F_0}{\sin kh} \sin ikh + \sum_{j=0}^{i} h^2 F_j \frac{\sin k(i-j)h}{\sin kh} .$$

Using this result we can transform (B.I.2) into the form

$$y_i = \bar{y}_i - \frac{h^2 F_0}{\sin kh} \sin kih + \sum_{j=0}^{i} h^2 F_j \frac{\sin k(i-j)h}{\sin kh} ,$$

where $h^2 F_j = h^2(\bar{\mu} - \mu) y_j + h^2 q_j y_j$.

$$\therefore |y_i| \leq |\bar{y}_i| + \frac{4\max|q|}{2h^{-1}\sin kh} \frac{i+2}{n} \max|y| .$$

Now $2h^{-1}\sin kh = \sqrt{\bar{\mu}} > 2(p-1)$ if $\bar{\mu}$ is the p^{th} eigenvalue of A . Thus the maximum value of y_i , the p^{th} eigenvector of A , satisfies the inequality

$$\max|y| \leq \frac{\max|\bar{y}|}{1 - \frac{2\max|q|}{p-1}(1 + \frac{2}{n})} \qquad \text{(B.I.3)}$$

provided $\frac{2\max|q|}{p-1}(1 + \frac{2}{n}) < 1$. This condition is always satisfied provided p and n are large enough .

Lemma 5 The eigenvectors of the matrix A , normalised so that their first elements are unity , have their elements of maximum modulus uniformly bounded independent of n .

This result follows readily for the lower eigenvectors (say y_1 , y_2 , ... y_r , r fixed independent of n) can be bounded independent of n by using our results for the initial value problem . If r is such that $\frac{4\max|q|}{r-1} < 1$ (this condition can always be satisfied) then the higher eigenvectors y_s , $s \geq r$, are bounded by comparison with $\bar{y}_s$ using (B.I.3) .

We note that our method of normalising the eigenvectors by taking $y_0 = 1$ precludes us discussing the case where y_0 is prescribed = 0 . Here it is convenient to normalise the eigenvector by taking $\mu y_0 = h$. Again the difference $(y_p - \bar{y}_p)$ satisfies zero initial conditions so that (B.I.3) also applies to this case .

(B.2) In this section we consider the eigenvalue problem

$$-L(\varphi) = \lambda\varphi$$

where L is the differential operator of equation (B.I) , for homogeneous boundary conditions of the type specified by equation (B.2) . Using the results of chapter (III) - equations (C.3.2) or (C.3.6) for the difference equation : equations (C.3.9) or (C.3.IO)for the boundary conditions - we see that the solution of the differential equation also satisfies the difference equation (in matrix form)

$$(A + h^2\lambda I)\underset{\sim}{\varphi} = h\,\underline{v}$$

where λ is an eigenvalue of the homogeneous differential equation , $\underset{\sim}{\varphi}$ is a vector with components $\varphi_i = \varphi(ih)$ where $\varphi(x)$ is the corresponding eigenfunction , and $\underline{v}$ is a vector with components constructed from the expressions for the truncation error .

The finite difference equation is

$$(A + h^2\mu I)\,\underline{y} = 0$$

so that , by subtraction ,

$$(A + h^2\mu I)(\underset{\sim}{\varphi} - \underline{y}) = h^2\underline{v} - h^2(\lambda - \mu)\,\underset{\sim}{\varphi} \qquad \text{(B.2.I).}$$

If $\varphi(x)$ has been normalised so that $\varphi(0) = I$, and the vector $\underline{y}$ normalised so that $y_0 = I$, then $\underset{\sim}{\varphi} - \underline{y}$ also satisfies the difference equation

$$\left\{\delta^2 + h^2(\mu - q_i)\right\}(\varphi_i - y_i) = h^2 v_i - h^2(\lambda-\mu)\,\varphi_i$$

with the initial conditions

$$\varphi_0 - y_0 = 0 , \quad h^{-1}\mu\delta(\varphi_0 - y_0) = \int_{-h}^{h} V\varphi''\,dx$$

as in section (A) pages 73 – 75 .

As μ is an eigenvalue of A the left hand side of equation (B.2.I) is singular ; and the condition that a solution exist is

$$\underline{y}^{*t}(h\underline{v} - h^2(\lambda-\mu)\underline{\varphi}) = 0 .$$

$$\lambda - \mu = \frac{\underline{y}^{*t}\underline{v}}{\underline{y}^{*t}\underline{\varphi}} \qquad (B.2.2)$$

If we denote the other eigenvalues and eigenvectors of A by $h^2\mu_i$ and $\underline{y}_i$ respectively then we have

$$\underline{\varphi} - \underline{y} = K\underline{y} + h^2 \sum_{i=1}^{n} \frac{\underline{y}^{*t}\underline{\psi}}{\underline{y}^{*t}\underline{y}} \frac{\underline{y}_i}{h^2(\mu-\mu_i)} \qquad (B.2.3)$$

where

$$\underline{\psi} = \underline{v} - (\lambda-\mu)\underline{\varphi} ,$$

and K is a constant which is determinate when the scales of $\underline{\varphi}$ and $\underline{y}$ are fixed . Using (B.2.3) we see that (B.2.2) can be written

$$= \frac{\underline{y}^{*t}\underline{v}}{(I+K)\underline{y}^{*t}\underline{y}} .$$

Now $$\frac{\underline{y}^{*t}\underline{v}}{\underline{y}^{*t}\underline{y}} = \frac{\frac{1}{2}y_0v_0 + y_Iv_I + \cdots\cdots\cdots + \frac{1}{2}y_nv_n}{\frac{1}{2}y_0y_0 + y_Iy_I + \cdots\cdots\cdots + \frac{1}{2}y_ny_n}$$

and as the eigenvector $\underline{y}$ can be found by solving an initial value problem , we have that $\max|y_i| \leq B$.

$$\therefore \left|\frac{\underline{y}^{*t}\underline{v}}{\underline{y}^{*t}\underline{y}}\right| \leq \frac{B\max|v_i|}{\frac{I}{n}\left\{\frac{1}{2}y_0y_0 + y_Iy_I + \cdots\cdots\frac{1}{2}y_ny_n\right\}}$$

Also the denominator (for large n) approximates to $\int_0^1 y^2 dx$ where y is the solution to the initial value problem

$$\begin{cases} \frac{d^2y}{dx^2} + (\mu - q(x))y = 0 , \\ y(0) = I , \ \frac{dy(0)}{dx} = \frac{A_0}{B_0} , \end{cases}$$

and is thus strictly greater than zero (note that we require only that μ lie in some bounded interval for all h to guarantee these results) . Thus there is some positive number ρ bounded independent of n (~~perhaps provided it is large enough~~) for which

$$\left| \frac{\underset{\sim}{y}^{*\prime}\underset{\sim}{v}}{\underset{\sim}{y}^{*\prime}\underset{\sim}{y}} \right| \leq \rho \max|v_i| \qquad (B.2.4)$$

As $\max|v_i| \to 0$ as $h \to 0$ it follows that $|\lambda - \mu| \to 0$ unless $K \to -I$. Now if $|\lambda - \mu| \to 0$ as $h \to 0$, then $\max|\psi_i|$ also tends to zero , and we can apply the argument of section A pages 73 – 75 to the initial value statement of equation (B.2.I) to show that $\max|\varphi_i - y_i| \to 0$. Thus provided $K \neq -I$, $K \not\to -I$, $h \to 0$, then the components of the eigenvector $\underset{\sim}{y}$ tend pointwise (to point values) of the eigenfunction $\varphi(x)$. The converse is also true for if $\underset{\sim}{y}$ tends to the eigenfunction pointwise then

$$\lim_{n\to\infty} \frac{1}{n}\left\{\tfrac{1}{2}y_0\varphi_0 + y_1\varphi_1 + \cdots\cdots + \tfrac{1}{2}y_n\varphi_n\right\} = \int_0^1 \varphi^2\,dx$$

as φ is certainly R-integrable . Thus $\underset{\sim}{y}$ cannot ~~take~~ be orthogonal to $\underset{\sim}{\varphi}$ (at least if n is large enough) , and therefore K cannot take the value -I .

Now $|\varphi_i - y_i|$ cannot tend to zero if $\underset{\sim}{\varphi}$ and $\underset{\sim}{y}$ have different oscillation properties so that $K \to -I$ unless $\underset{\sim}{\varphi}$ and $\underset{\sim}{y}$ exhibit the same number of changes in sign on (0,I) . Obviously the fundamental eigenvector $\underset{\sim}{y}_0$ ~~[illegible]~~ can never be orthogonal ~~[illegible]~~ to the vector ~~[illegible]~~ $\underset{\sim}{\varphi}_0$ constructed from the fundamental eigenfunction $\varphi_0(x)$ as all their components are one signed . Thus certainly $\underset{\sim}{y}_0$ tends pointwise to $\varphi_0(x)$ and $\mu_0 \to \lambda_0$ as $h \to 0$.

This must also be true for the higher eigenvectors and eigenvalues where the eigenvalues are ordered from the least positive (that y_p shows p changes of sign is then guaranteed by lemma I.) . Let us assume that the p^{th} eigenvector fails to tend to an eigenfunction . As μ_p lies in some bounded range (we have shown this - lemma 4 - for positive μ : for negative μ we can again calculate a lower bound $\bar{\mu}$ - lemma 3 - explicitly) there is at least one convergent subsequence of the $\mu_p(h)$ as $h \to 0$; and we can associate with this limiting value a continuous and non-zero function (non-zero as we can impose the initial condition $y_0 = I$) as in section (A) . Now this function must be orthogonal to all $\varphi_r(x)$ as otherwise $K \not\to -I$ for some $\varphi_r(x)$ and the sequence of values of h chosen , and this would imply $y \to \varphi_r(x)$ contrary to our assumption . However this gives a contradiction as the only function orthogonal to all φ_r is zero . It follows that y_p tends pointwise to $\varphi_p(x)$ for all p as $h \to 0$ ($n \to \infty$) as this ordering leads to identical oscillation properties .

This demonstrates the convergence of the solution of the standard finite difference approximation to the solution of the differential equation as $h \to 0$ for eigenvalue problems of second order differential equations in normal form .

Remark : If the eigenvalue occurs multiplied by some positive weight function - that is $-L(\varphi) = \lambda \rho \varphi$ ($\rho > 0$) instead of $L(\varphi) = \lambda \varphi$ - the same approach can be used to demonstrate the convergence of the finite difference methods . Lemma 3 can be amended

can be amended to bracket the eigenvalues of the difference equation in this case.

As with the initial value problems the two expressions for the truncation error fill complementary roles. Equation (C.3.6) of chapter (III) ensures convergence provided $q(x)$ is continuous, while equation (C.3.2) tells us that the error in the solution is at most $O(h^2)$ provided φ has a bounded fourth derivative.

(B.3) The boundary value problem which is given by the system of equations (B.1) and (B.2) can be written as the matrix problem

$$A \underset{\sim}{\varphi} = h^2 \underset{\sim}{f} + h^2 \underset{\sim}{V}$$

where $\underset{\sim}{V}$ is the vector representing the truncation error in the standard finite difference approximation (B.5). We note that the components of $\underset{\sim}{V}$ can be constructed (as in the previous subsection and in section A) from the formulae of chapter (III).

Thus we see that the error vector $\underset{\sim}{\varphi} - \underset{\sim}{y}$ satisfies the equation

$$A(\underset{\sim}{\varphi} - \underset{\sim}{y}) = h^2 \underset{\sim}{V}$$

whence

$$\underset{\sim}{\varphi} - \underset{\sim}{y} = h^2 A^{-1} \underset{\sim}{V}$$

$$= - \sum_{i=0}^{m} \frac{\underset{\sim}{y}_i^{*\prime} \underset{\sim}{V}}{\underset{\sim}{y}_i^{*\prime} \underset{\sim}{y}_i} \frac{\underset{\sim}{y}_i}{\mu_i}$$

where $\underset{\sim}{y}_i$ and $-h^2\mu_i$ are the eigenvectors and eigenvalues of the matrix A. By lemma 4 we know that $1/\mu_i \to 0$ at least with $1/4(i-1)^2$ as $i \to \infty$. Thus $\sum_{i=0}^{m} \frac{1}{|\mu_i|}$ is bounded for all m unless, for some

n, one of the μ_i happens to be zero. To estimate $\frac{\underset{\sim}{y}_i^{*\prime} \underset{\sim}{V}}{\underset{\sim}{y}_i^{*\prime} \underset{\sim}{y}_i}$ it is convenient to first normalise the $\underset{\sim}{y}_i$ by requiring that $\underset{\sim}{y}_i^{*\prime} \underset{\sim}{y}_i = n$. This condition is the analogue of normalising the corresponding eigenfunction φ_i by requiring that $\int_0^1 \varphi_i^2 \, dx = 1$.

Thus we have (as in (B.2.4)

$$\max |\varphi_i - y_i| \leq \max |V_i| \max y_i^2 \sum_{i=0}^{n} \frac{1}{|\mu_i|}$$

Using lemma 5 we have that y_i^2 can be bounded independent of n*. Thus, as $\max |V_i| \to 0$ as $h \to 0$, we have $\max |\varphi_i - y_i| \to 0$ as $h \to 0$ unless some μ_i also tends to zero. As the μ_i tend to eigenvalues of the homogeneous differential equation this exceptional case can only occur if the differential operator has a zero eigenvalue; and in this case the solution of the differential equation is not unique if it exists at all.

Thus sufficient conditions for the solution of the standard finite difference approximation to tend pointwise to the solution of the differential equation boundary value problem as $h \to 0$ are

(1) that the differential equation have a unique solution,

and (2) that $q(x)$ and $f(x)$ be continuous.

If the solution of the differential equation has a bounded fourth derivative then the error in the solution is ultimately $O(h^2)$. We must qualify the $O(h^2)$ by ultimately as we have no guarantee that one of the μ_i may not pass through zero as it approaches its limiting value. We may note that the paper by Mitchell [3] giving an example

* We actually have $|y_j - \bar{y}_j| = O(1/p)$ for the p^{th} eigenvectors $j = 0, 1, 2, \cdots, n$.

where the solutions of the differential equation and of the difference equation may be made to differ by arbitrarily large amounts by suitable choice of h makes use of the exceptional case of a zero eigenvalue (actually he introduces a parameter which enables him to vary a differential equation eigenvalue through zero, and then tabulates the solution of the differential equation and the finite difference approximation for different values of the parameter).

Convergence proofs of the type given by Kantarovich and Krylow [4] give sufficient conditions for both the differential equation and the difference equation to have positive eigenvalues. They consider a subclass of the operators monotonic in the sense of Collatz [5]. The condition that an operator be monotonic restricts both the coefficients in the differential equation and the form of boundary conditions.

Typical sufficient conditions that ensure that the difference equation (and the differential equation) always have positive eigenvalues are (equations (B.1), (B.2))

(1) $y(0) = y(1) = 0$, $q(x) > -8$ (or better $q(x) > -4h^{-2}\sin^2\frac{\pi h}{2} = -8$ when $h = \frac{1}{2}$), and

(2) $y'(0) = y'(1) = 0$, $q_0(x) > 0$. A more general sufficient condition of the same type but putting some restriction on h is

$$q(x) > -\bar{\mu}_0(h)$$

which guarantees that the eigenvalues of the difference equation are positive by lemma 3.

The condition that all the functions appearing in the differential equation be continuous which has been a sufficient condition for the pointwise convergence of the solutions of the difference equation in all three cases (initial value, eigenvalue, and boundary value problems) considered does not appear capable of being weakened. There are two reasons for this:

(a) the difference equation would be ambiguous if a point of discontinuity happened to be an ordinate point,

and (b) additional conditions (for example the matching conditions in the appendix to chapter I) are usually required at a point of discontinuity in order to specify the solution of the differential equation.

APPENDIX 1: Discontinuous coefficients.

Here we consider further the case of the differential equation with discontinuous coefficients. The occurrence of equations of this type in problems with physical application (as in chapter (I)) suggests that one way of imposing additional conditions at the discontinuity is to attempt to define the differential equation as the solution of a problem in the calculus of variations. Let us consider for example the equation

$$\mathcal{L}(y) = \frac{d}{dx}\left(p\frac{dy}{dx}\right) + q(x)\,y = 0$$

If the coefficients of this equation are continuous (p absolutely continuous), and if the boundary values are such as to make up a self adjoint system ($\mathcal{L}$ is formally self adjoint), then y is also the minimising function for the variational problem

$$I = (y, \mathcal{L}(y))\Big|_a^b \qquad \text{to be stationary.}$$

The definition of y in this manner is fully discussed by Gould, ref [2].

Turning to the discontinuous case we assume that the coefficients in the differential equation have a discontinuity at $x=c$, $a<c<b$.

We consider the variational problem

$$I+\delta I = (y+\varepsilon\eta, \mathcal{L}(y+\varepsilon\eta))\Big|_a^{c-\delta}\Big|_{c+\delta}^{b},$$

$$= (y, \mathcal{L}(y))\Big|_a^{c-\delta}\Big|_{c+\delta}^{b} + \varepsilon\left[(\eta, \mathcal{L}(y)) + (\mathcal{L}(\eta), y)\right]\Big|_a^{c-\delta}\Big|_{c+\delta}^{b} + O(\varepsilon^2).$$

Integrating the $\mathcal{E}$ term by parts we get

$$\delta I = \mathcal{E}\left\{ a(\eta, \lambda(y))\Big|_{a}^{c-\delta} + a(\eta, \lambda(y))\Big|_{c+\delta}^{b} + \left[P\eta y' - P\eta' y\right]\Big|_{c-\delta}^{c+\delta} \right\}$$

where we have assumed that the terms involving the boundary values vanish (i.e. that the boundary conditions are such as to make an equation with sufficiently regular coefficients self adjoint).

Now our aim is to seek conditions on the integrated term so that it vanishes in limit as $\delta \to 0$ for all suitably restricted variations (from the form of the integrated term any condition on y implies a similar condition on η and vice versa).

Writing

$$y_+ = A y_- + B y_-' \quad , \quad \eta_+ = A \eta_- + B \eta_-' \quad ,$$
$$y_+' = C y_- + D y_-' \quad , \quad \eta_+' = C \eta_- + D \eta_-'$$

where the $+$ and $-$ indicate limiting values at the discontinuity approached from $x > c$ and $x < c$ respectively, the condition that the integrated term vanish becomes

$$AD - BC = \frac{P_-}{P_+} \tag{4.1}$$

Any values of A, B, C, D satisfying this equation specify a solution of the variational problem. We also have

$$\left(\eta, \lambda(y)\right)\Big|_{a}^{b} = \left(\lambda(\eta), y\right)\Big|_{a}^{b}$$

so that the completed system is self adjoint.

The condition of the appendix to chapter I is obtained by putting

$A = 1, \quad B = C = 0, \quad D = \frac{P_-}{P_+}$ so that

$$\left.\begin{aligned} y_+ &= y_- \\ \alpha\, \rho_+ y_+' &= \rho_- y_-' \end{aligned}\right\}$$

where, in this case, $\rho = 1/\rho$. The above solution of (1) is not the only one of physical interest for, in chapter I, if we had taken a velocity potential instead of a pressure potential the appropriate solution of (1) would be $A = \rho_-/\rho_+ , B = C = 0 , D = 1$.

We now turn to the problem of constructing finite difference approximations at the points of discontinuity. Here a useful device which is often possible is the introduction of pseudo points.

For example, if $q(x)$ in equation (B.1) is equal to

$$\left.\begin{aligned} &q_1(x) && x < c \\ &q_2(x) && x > c \end{aligned}\right\}$$

where $q_1(x)$ is a function which is defined for $x > c$ and $q_2(x)$ is a function which is defined for $x < c$ (and where both functions are at least continuous throughout their domain of definition), then the equation

$$\frac{d^2 y_1}{dx^2} - q_1(x)\, y_1 = f(x)$$

has its solutions defined for $x > c$, and the equation

$$\frac{d^2 y_2}{dx^2} - q_2(x)\, y_2 = f(x)$$

has its solutions defined for $x < c$.

We will assume that the matching conditions are

$$\left.\begin{aligned} y_1 &= y_2 \\ y_1' &= y_2' \end{aligned}\right\} , \quad x = c .$$

We can approximate the second condition by setting

$$h y_1' = \tfrac{1}{2}\{y_1(c+h) - y_1(c-h)\},$$

and $$h y_2' = \tfrac{1}{2}\{y_2(c+h) - y_2(c-h)\},$$

where $y_1(c+h)$ is defined by the difference equation

$$y_1(c-h) - (2 + h^2 q_1(c))\, y_1(c) + y_1(c+h) = h^2 f(c),$$

and $y_2(c-h)$ by the difference equation

$$y_2(c-h) - (2 + h^2 q_2(c))\, y_2(c) + y_2(c+h) = h^2 f(c).$$

In these cases we can evaluate the expressions for the truncation error in these equations because the solutions of the corresponding differential equations can be extended as far as the pseudo points ($y_1(c+h)$ and $y_2(c-h)$ respectively) by the remarks made above.

The matching conditions now become

$$y_1(c) = y_2(c),$$

$$\left(1 + \tfrac{h^2}{2} q_1(c)\right) y_1(c) - y_1(c-h) + \tfrac{h^2}{2} f(c)$$

$$= y_2(c+h) - \left(1 - \tfrac{h^2}{2} q_2(c)\right) y_2(c) - \tfrac{h^2}{2} f(c)$$

If these equations are used at the point of discontinuity and the standard finite difference equation used at the remaining ordinate points then it is probable that arguments similar to those of the preceding sections can be used to show that the error in the solution of this finite difference system tends to zero as the mesh length tends to zero. The appropriate differential equation on which to base the estimates for the eigenvalues (as in lemma 3, etc.) is one in which $q(x)$ is a suitably chosen step function. This eigenvalue problem is not without interest. It is similar to the problem discussed in the appendix to chapter I.

Differential equations with discontinuous coefficients have been discussed by Fox [6] . He suggests a method of difference correction to improve the accuracy of the solution to the standard difference equation.

APPENDIX 2: Deferred approach to the limit and difference correction.

We have discussed in [7] an approach to the techniques of 'deferred approach to the limit' (h^2 extrapolation), and difference correction. This paper is bound with the thesis.

At this stage it seems that the argument made in §5 of this paper to justify the estimate

$$\left| \frac{d^p}{dx^p} \frac{\partial^q g}{\partial h^q} \right| \leq \frac{p!}{\rho^p} K$$

(where K is independent of p, q, x and is bounded) is insufficient. If this is so then the argument of the paper needs to be modified. A possible method of attacking this problem will be given in chapter (V.) when we discuss some problems of partial differential equations.

APPENDIX 3: Computation of Eigenvalues.

In this appendix we give a summary of some computations of eigenvalues, eigenvectors, and group velocities for problem 1 of chapter I.

The programme was first written for the Ferranti Pegasus electronic computer and subsequently adapted for the Ferranti Mercury at the University Computing Unit. A particular consideration when writing the first programme was the small high speed store of the Pegasus. Also the comparative slowness of this computer makes it desirable to work fixed point (incorporating floating point arithmetic only where necessary).

The difference equation adopted was (A.1) of chapter (III). This equation is solved in a number of stages. First we considered the standard finite difference approximation: and we solved for the eigenvalues of this

equation by finding an interval in which the Sturm count (Lemma 1) changed by 1 and then, by a process of bisections, reducing the length of this interval until it is less than a prescribed tolerance. The eigenvectors are then found by solving the initial value problems for the calculated eigenvalues. Next we calculated an improvement to the calculated eigenvalue by

$$\Delta\mu^{*} = \frac{1}{12}\,\frac{\sum_{i=0}^{n} y_i \delta^4 y_i}{\sum_{i=0}^{n} y_i^2}$$

(see reference [7]). The fourth differences at the boundary points require the solution of the difference equation outside the range in which the problem is set; but in this case these values can be calculated by an easy extrapolation using the difference equation (compare with sections C, D chapter (V.)).

The solution is completed by using the approximate eigenvalue to compute approximate right and left eigenvectors for equation (A.1) of chapter (III) treating it as initial value problem. We then compute the Rayleigh Quotient

$$\mu = \frac{\underset{\sim}{y}^{*\prime} M \underset{\sim}{y}}{\underset{\sim}{y}^{*\prime} N \underset{\sim}{y}}$$

where

$$M = \left[\; 1 + \frac{h^2 q_{i-1}}{12} \qquad -2 + \frac{5h^2 q_i}{6} \qquad 1 + \frac{h^2 q_{i+1}}{12} \;\right],$$

* This formula is appropriate for the boundary conditions $y(0) = y(1) = 0$.

and $$N = \begin{bmatrix} \frac{h^2}{12} & \frac{5h^2}{6} & \frac{h^2}{12} \end{bmatrix}.$$

We then take this value of μ and repeat the cycle.

We continue the iteration until μ is constant to within the desired tolerance.

In this last part of the calculation the components of the right and left eigenvectors satisfy similar three term recurrences, and it is convenient to calculate them together and to simultaneously accumulate the terms in the Rayleigh Quotient. The iteration gives a quadratic convergence provided the eigenvectors are calculated with sufficient accuracy; and a floating point routine should be used in their calculation to guard against loss of significant figures.

The Sturm sequence routine was particularly useful in the calculations made on the Pegasus computer. Here it could be kept in the high speed store as a self preserving subroutine. This advantage far outweighed its comparative slowness as any more elaborate method (for example the version of Newton's method described by Fox [63]) would have required programme transfers from the backing store. On the Mercury the Sturm technique was used to isolate the root and to form a rough approximation only. The final computation was done by iterating with the Rayleigh quotient for the standard finite difference equation to get a process with quadratic convergence.

The process outlined above is completely satisfactory providing that the computation of the eigenvectors by means of a marching technique

is stable. In the problem of chapter (I) the main occurrence of instability is likely to be in the computation of the exponentially decaying eigenfunctions associated with very great ('infinite') depths of fluid. In this case we 'marched' from both boundaries to some convenient internal ordinate point and matched the two solutions by requiring that

(1) function values agree (this then fixes the scale for the whole calculation), and

(2) that the difference equation must be satisfied at this ordinate point.

Condition (2) provides a check on the accuracy of our working as does the terminal boundary condition in a straightforward computation. This check is essential as it provides an indication of the stability achieved by our choice of matching point. In computations of this kind there is an inevitable loss of accuracy even in a stable procedure due to build up of rounding errors. As an example of the loss of accuracy due to marching in a well behaved case we give in the table 1 some values of the check against the order of magnitude of φ . The computations were carried out with $n = 40$; and the solutions were matched at φ_8 . The floating point registers held approximately 8 significant figures.

Check	g_2
8×10^{-7}	7
-5×10^{-7}	5
5×10^{-6}	7
-5×10^{-6}	7
-2×10^{-5}	20
1×10^{-6}	-2

Table 1

It is apparent that 2 figures have been lost representing 25% of the available significance yet the matching point was carefully adjusted for maximum stability.

Although instability can be a problem in computing the eigenvector it has very little effect on the calculation of the eigenvalue by using the Sturm sequence. The reason for this is that the unwanted solution which may ruin the calculation of the exact eigenvector, is present by right when μ is not exact; and trouble from the component of this solution introduced by rounding errors can only occur when μ is very close to its exact value.

An essential point in this argument is that the order of the difference equation and differential equation are the same so that their fundamental solutions correspond. It will not hold in general if the order of the difference equation is greater than that of the differential equation.

In calculating the eigenfunction for a fluid of infinite depth one is forced to approximate by taking the depth large but finite. I do not

know of any general method for checking this approximation other than that of comparison between solutions for two or more depths. Another disadvantage is that one choice of the depth is not likely to be uniformly good for all eigenfunctions. To illustrate this point we have tabulated the first and eighth eigenfunctions for a particular case (taking $\eta = h0$ and tabulating every second value).

	1			8
0.	000	000 0		0. 000 000 0
	8	164 1		38 752 4
	23	410 1		19 527 4
	44	846 5	−	33 743 1
	64	182 3	−	14 094 0
	71	990 5		36 378 5
	65	379 6		5 386 9
	49	250 7	−	38 190 7
	31	444 6	−	352 4
	17	226 0		39 544 4
	8	261 7		3 694 5
	3	4 87 6	−	40 374 3
	1	9 11 2	−	19 127 2
		4 4 2 8		39 691 0
		1 3 5 3		42 971 25
		3 7 7		6 2 935
		9 6	−	37 7943
		2 3	−	36 5415
		5	−	47 5789
		1	−	24 5834
		0		0

It is obvious that 1 will provide a much better approximation to the actual function than will 2.

Chapter (V). Some Problems in the Numerical Solution of Partial Differential Equations.

This chapter is divided up in the following manner. In the first section we consider the extension of the methods of chapter (III) to partial differential equations, while the bulk of the remainder of this chapter is devoted to the consideration of the feasibility and convergence of the difference correction method for the solution of partial differential equations of elliptic type.

A. Finite difference approximations to partial differential equations.

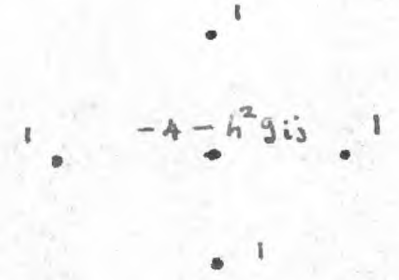
The finite difference formulae of chapter (II) can be used to approximate to the derivatives in a partial differential equation to give an approximate finite difference equation. In this section we will restrict ourselves to differences taken on a square mesh of side h - the extension to rectangular meshes is immediate while accounts of triangular and hexagonal meshes may be found in the literature (for example Collatz [1]). Consider the differential equation

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} - g(x,y)\,\varphi = 0 .$$

In this case the approximate difference equation is

$$\left(\varphi_{i-1,j} - 2\varphi_{ij} + \varphi_{i+1,j}\right) + \left(\varphi_{i,j-1} - 2\varphi_{ij} + \varphi_{i,j+1}\right) - h^2 g(ih, jh) = 0 \qquad (A.1).$$

This equation is often displayed by means of the array



For partial differential equations the construction of more accurate finite difference approximations is much more difficult than it is in the case of ordinary differential equations. Quite apart from the additional labour that the computation of the solution of a p.d.e. necessarily involves, we find that many of the methods of chapter (III) do not generalise to the higher dimensional case. For example we find the analogue of the result that the solution of an ordinary linear differential equation exactly satisfies a linear difference equation of the same order is the Green's formula

$$\varphi(P) = -\int_S \frac{\partial G}{\partial n}\varphi\, ds$$

where S is a closed curve and P any interior point of this curve. Thus the analogue of the one dimensional difference equation is an integral equation.

We do, however, have the method of polynomial interpolation which we outlined in section B of chapter (III). To derive the basic finite difference equation (A.1) by this method we use the values of the solution at the mesh points of the array, and the differential equation at the central point. There are six independent polynomials of degree

≤ 2 in x and y,

$$1, \quad x, \quad y, \quad x^2, \quad xy, \quad y^2.$$

However, xy vanishes at every point on the array and therefore cannot contribute to any condition on the data given at these points. Thus we have six conditions to determine five unknowns (the coefficients of the non zero terms). We readily verify that (A.1) gives the necessary condition on the data for the interpolation to be possible.

In the case of Laplace's equation we can make use of the fact that it has a special family of polynomial solutions (the harmonic polynomials) given by the real and imaginary parts of z^n. The first few of these are

$$1,$$

$$x, \quad y,$$

$$x^2-y^2, \quad xy,$$

$$x^3-3xy^2, \quad 3x^2y-y^3,$$

$$x^4-6x^2y^2+y^4, \quad 4x^3y-4xy^3,$$

$$x^5-10x^3y^2+5xy^4, \quad 5x^4y-10x^2y^3+y^5.$$

Here we do not need to use the condition that the polynomial satisfy Laplace's equation at the ordinate points because this is automatically satisfied if we expand in terms of the harmonic polynomials.

For the array of equation (A.1) we obtain the correct degree of overspecification if we pose the solution values at the points of the array (five conditions), and take an interpolation polynomial of degree two as there are four harmonic polynomials of degree ≤ 2 non zero at these points (the exception is, as before, xy).

The equations determining the coefficients in the interpolating polynomial

$$y = A + Bx + Cy + D(x^2-y^2)$$

are

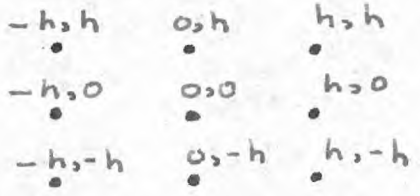
$$\begin{aligned}
y_{-h,o} &= A - Bh + Dh^2 , \\
y_{h,o} &= A + Bh + Dh^2 , \\
y_{o,o} &= A , \\
y_{o,h} &= A + Ch - Dh^2 , \\
y_{o,-h} &= A - Ch - Dh^2 .
\end{aligned}$$

Thus

$$y_{-h,o} + y_{h,o} + y_{o,h} + y_{o,-h} - 4y_{oo} = 0 ,$$

and this is the desired difference equation. It is just equation (4.1) applied to Laplace's equation. We can readily verify that it is satisfied by the harmonic polynomials of degree three but not by both those of degree four.

If we consider the array



and seek a difference approximation to Laplace's equation on it we see that we have 9 function values and 9 harmonic polynomials of degree ≤ 4. However, the polynomial $4(x^3y-xy^3)$ vanishes at every point of the array and can thus be ignored in the interpolation.

We put

$$y = A + Bx + Cy + D(x^2-y^2) + Exy + F(x^3-3xy^2) + G(3x^2y-y^3) + \\ + H(x^4-6x^2y^2+y^4) .$$

The equations determining the unknowns are

$$\begin{aligned}
y_{-h,h} &= A - Bh + Ch - Eh^2 + 2Fh^3 + 2Gh^3 - 4Hh^4 \\
y_{-h,o} &= A - Bh + Dh^2 - Fh^3 + Hh^4 \\
y_{-h,-h} &= A - Bh - Ch + Eh^2 + 2Fh^3 - 2Gh^3 - 4Hh^4 \\
y_{o,-h} &= A - Ch - Dh^2 + Gh^3 + Hh^4 \\
y_{o,o} &= A \\
y_{o,h} &= A + Ch - Dh^2 - Gh^3 + Hh^4 \\
y_{h,h} &= A + Bh + Ch + Eh^2 - 2Fh^3 + 2Gh^3 - 4Hh^4 \\
y_{h,o} &= A + Bh + Dh^2 + Fh^3 + Hh^4 \\
y_{h,-h} &= A + Bh - Ch - Eh^2 - 2Fh^3 - 2Gh^3 - 4Hh^4
\end{aligned}$$

We have

$$(\delta_x^2 + \delta_y^2)y_{oo} = 4Hh^4 ,$$

and $$\sum_{i,j\neq o} y_{ij} = -12Hh^4 + 8y_{o,o} ,$$

$$\therefore \quad 3(\delta_x^2 + \delta y^2)y_{oo} + \sum_{i,j\neq o} y_{ij} - 8y_{oo} = 0 ,$$

and

·1	·4	·1
·4	·-20	·4
·1	·4	·1

is the corresponding array.

We readily verify that the equation is satisfied by harmonic polynomials of degree five.

In all the previous examples we were able to get the correct degree of overdetermination only because certain of the polynomials vanished at all the ordinate points and therefore could not contribute to any relation on the data. This would seem to be due to the symmetry of the arrays. This point may cause serious difficulty if it is desired to compute the difference equations because it means that the exact degree of overdetermination may be obscure. Another difficulty is that the number of points in a rectangular array does not bear any satisfactory relation to the number of coefficients in the interpolating polynomials.

Both these difficulties can be removed by going to asymmetric arrays. However, the magnitude of the problem remains large. For example there are $\frac{(n+1)(n+2)}{2}$ independent polynomials of degree $\leq n$. If it is desired to use interpolation polynomials of degree 10 (say), then to compute the difference equation a matrix of order 66×66 has to be decomposed into upper and lower triangular matrices at each point in the domain. The minimum requirements would be something like 25 interior points (plus 19 boundary values). It will be seen that the amount of work is necessarily considerable.

On the credit side we will have no difficulty in grouping points in regions where the solution can be expected to change rapidly, and no additional measures have to be taken to deal with curved boundaries. Professor Bickley has pointed out to me that triangular meshes are correct for two dimensional interpolation. If these are employed then the irregular stars need only be used in the vicinity of the boundary.

B. Difference methods for the solution of p.d.e.'s

In this section we will consider in outline some of the finite difference techniques available for the solution of elliptic partial differential equations. For convenience we restrict ourselves to a discussion of the Poisson equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f(x,y) \qquad (B.1)$$

given in some finite region R on whose boundaries ϕ takes prescribed values. Differences will be calculated on a rectangular mesh with spacings $\Delta x = h$ and $\Delta y = k$. The mesh is assumed to be of sufficient extent to enable differences of any required order to be calculated at any point of R.

The basic finite difference equation is

$$h^{-2}\delta_x^2 \Phi + k^{-2}\delta_y^2 \Phi = f(x,y) \qquad (B.2)$$

We will assume for the moment that the boundary of R intersects the mesh at grid points and, further, that there are a sequence of values of h and k tending to zero such that this remains true. The boundary condition on (2.2) is then that $\Phi = \phi$ at the grid points on the boundary of R.

Sufficient conditions for the solution of (B.2) to differ by as little as we please from the corresponding point values of ϕ provided h and k are small enough are well known.

For example, Collatz [2] shows that the magnitude of the error in the solution of (B.2) is $\leq h^2 \frac{M_4 \rho^2}{2^4}$ (assuming $h = k$) where ρ is the radius of a circle enclosing R, and M_4 is a bound for the fourth partial derivatives of ϕ. A similar discussion is given in Kantorovich and Krylov [3].

We can obtain much more information about the manner in which approximates to ϕ if we strengthen the conditions on the differentiability of ϕ. For example if ϕ is at least $2n+2$ times continuously differentiable in both variables then Φ can be expressed as the sum of ϕ, a polynomial of degree $2n-2$ in h and k involving only even powers of h and k and having quadratic lowest order terms (the coefficients in the polynomial being functions of x and y), and a function which is small in the sense of being of degree $2n$ in h and k. We will show this for the case $n=2$.

The solution of (B.2) is a function of h and k as well as of x and y. We will assume that it can be represented in the form

$$\begin{aligned}\Phi(x,y;h,k) = \phi_0(x,y) &+ h\phi_{11}(x,y) + k\phi_{12}(x,y) \\ &+ h^2\phi_{21}(x,y) + hk\phi_{22}(x,y) + k^2\phi_{23}(x,y) \\ &+ g(x,y;h,k)\end{aligned}$$

where, in particular, g is at least of third degree in h and k.

We have

$$h^{-2}\delta_x^2\phi_{ij} = \frac{\partial^2\phi_{ij}}{\partial x^2} + \frac{h^2}{12}\frac{\partial^4\phi_{ij}}{\partial x^4} + O(h^4), \text{ and}$$

$$k^{-2}\delta_y^2\phi_{ij} = \frac{\partial^2\phi_{ij}}{\partial y^2} + \frac{k^2}{12}\frac{\partial^4\phi_{ij}}{\partial y^4} + O(k^4).$$

The expression for Φ must satisfy (B.2) identically. If we group terms with similar dependence on h and k together the resulting expression must also vanish identically as h and k can vary independently.

This gives the series of equations

$$\frac{\partial^2 \phi_0}{\partial x^2} + \frac{\partial^2 \phi_0}{\partial y^2} = f(x,y) ,$$

$$\frac{\partial^2 \phi_{11}}{\partial x^2} + \frac{\partial^2 \phi_{11}}{\partial y^2} = \frac{\partial^2 \phi_{12}}{\partial x^2} + \frac{\partial^2 \phi_{12}}{\partial y^2} = 0 ,$$

$$\frac{\partial^2 \phi_{21}}{\partial x^2} + \frac{\partial^2 \phi_{21}}{\partial y^2} = -\frac{1}{12} \frac{\partial^4 \phi_0}{\partial x^4} ,$$

$$\frac{\partial^2 \phi_{22}}{\partial x^2} + \frac{\partial^2 \phi_{22}}{\partial y^2} = 0 ,$$

$$\frac{\partial^2 \phi_{23}}{\partial x^2} + \frac{\partial^2 \phi_{23}}{\partial y^2} = -\frac{1}{12} \frac{\partial^4 \phi_0}{\partial y^4} , \quad \text{and}$$

$$\left\{ h^{-2} \delta_x^2 + k^{-2} \delta_y^2 \right\} g = -\frac{1}{12} \left\{ h^3 \frac{\partial^4 \phi_{11}}{\partial x^4} + h^2 k \frac{\partial^4 \phi_{12}}{\partial x^4} + h k^2 \frac{\partial^4 \phi_{11}}{\partial y^4} + k^3 \frac{\partial^4 \phi_{12}}{\partial y^4} \right\} + O(h^4 + k^4) .$$

As the boundary conditions are independent of h and k, $\phi = \phi_0$ on the boundary of R, and the other functions satisfy the boundary conditions $\phi_{ij} = 0$ (and $g = 0$). Thus ϕ_0 is seen to be identical with ϕ the solution of (2.1) while ϕ_{11}, ϕ_{12} (terms involving odd powers of h and k), and ϕ_{22} vanish identically. In particular $g(x,y : h,k) = O(h^4 + k^4)$ at most (we can use the results of [2] and [3] quoted earlier to guarantee this).

An immediate consequence is that the classical technique of the deferred approach to the limit (h^2-extrapolation) can be used to refine solutions of (B.2).

Another method which, like the technique of h^2-extrapolation, seeks to determine point values of the solution of (B.1) by refining the solution of the basic difference equation is the technique of difference correction [4] . Here we make use of the substitution (chapter (II), equation (A.4))

$$h^2\delta^2 = \delta^2 - \frac{1}{12}\delta^4 + \frac{1}{90}\delta^6 - \dots$$

to write (B.1) in the form

$$\left\{ h^{-2}\delta^2_x + k^{-2}\delta^2_y \right\} \phi = f(x,y) + \mathcal{C}\phi \qquad (B.3)$$

where $$\mathcal{C} = \frac{1}{12}(h^{-2}\delta^4_x + k^{-2}\delta^4_y) - \frac{1}{90}(h^{-2}\delta^6_x + k^{-2}\delta^6_y) + \dots$$

We take Φ (the solution of (B.2)) as a first approximation to ϕ and set

$$\phi = \Phi + \eta_1$$

where η_1 satisfies the equation

$$\left\{ h^{-2}\delta^2_x + k^{-2}\delta^2_y \right\} \eta_1 = \mathcal{C}\Phi + \mathcal{C}\eta_1 .$$

We define $\bar{\eta}_1$ by the equation

$$\left\{ h^{-2}\delta^2_x + k^{-2}\delta^2_y \right\} \bar{\eta}_1 = \mathcal{C}\Phi \qquad (B.4),$$

and successive $\bar{\eta}_i$ by the recurrence

$$\left\{ h^{-2}\delta^2_x + k^{-2}\delta^2_y \right\} \bar{\eta}_i = \mathcal{C}\bar{\eta}_{i-1} \qquad (B.5).$$

As $\phi = \Phi$ at the boundary mesh points we take $\bar{\eta}_i = 0$ as the boundary conditions on (B.4) and (B.5). Assuming that the computation of the $\bar{\eta}_i$ can be carried out we then have

$$\phi = \Phi + \sum_{i=1}^{\infty} \bar{\eta}_i \qquad (B.6)$$

as a formal solution to equation (B.3). Discussion of this result and its implications will occupy the bulk of the remainder of the paper. Here we

will restrict ourselves to the following remarks.

(A) An immediate consequence of chapter (II) is that a regular function bounded on the real axis which can be differentiated exactly by means of the finite difference formulae is necessarily an integral function of exponential type. No such restrictions apply to the solution of equation (B.1). This implies that equation (B.3) cannot in general be an equivalent statement of equation (B.1). Hence it will be necessary to discuss the convergence of (B.6) in both of the senses used in chapter (II). Some results in this direction will be given in sections D and E.

(B) In practice the computation of $\overline{\eta}_i$ requires the solution of a finite system of linear equations, and to set up these equations we have to calculate $\delta \overline{\eta}_{i-1}$. This requires the knowledge of $\overline{\eta}_{i-1}$ outside the region in which the problem was originally specified. In accounts of the computational technique (for example [5], p. 78) it is suggested that the difference equation can be used to perform the extrapolation. We will discuss this point further in the next section.

C. Some Problems associated with the Application of the Difference Correction

Although there is at present little rigorous justification for the technique of difference correction, there is considerable evidence of its utility in practice. This is especially true for the boundary value problems of ordinary differential equations (reference [6] is devoted to the subject). We are concerned with the application of difference correction to the numerical solution of elliptic partial differential equations, and here the problem is more complicated.

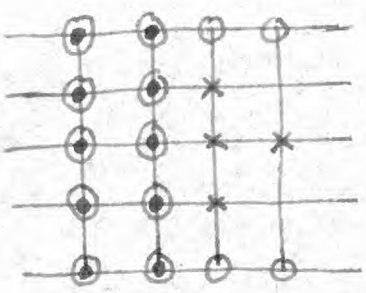
The main reasons for this are the following:

(1) The boundary of the region inwhich the problem is posed may not intersect the mesh at grid points so that we have to proceed (a) by using interpolation formulae to compute values at the internal grid points adjacent to the boundary, or (b) (more crudely) by transferring the boundary values to the nearest grid points.

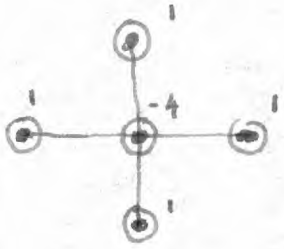
(2) In general we cannot obtain high order central differences of our approximate solutions at grid points in the neighbourhood of the boundary by using the difference equation to extrapolate the solution across the boundary as such a continuation is usually not defined without additional information (and even when defined it may be highly unstable).

In case 1(a) the difference correction formulae are considerably complicated at the grid points adjacent to the non-grid boundary mesh points; and in general, each of these points will need special treatment.

In case 1(b) difference correction is hardly appropriate as any correction process must take account of the modifications made to the original boundary.



(a)



(b)

Figure 1. The Continuation Problem

(a) Solution Values: ⊙

Continuation by five point formula: ×

Data required to complete the continuation: ○

(b) 'Five Point' formula for Laplace's Equation

(equation A.1)

If we consider problems set on rectangular regions (the simplest case) then we can illustrate the continuation problem as in figure 1. Without additional information the difference scheme specifies the continuation only in a triangular region whose dimensions depend on the ratio $h/k = \Delta x/\Delta y$ and on the length of the boundary. We see that the continuation is sufficient to give no more than the fourth central differences at an internal point adjacent to a boundary corner.

But even the existence of the continuation into this triangular region raises an interesting problem. Let us assume that the original problem is $\nabla^2\phi = 0$ in the interior of a rectangle with ϕ specified round the boundary; and let us assume that the prescribed values of ϕ are continuous everywhere, and that their first derivative in the direction of the boundary is continuous except at isolated boundary points. We have seen that the solution of the difference equation (B.2) converges to the true solution everywhere in the interior of the rectangle as the mesh tends to zero. Let us assume that the ratio $\Delta x/\Delta y$ is held constant. This then fixes the triangular extension. In this region the solution of the difference equation cannot tend to a function which is a harmonic continuation of the solution in the rectangle. This would imply the existence of a harmonic function which has isolated singularities (the points of discontinuity of the first derivative in the direction of the boundary) in whose neighbourhood it is bounded which is impossible [7].

Let us consider the difference equation at a point on the x = constant boundary which has the interior of the rectangle on the side x decreasing.

This can be written

$$\left[\Phi(x+h,y) - \Phi(x,y)\right] - \left[\Phi(x,y) - \Phi(x-h,y)\right]$$
$$= -\left[\Phi(x,y+k) - \Phi(x,y)\right] + \left[\Phi(x,y) - \Phi(x,y-k)\right] .$$

If x,y is a point of continuity of $\frac{\partial \phi}{\partial y}$ we have

$$\lim_{k\to 0} \frac{1}{k}\left\{\left[\Phi(x,y+k) - \Phi(x,y)\right] - \left[\Phi(x,y) - \Phi(x,y-k)\right]\right\} = 0$$

as $\phi = \Phi$ on the boundary.

In section B we showed that the error in Φ in the interior of R is $O(h^n)$. Thus if $\lim_{h\to 0} \frac{\phi(x,y) - \phi(x-h,y)}{h}$ exists then so will $\lim_{h\to 0} \frac{\Phi(x,y) - \Phi(x-h,y)}{h}$ and these limits will be equal. If we assume that these limits exist then, as the ratio h/k is fixed, the difference equation insists that $\frac{\partial \phi}{\partial x}$ must be continuous across the boundary.

This would imply a harmonic continuation into the triangular extension [8]; and we have already shown this to be impossible. In this case we must conclude that the difference equation must fail in the limit.

It will be seen that the boundary of the rectangle is a natural boundary of the solution to the problem we have been considering.

As an example to illustrate the above discussion consider the solution* of Laplace's equation in an infinite strip with the imposed boundary conditions

(a) $\phi(x,0) = x$, $0 \le x < \frac{1}{2}$,

(b) $\phi(x,0) = 1-x$, $\frac{1}{2} \le x \le 1$,

(c) $\phi(0,y) = \phi(1,y) = 0$, $-\infty < y \le 0$,

(d) $\phi(x,y) \to 0$, $y \to -\infty$.

---

* This example was suggested by Mr. Sidney Michaelson and Professor Bickley.

This problem has the solution

$$\phi = \frac{4}{\pi} \sum_{i=0}^{\infty} \frac{(-1)^i \sin(2i+1)\pi x \, e^{(2i+1)\pi y}}{(2i+1)^2} \qquad (C.1)$$

At $y = 0$ the normal derivative is given by

$$\frac{\partial \phi}{\partial y} = \frac{4}{\pi} \sum_{i=0}^{\infty} \frac{(-1)^i \sin(2i+1)\pi x}{2i+1}$$

$$= 1, \quad 0 < x < 1 .$$

Now let us assume that a harmonic continuation is possible in a small circle centre $(\bar{x},0)$, $0 < \bar{x} < \frac{1}{2}$. Then this continuation must be possible by means of power series (double Taylor series); and this series must agree with the solution of the Cauchy problem for $\nabla^2 \phi = 0$ with $\phi = x$ and $\frac{\partial \phi}{\partial n} = \frac{\partial \phi}{\partial y} = 1$ on the corresponding small section of the boundary by the Cauchy-Kowaleski theorem [8]. The solution of this Cauchy problem is $\phi = x+y$. This agrees with (C.1) nowhere in the interior of the given strip contradicting the supposition that the continuation was possible. Thus it follows that the segment of the boundary $0 \leq x \leq 1$ is a natural boundary of (3.1) - the case $\bar{x} > \frac{1}{2}$ is exactly similar.

For this equation we can also get an explicit solution for the approximate difference equation (B.2) (this is the equation that results if we use the five point formula of fig. 1b). We assume that $h = k$. To do this we carry out a finite harmonic analysis of $\phi(x)$ on $y = 0$, and then weight the trigonometric terms ($\sin i\pi x$: $i = 1, 2, \ldots, n-1$, $n = 1/h$) with the functions $e^{\beta_i y}$ to give the correct decay as $y \to -\infty$. We must have

$$\left\{ \delta^2_x + \delta^2_y \right\} \sin i\pi x \, e^{\beta_i y} = 0 ,$$

which gives

$$4 \sin^2 \frac{i\pi h}{2} = 4 \sinh^2 \frac{\beta_i h}{2},$$

whence $\beta_i = 2n \sinh^{-1} \left\{ \frac{1}{2} \sin \frac{i\pi}{2n} \right\}$.

For any finite value of n the solution of the difference equation is defined for all x and $y < +\infty$ but, as $\beta_{n-1} \to \infty$ as $h \to 0$, the solution tends to a finite limit nowhere in $y > 0$ as $h \to 0$.

As the solution of the difference equation is defined for all finite x and y for any $h > 0$, there is no continuation problem in calculating the first stage (B.4) of the difference correction; and here another feature becomes important. In this example the trigonometric factors are already exact and difference correction does not alter this, also their coefficients at $y = 0$ are fixed by the boundary conditions on the difference equation.

Now, assuming that the difference correction procedure converges, this implies that we get at the grid points not the values of the solution of the original problem but those of a modified problem in which the original boundary condition on $0 \leq x \leq 1$, $y = 0$ is replaced by its finite harmonic sum approximation on the mesh we are considering.

Using the maximum modulus theorem (which applies to harmonic functions) we have that the magnitude of the error in the solution obtained by difference correction is less than the maximum modulus of the error in the approximation to the original boundary conditions.

This example highlights an interesting defect of difference correction when applied to partial differential equations. Let us assume that all other difficulties have been overcome and that we have obtained satisfactory

convergence to a solution (we will see that this need not imply that the difference correction procedure converge). The solution whose values we get at the mesh points satisfies not the prescribed boundary conditions but an m point interpolation of them; and the accuracy we get depends on the rate of convergence of this interpolation. There is thus a case for solving the problem again on a finer mesh even after we have calculated the difference correction. This point has been made before from a somewhat different point of view in [9] and elsewhere. Also some recent work by Collatz [10] is of interest because, although his methods are quite remote from our own, it illustrates the importance of adequately interpolating to the boundary conditions.

D. Calculation of the Difference Correction

Let us consider the solution of the Poisson equation

$$\nabla^2 \phi = f(x,y) \tag{B.1}$$

on a square of side unity with $\phi = 0$ being the prescribed boundary condition. With this boundary condition the operator ∇^2 has the eigenfunctions

$$\phi_{ij} = \sin i\pi x \sin j\pi y ,$$

and the eigenvalues

$$\lambda ij = i^2 \pi^2 + j^2 \pi^2 .$$

The solution of (B.1) is then

$$\phi = 4 \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} - \frac{(f,\phi_{ij})}{\lambda ij} \phi_{ij} \tag{D.1}$$

where $(f,\phi_{ij}) = \int_0^1 \int_0^1 f\phi_{ij} \, dx \, dy$ - the scalar product of f and the eigen function ϕ_{ij}.

Let us assume that $f(x,y)$ is defined <u>for all values of</u> x <u>and</u> y by the expansion

$$f = 4 \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} (f,\phi_{ij}) \phi_{ij} \tag{D.2}$$

then the function ϕ defined by (D.1) satisfies (B.1) for all values of x and y. It is thus reasonable to speak of it as valid in the whole plane.

We now consider the application of difference correction to (B.1) with $f(x,y)$ defined as a periodic function by (D.2). <u>This specification of</u> $f(x,y)$ <u>as a periodic function is essential to our argument</u>.

For convenience we will set $h = k$. In this case we consider the difference operator $\delta_x^2 + \delta_y^2$. The eigenfunctions of this operator which satisfy the boundary condition zero on a square of side unity are

$$\phi_{ij} = \sin i\pi x \sin j\pi y$$

with $i, j = 1, 2, \ldots, n-1$, $(n = 1/h)$.

The eigenvalues are

$$\mu_{ij} = 4 \sin^2 \frac{i\pi}{2n} + 4 \sin^2 \frac{j\pi}{2n} .$$

The solution of the difference equation (B.2) is

$$\Phi = \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} - H_{ij} \frac{\phi_{ij}}{\mu_{ij}} ,$$

where $H_{ij} = \frac{4}{n^2} \sum_{r=1}^{n-1} \sum_{s=1}^{n-1} h^2 f(\frac{r}{n}, \frac{s}{n}) \phi_{ij}(\frac{r}{n}, \frac{s}{n})$, and

$$g(x,y) = h^{-2} \sum_{r=1}^{n-1} \sum_{s=1}^{n-1} H_{ij} \phi_{ij}$$

is a finite harmonic sum approximation to $f(x,y)$ - that is

$$g(\frac{r}{n}, \frac{s}{n}) = f(\frac{r}{n}, \frac{s}{n}) \; ; \; r, s = 1, \ldots, n-1 .$$

Now, using the periodicity of both f and g, we see that $g(x,y)$ is a finite harmonic sum approximation everywhere in the x,y plane. Hence Φ is defined everywhere and satisfies (B.2) for all values of x and y. We can now calculate $\mathcal{C}\Phi$ which is again defined in the whole plane as a finite sum of the ϕ_{ij}. The problem of solving (B.4) is thus technically the same as that of solving (B.2); and this is also true of each of the equations (B.5).

Thus we have

$$\bar{\eta}_{i-1} = \sum_{r=1}^{n-1}\sum_{s=1}^{n-1} A_{rs}^{(i-1)}\,\phi_{rs}\,,$$

and $$\delta\,\bar{\eta}_{i-1} = \sum_{r=1}^{n-1}\sum_{s=1}^{n-1} A_{rs}^{(i-1)}\,\delta\,\phi_{rs}\,.$$

Now $\delta\,\phi_{rs}$ is given by $-(h^2D^2 - \delta^2)$ * operating on ϕ_{rs}, that is by

$$\delta\,\phi_{rs} = \left[h^2(r^2\pi^2 + s^2\pi^2) - 4\sin^2\frac{r\pi}{2n} - 4\sin^2\frac{s\pi}{2n}\right]\phi_{rs}$$
$$= \left[h^2\lambda_{rs} - \mu_{rs}\right]\phi_{rs}\,.$$

As the eigenfunctions of $\delta_x^2 + \delta_y^2$ are orthogonal with respect to summation over the mesh we have

$$\bar{\eta}_i = \sum_{r=1}^{n-1}\sum_{s=1}^{n-1} A_{rs}^{(i-1)}\,\frac{h^2\lambda_{rs} - \mu_{rs}}{-\mu_{rs}}\,\phi_{rs}\,,$$

$$\therefore\ A_{rs}^{(i)} = -A_{rs}^{(i-1)}\,\frac{h^2\lambda_{rs} - \mu_{rs}}{\mu_{rs}}\,.$$

For the series $\sum_{i=1}^{\infty}\bar{\eta}_i$ to be convergent we must have

$$\max_{r,s}\ \frac{h^2\lambda_{rs} - \mu_{rs}}{\mu_{rs}} = \max_{r,s}\ \frac{r^2\pi^2 + s^2\pi^2}{4h^{-2}(\sin^2\frac{r\pi}{2n} + \sin^2\frac{s\pi}{2n})} - 1 \quad < 1\,.$$

The maximum occurs when $r = s = n-1$. Putting $(n-1)\pi/n = \rho$, the condition becomes

$$\frac{\rho^2}{4\sin^2\rho/2} - 1 \quad < 1\,.$$

As $n \to \infty$, $\rho \to \pi$, and the left hand side of this inequality tends to $\pi^2/4 - 1$ or about 1.5. Thus for n greater than a certain finite value (in fact $n = 8$) the difference correction procedure fails to con-

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* by the equivalence of the finite difference formulae with differentiation for $\sin\lambda x$ $(\lambda < \pi/n)$.

verge for this problem. But we can say more for, even when the difference correction procedure converges, we obtain not point values of the solution of (B.1), but point values of the solution of a modified problem in which $f(x,y)$ is replaced on the right hand side of (B.1) by a finite harmonic sum approximation to it on the given mesh. We now give a proof of the result.

From the manner of its construction we have that $\eta_1 = \sum_{i=1}^{\infty} \bar{\eta}_i$ satisfies the difference equation

$$\left[\delta_x^2 + \delta_y^2 - \mathcal{C}\right]\eta_1 = \mathcal{C}\Phi .$$

Now, as $\sin r\pi x$ satisfies the equation

$$h^2 \frac{d^2}{dx^2} \sin r\pi x = \left[\delta^2 - \frac{1}{12}\delta^4 + \frac{1}{90}\delta^6 \ldots\right] \sin r\pi x$$

with $r = 1, 2, \ldots, n-1$, we also have that η_1 satisfies the differential equation

$$\frac{\partial^2 \eta_1}{\partial x^2} + \frac{\partial^2 \eta_1}{\partial y^2} = h^{-2}\mathcal{C}\Phi$$

$$= \sum_{i=1}^{n-1}\sum_{j=1}^{n-1} -\frac{H_{ij}}{\mu_{ij}} h^{-2}\mathcal{C}\phi_{ij} ,$$

and, hence, that

$$\eta_1 = \sum_{i=1}^{n-1}\sum_{j=1}^{n-1} -\frac{H_{ij}}{\mu_{ij}} \frac{\lambda_{ij} - h^{-2}\mu_{ij}}{-\lambda_{ij}} \phi_{ij} ;$$

$$= \sum_{i=1}^{n-1}\sum_{j=1}^{n-1} \frac{H_{ij}}{\mu_{ij}} \phi_{ij} + h^{-2} \sum_{i=1}^{n-1}\sum_{j=1}^{n-1} -\frac{H_{ij}}{\lambda_{ij}} \phi_{ij}$$

$$= -\Phi + \Psi(x,y) .$$

We see that $\Psi(x,y)$ satisfies the Poisson equation

$$\nabla^2 \Psi = g(x,y)$$

which establishes the stated result.

E. Nature of the approximation by Difference Correction

In sections C and D we have illustrated the fact that equations (B.1) and (B.3) are not equivalent statements of the same problem (a) because the information necessary to enable the high order differences in $\mathcal{C}\phi$ to be computed may not be available, and (b) because even when the procedure outlined in section B can be carried through (as in section D the solution of (B.3) is, in general, not the same function as the solution of (B.1)). It is not even cotabular with it at the grid points in the interior of the specified region.

For these reasons we will consider in this section not equation (B.3) but the equation

$$\left[\delta^2_{x^*} + \delta^2_{y^*}\right] \chi = h^* f + \mathcal{C}_m \chi \qquad \text{(E.1)}$$

where $\mathcal{C}_m$ has been written for the expression obtained by truncating at differences of order $2m$. We see that ϕ satisfies this equation with an error which tends to zero with h^{2m+2} provided the order of $\mathcal{C}_m$ has been suitably restricted. The factors determining the order of $\mathcal{C}_m$ are our ability to continue ϕ beyond the boundaries of the region R, and the differentiability of ϕ in the extended region. The error estimate for ϕ may be derived by using the Taylor expansion (in general the finite expansion plus remainder term) in the calculation of the differences occurring in (E.1).

Two other estimates of this type which we will need in this section are

$$\left[\delta^2_{x^*} + \delta^2_{y^*}\right] g(x, y) = O(h^* g) \qquad \text{(E.2)}$$

and

$$\mathcal{E}_m\, g(x, y) = O(h^4 g) \qquad (E.3)$$

Provided h (mh in (E.3)) is less than the radius of convergence of the Taylor series for g about the point x,y. The condition that g be regular is stronger than we need; and it is sufficient that g can be represented by a polynomial of order at least that of the highest order difference considered plus a remainder term which remains uniformly small. The first estimate (equation (E.2)) is easily derived. We have

$$\delta_x^2 g(x,y) = g(x+h,y) - 2g(x,y) + g(x-h,y)$$

$$= \sum_{i=1}^{\infty} \frac{h^i}{i!} \frac{d^i g}{dx^i}\Big|_{x,y} + \sum_{i=1}^{\infty} \frac{(-h)^i}{i!} \frac{d^i g}{dx^i}\Big|_{x,y} ,$$

$$= h^2 \frac{d^2 g}{dx^2} + \frac{h^4}{12} \frac{d^4 g}{dx^4} + \ldots = O(h^2 g) , \text{ and the second}$$

difference in the y direction can be computed in the same way.

Instead of the sequence of equations (B.2), (B.4), (B.5) which define the recursion for the difference correction we now consider the system

$$\left[\delta_x^2 + \delta_y^2\right] \Phi = h^2 f ,$$

$$\left[\delta_x^2 + \delta_y^2\right] \xi_1 = \mathcal{E}_m \Phi ,$$

$$\cdots\cdots\cdots$$

$$\left[\delta_x^2 + \delta_y^2\right] \xi_i = \mathcal{E}_m \xi_{i-1} , \quad i = 2, 3, \ldots, m-1 .$$

A formal application of equation (E.3) gives

$$\left[\delta_x^2 + \delta_y^2\right] \xi_i = O(\mathcal{E}_m \xi_i) = h^4 O(\xi_{i-1}) .$$

Thus $\xi_i = h^2 O(\xi_{i-1})$. Also $\Phi = O(1)$ so that

$$\xi_i = O(h^{2i}) .$$

Now $\Psi = \Phi + \sum_{i=1}^{m-1} \xi_i$ satisfies the equation

$$\left[\delta_x^2 + \delta_y^2\right]\Psi = h^2 f + \mathcal{C}_m \Psi - \mathcal{C}_m \xi_{m-1} .$$

$$= h^2 f + \mathcal{C}_m \Psi + O(h^{2m+2}) ,$$

so that $(\Psi - \phi)$ satisfies the difference equation

$$\left[\delta_x^2 + \delta_y^2 - \mathcal{C}_m\right](\Psi - \phi) = O(h^{2m+2}) . \qquad (E.4)$$

We can make this result definite for the example of section D by deriving the estimates for the ξ_i by a direct method. Starting with the equation

$$\left[\delta_x^2 + \delta_y^2\right]\xi_i = \mathcal{C}_m \xi_{i-1}$$

we have

$$\left[\delta_x^2 + \delta_y^2\right]^2 \xi_i = \left[\delta_x^2 + \delta_y^2\right]\mathcal{C}\,\xi_{i-1}$$

$$= \mathcal{C}_m^2 \xi_{i-2} .$$

This procedure can be repeated and gives finally

$$\left[\delta_x^2 + \delta_y^2\right]^{i+1} \xi_i = h^2 \left[\mathcal{C}_m\right]^i f .$$

To specify the solution of this equation we must impose i boundary conditions in addition to the boundary condition $\xi_i = 0$. As the ξ_p, $p = 1, 2, \ldots, m-1$ can be expressed in terms of the ϕ_{ij} (of section D), the expansions being valid in the whole plane, and as the even order differences of ϕ_{ij} are proportional to ϕ_{ij} which vanishes on the boundary of the square, the most convenient boundary conditions to impose are

$$\left[\delta_x^2 + \delta_y^2\right]^p \xi_i = \mathcal{C}_m^p \xi_{i-p} = 0 , \quad p = 1, 2, \ldots, i .$$

We see that the iterated difference operator has the same eigenfunctions

for the square as the operator $\delta_x^2 + \delta_y^2$ (that is the ϕ_{ij}), and that its eigenvalues are those of the operator $[\delta_x^2 + \delta_y^2]$ raised to the (i+1)st power. Thus we have

$$\xi_i = \sum_{p=1}^{n} \sum_{q=1}^{n} \frac{h^2(\phi_{pq}, \mathcal{C}_m^i f)}{(\phi_{pq}, \phi_{pq})} \frac{\phi_{pq}}{-(\mu_{pq})^{i+1}}$$

where the scalar product here implies summation not integration.

Now $h^{-2}\mu_{ij} > 4((i-1)^2+(j-1)^2)$, and $(\phi_{pq}, \phi_{pq}) = n^2/4$ so that the components of ξ_i satisfy the inequality

$$|\xi_i| < 4\, h^{-2i} \max |\mathcal{C}_m^i f| \sum_{p=1}^{n} \sum_{q=1}^{n} \frac{1}{(h^{-2}\mu_{pq})^{i+1}},$$

and we have $\sum_{p=1}^{n} \sum_{q=1}^{n} \frac{1}{(h^{-2}\mu_{pq})^{i+1}}$ bounded for all n by comparison with the series $\sum_{p=1}^{n} \sum_{q=1}^{n} \frac{1}{4(i^2+j^2)^{i+1}}$ with $i \geq 1$. Therefore $\xi_i = O(h^{2i})$ provided that equation (E.3) can be applied recursively to estimate $\mathcal{C}_m^i f$.

To justify the estimates for the ξ_i in the general case is more difficult. As ξ_i is the solution of a difference equation it is defined only at a discrete set of points; and a possible approach is to show that ξ_i is cotabular with a function for which the estimate of (E.2) and (E.3) are valid. A result of this type was indicated in section B.

For the example of section D we can also invert equation (E.4) to estimate $(\phi-\psi)$. Equation (E.4) is a difference equation of order 2m. Therefore to specify the solution of this equation posed as a boundary

value problem it is necessary to give m boundary conditions. Here it is convenient to specify the even order differences normal to the boundary of order up to $2m-2$ as well as the value of the function on the boundary. As both ϕ and ψ are expressible in terms of the ϕ_{ij} (the expressions being valid in the whole plane as in section D) we see that the boundary conditions are

$$\left[1, \delta_\nu^2, \delta_\nu^4, \ldots, \delta_\nu^{2m-2}\right](\phi - \psi) = 0 \qquad (E.5)$$

where ν denotes that differences are taken in the direction normal to the boundary.

We see that the operator $\delta_x^2 + \delta_y^2 - \rho_m$ has the eigenfunctions ϕ_{ij}, and the eigenvalues

$$\rho_{ij} = 4\sin^2\left(\frac{i\pi}{2n}\right) + 4\sin^2\left(\frac{j\pi}{2n}\right) + \frac{1}{12}\left[\left(4\sin^2\frac{i\pi}{2n}\right)^2 + \left(4\sin^2\frac{j\pi}{2n}\right)^2\right] + \ldots .$$

In particular we see that

$$\rho_{ij} > \mu_{ij} = 4\sin^2\frac{i\pi}{2n} + 4\sin^2\frac{j\pi}{2n} .$$

If we write equation (E.4) as

$$\left[\delta_x^2 + \delta_y^2 - \rho_m\right](\phi - \psi) = h^{2m+2} g$$

then, by an easy estimate of the eigenfunction expansion of the solution, we have

$$\max|\phi - \psi| < h^{2m}\, 4 \max|g| \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{1}{h^{-2}\mu_{ij}} .$$

As $\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{1}{i^2+j^2} = O(\log n)$ for large n we have that

$$\max|\phi - \psi| \le K h^{2m} \log\left(\tfrac{1}{h}\right) \qquad (E.6)$$

where K is some number independent of h.

It is of interest to analyse $(\phi - \psi)$ directly. A typical term $(i, j < n)$ would be

$$\Delta_{ij} = -\frac{\phi_{ij}}{\lambda_{ij}} \left\{ (f, \phi_{ij}) - H_{ij} \frac{\lambda_{ij}}{\rho_{ij}} \left(1 + \sum_{k=1}^{m-1} A_{ij}^{(k)}\right) \right\}$$

where the $A_{ij}^{(k)}$ are here defined by the recursion (compare with section D)

$$A_{ij}^{(k)} = -A_{ij}^{(k-1)} \frac{\rho_{ij} - \mu_{ij}}{\mu_{ij}} .$$

The expression for Δ_{ij} simplifies to

$$-\frac{\phi_{ij}}{\lambda_{ij}} \left\{ (f, \phi_{ij}) - H_{ij} \frac{\lambda_{ij}}{\rho_{ij}} \left(1 + \left(\frac{\mu_{ij} - \rho_{ij}}{\rho_{ij}}\right)^m\right) \right\} .$$

Now $H_{ij} = h^{\alpha}(f, \phi_{ij}) + h^{\alpha}$ $\times$ coefficients of terms in the Fourier series (D.2) corresponding to harmonics with i and $j > n$, so that the goodness of the approximation of ψ to ϕ depends on two factors (1) the improvement in the approximation to the lower eigenvalues ($h^{-2}\rho_{ij}$ is a better approximation to λ_{ij} than $h^{-2}\mu_{ij}$), and (2) the rate of decrease of the Fourier coefficients in equation (D.2).

The second condition is really the critical one as it is on the differentiability properties of f that those of ϕ depends, and these are reflected in the rate of decrease of the Fourier coefficients. In particular we see that the type of continuation used in section D is suitable only for functions f which have the correct periodicity properties.

It seems that the difference correction in the form described in this section gives, where applicable, a better approximation to the

solution ϕ of the differential equation. Using the terminology of Chapter (II), subsection C, we may interpret equation (B.3) as the formal statement of an asymptotic relation. The difference correction procedure is thus a method of computing the solution of an equation which lies close to this asymptotically satisfied difference equation. A general proof that this solution is a good approximation to ϕ is more difficult than in the example of this section as the boundary values (B.3) are not in general zero, and further analysis must be done to show that they are sufficiently small. However, the method of approach used in this section should be capable of extension to more general problems.

6. Difference Correction and h^2-Extrapolation

It must be pointed out that no discrepancy between the theory and practice of difference correction has been noted precisely because the numerical technique has been treated as an asymptotic expansion. For example, in reference [6], it is recommended that only converging differences be kept at any stage as the diverging, high order differences will be severely contaminated by round off errors.* This then ensures a recursion of the type considered in the previous section. Moreover, this recursion is continued only until the terms become small - one again the probability that rounding errors will dominate all subsequent calculations is sufficient reason for stopping the computation at this point. Thus, provided h is chosen small enough so that differences of some convenient order are negligible, we can be confident that difference correction leads to numerical values that are as accurate as rounding errors will permit.

When solving partial differential equations considerably less is attempted. In reference [4] only the fourth differences of the solution to the difference equation are calculated at the grid points in R, and these are found by using the difference equation to extrapolate the solution to the exterior grid points adjacent to the boundary. These values are then used to compute a first approximation to the required correction. It is noted that in every case the result gave a marked improvement to the solution of the basic difference equation.

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* The effect of round off error on differences is very similar to that of the dominance of high order harmonics.

Here it seems that the difference correction gives an h^8-extrapolation of the solution of (B.2). In fact the correction is given by solving the basic difference equations approximating to the differential equations determining the h^8 terms in Φ (the solution of (B.2)). We must show that the error in setting up the right hand sides of these equations is $O(h^8)$.

As $\Phi = \phi + O(h^8)$, and $\delta^4 = h^4 D^4 + O(h^6)$ this result is immediate everywhere in the interior of R except for the mesh points adjacent to the boundary where an exterior value must be used in calculating at least one of the fourth differences. It is probable that it also holds at these points. To see this we note that it is possible (for any fixed h) to find polynomial solutions to (B.2) cotabular everywhere in R. These polynomials will differ from ϕ by an error term which is $O(h^8)$ in R. This will also be true of the error in approximating the fourth derivatives of ϕ by means of the fourth derivatives of these polynomials, and hence by means of fourth differences of the solution of the difference equation. This will be true everywhere in R.

The use of special sets of polynomials in the solution of Laplace's equation has been discussed in reference [11]. It is here noted that the polynomial expansions are not unique. This affords another illustration of the continuation problem.

Appendix. Solution of Reynold's equation

We follow several previous workers in using finite difference methods to integrate this equation (for example, Christopherson [12], or Raimondi and Boyd [13]).

As a first step it is convenient to transform the differential equation by introducing the new variable η by means of the relation

$$P = \eta / h^{3/2} . \tag{1}$$

This transformation serves two purposes. First it reduces the differential equation to normal form; and second it gives a dependent variable which changes far more smoothly in regions where h is small. It is thus advantageous for numerical work. This transformation is used in Christopherson [12]. It is readily verified that the boundary conditions on η are identical with those on P.

In the usual non-dimensional form the equation becomes

$$\frac{\partial^2 \eta}{\partial \theta^2} + \alpha^2 \frac{\partial^2 \eta}{\partial y^2} + \frac{3}{4} \frac{2\varepsilon\cos\theta + \varepsilon^2\cos 2\theta + \varepsilon^2\cos^2\theta}{(1+\varepsilon\cos\theta)^2} \eta = -\frac{6\varepsilon\sin\theta}{(1+\varepsilon\cos\theta)^{3/2}} \tag{2}$$

where $\alpha = \frac{\text{radius of bearing R}}{\text{breadth of bearing h}}$, and ε is the eccentricity of the bearing. In the numerical work that has been carried out to this stage we have used the standard finite difference equation (A.1). This is also the equation which has been used by the other investigators.

The boundary of the lubricating film is unknown and must be calculated by some kind of iteration procedure. This has been done by Raimondi and Boyd using the Liebman iteration, and by Christopherson using relaxation by requiring that the solution of the approximate difference equation never take negative values.

Our approach has been to approximate the end boundary by a straight line and to ask that $\frac{\partial \eta}{\partial \theta} = 0$ at the mid point of this line as well as $\eta = 0$ on it. We solve for η for a trial rectangular region with $\eta = 0$ as boundary condition, and then compute $\frac{\partial \eta}{\partial \theta}$ at the said mid point of the end boundary. If this is not zero then this boundary position is adjusted.

Programmes to carry out this part of the computation has been completed. It is hoped to finish the computation by calculating values of η on the rectangular end edge which will make η and $\frac{\partial \eta}{\partial \theta}$ vanish on some interior line; and we have worked out formulae to do this. This will add another stage to the iteration. However, it will not be necessary to know much more about the initial guess of the film extent than that it is an over estimate.

The initial approximation turns out to be a useful one, and spot checks have shown good agreement with the results of previous investigators (for example Sassenfeld and Walther [14]). The disagreements (up to 5% for $\varepsilon = .95$) can be explained in part by the inadequacy of the integration routine for evaluating the resultant thrust on the bearing. In the original programme we used the trapezoidal rule; and this has now been modified to use Simpson's rule. This appears to give an improvement having the right order of magnitude.

We will now describe in greater detail the actual method used for the solution of the difference equation.

We write equation (2) as

$$\frac{\partial^2 U}{\partial \Theta^2} + \alpha^2 \frac{\partial^2 U}{\partial y^2} + a(\Theta)U = b(\Theta) .$$

Using this terminology the difference equation can be written

$$UX + YU = H , \qquad (3)$$

where U is the $(n \times m)$ matrix of the solution values at the grid points in the approximate lubricating film,

X is the $(n \times m)$ matrix $\left[h^{-2} \delta^2 + a \right]$ operating on the rows of U,

Y is the $(m \times m)$ matrix $\alpha^2 \left[k^{-2} \delta^2 \right]$ operating on the columns of U,

and H is the $(n \times m)$ matrix of the values of $b(\Theta)$ at the grid points.

We consider only half the bearing width as the flow will be symmetric about the centre line; and we take the boundary condition $\frac{\partial U}{\partial y} = 0$ at $y = \frac{1}{2}$ as in figure 1.

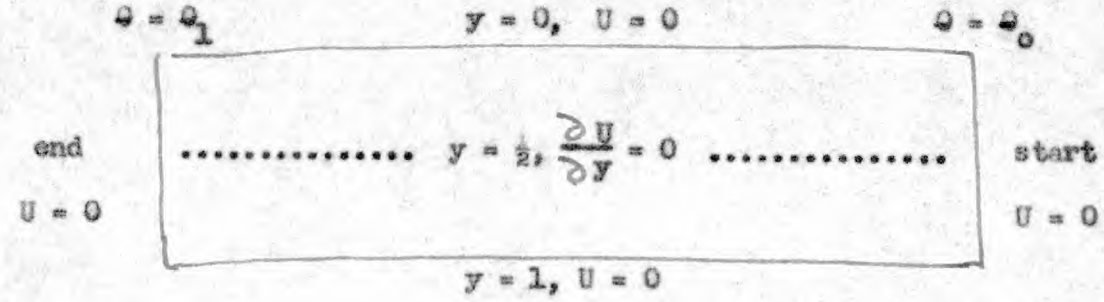


fig. 1

X is the matrix

$$\begin{bmatrix} -2h^{-2}+a_1 & h^{-2} & & \\ h^{-2} & -2h^{-2}+a_2 & h^{-2} & \\ \cdots & \cdots & \cdots & \cdots \\ & & h^{-2} & -2h^{-2}+a_n \end{bmatrix} ;$$

and Y is the matrix

$$\alpha^2 \begin{bmatrix} -2k^{-2} & k^{-2} & & & \\ k^{-2} & -2k^{-2} & k^{-2} & & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & & k^{-2} & -2k^{-2} & k^{-2} \\ & & & 2k^{-2} & -2k^{-2} \end{bmatrix} .$$

We see that the symmetry of Y is destroyed by the last row. Y has the eigenvalues

$$\lambda_j = -4\alpha^2 k^{-2} \sin^2 \left(\frac{2j+1}{2m}\pi\right), \quad k = \tfrac{1}{2}m, \; j = 0, 1, \ldots, m-1 ,$$

The right eigenvectors of Y are

$$(\underset{\sim}{\phi}_j)_s = \sin (2j+1)\pi \frac{s}{2m} , \quad s = 1, 2, \ldots, m ;$$

and the biorthogonal left eigenvectors are

$$(\underset{\sim}{\phi}^*_j)_s = \sin (2j+1)\pi \frac{s}{2m} , \quad s = 1, 2, \ldots, m-1 ,$$

$$(\underset{\sim}{\phi}^*_j)_m = \tfrac{1}{2} \sin (2j+1)\pi \frac{m}{2m} .$$

It will be necessary to normalise these vectors. We have

$$\frac{1}{2m}\left[\sum_{s=1}^{m-1} \sin^2 (2j+1)\pi \frac{s}{2m} + \tfrac{1}{2} \sin^2 (2j+1)\pi \frac{m}{2m}\right] ,$$

$$= \int_0^{\frac{1}{2}} \sin^2 (2j+1)\pi x \, dx = 1/4$$

as the trapezoidal rule is exact for this case.

$$\therefore \underset{\sim}{\phi}_j^{*'} \underset{\sim}{\phi}_j = \frac{m}{2} ,$$

and the normalised vector is $\sqrt{\frac{2}{m}}\,\underset{\sim}{\phi}_j$. In the actual programme the variable location V_3 contains $\frac{1}{2}m$ so that the normalising factor is

$$V = \phi \ \text{sqrt}(4V_3) .$$

The matrix H is given by

$$\begin{bmatrix} b(\theta_1) & b(\theta_2) & \ldots\ldots & b(\theta_n) \\ b(\theta_1) & b(\theta_2) & \ldots\ldots & b(\theta_n) \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ b(\theta_1) & b(\theta_2) & \ldots\ldots & b(\theta_n) \end{bmatrix} .$$

We can write equation (5) as

$$U X + H \Lambda M^{*'} U = H$$

where M , and M^* are the matrices of the normalised right and left eigenvectors of Y respectively, and Λ is the diagonal matrix whose elements are the eigenvalues.

We can now write this as

$$M^{*'} U X + \Lambda M^{*'} U = M^{*'} H ,$$

or $$V X + \Lambda V = G .$$

Let $\{V_j\}$ denote the j^{th} row of V, then we have

$$\{V_j\} X + \lambda_j \{V_j\} = \{G_j\} .$$

Transposing we have the equation

$$\left[X + \lambda_j I \right] \{V_j\}' = \{G_j\}' ,$$

$$j = 1, 2, \ldots, m \qquad (4)$$

This gives a system of m sets of linear equations to solve for the components of V. When this has been done the solution is given by the matrix product

$$U = N V .$$

The above procedure has been suggested by Bickley and MacNamee in a recent paper [15]. Our programme represents the first practical application of this technique which has an advantage over standard direct procedures (see for example [16]) in that the machine storage can be utilised more efficiently (our programme uses $2mn$ against the $(mn)^2 + (mn)$ storage locations needed in the triangulation of the partitioned matrix).

The derivative $\frac{\partial U}{\partial \Omega}$ at the end position is found from the formula

$$\frac{\partial U}{\partial \Omega} = h^{-1} \mu \delta U(n+1), m ,$$

$$= \frac{h^{-1}}{2} (U(n+2), m - Un, m) .$$

This formula involves the unknown grid value $U(n+2), m$; and this can be found from the difference equation centred on $Un+1, m$.

This gives

$$h^{-2}(U(n+2), m + Un, m) = b(n+1)$$

as all other terms have the value zero because U vanishes on the end line.

$$\therefore \quad \frac{\partial U}{\partial \theta} = h^{-1}\left(-U_{n,m} + \frac{h^2}{2} b(n+1)\right) \quad . \qquad (5)$$

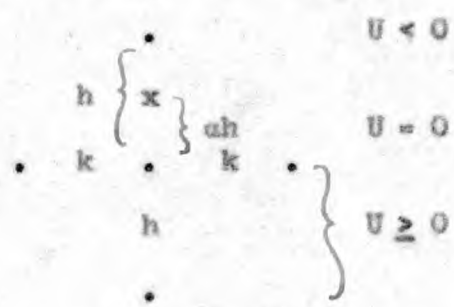
It is hoped that the following formulae will enable the position of the end line to be calculated more accurately. If we assume that our rectangular approximation to the film is too large, then the computed pressures will become negative near our approximate end line. We plan to compute a better approximation as follows.

(1) We compute the position of the interior line along which the pressure vanishes.

(2) We increase the values of U on the approximate end boundary to try and make $\frac{\partial U}{\partial \theta}$ vanish on the zero line computed in (1).

It will be seen that (2) will give a new boundary condition on the approximate end line; and the suggestion is that we recalculate our solution using this new boundary condition. The whole procedure is to be repeated until the solution settles down.

Stage (1) of the computation is the calculation of the line of zero pressure. We consider the stencil



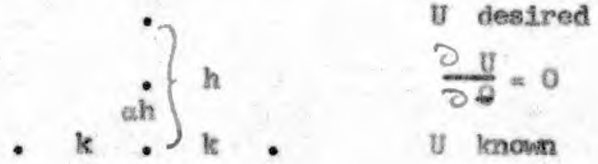
The problem is to find α such that $U = 0$. Perhaps the best formula to use for this is the finite difference formula approximating to the differential equation using unequal intervals in the $\theta(h)$

direction. For our equation the formula is

$$b_i = (a_i + k^{-2}\delta_y^2)U_{ij} + \frac{2h^{-2}}{\alpha^2+\alpha}\left\{ U_{i+1,j} + \alpha U_{i-1,j} - U_{ij}(1+\alpha).\right\} \quad (6) .$$

The value of α is found by setting $U_{i+1,j} = 0$ and solving the resulting equation for α .

In stage (2) of the computation we can assume the following stencil



Here we want to replace the U value which was previously < 0 by one which makes $\frac{\partial U}{\partial \Omega} = 0$ at the point αh . The difference equation linking these values is

$$h^2(1 - 2\alpha)\left[a_i U_{ij} + k^{-2}\delta_y^2 U_{ij} - b_i \right] + 2\left\{ (U_{i+1,j} - U_{ij}) - h\frac{\partial U}{\partial \Omega} \right\} = 0 . \quad (7)$$

In this case we put $\frac{\partial U}{\partial \Omega} = 0$, and solve for $U_{i+1,j}$.

Equations (6) and (7) are both obtained by fitting a quadratic interpolation polynomial to the given data. The details are very similar to those for the construction of the standard finite difference equation as described in section (A) .

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h^2-EXTRAPOLATION IN EIGENVALUE PROBLEMS

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SUMMARY

It is a common hypothesis that the error involved in a certain numerical process is an analytic function of a parameter which specifies in some way the closeness of the approximations used. We consider this hypothesis in detail for difference approximations to differential equation eigenvalue problems. Our approach is to construct the solution of this difference equation by determining a recurrence for the terms in its Taylor series. Existence is then guaranteed by the convergence of this series. The solution thus obtained is used as the basis for a discussion of methods by which h^2-extrapolation of the eigenvalues and eigenvectors of the difference equation could be obtained.

1. Introduction†

To make our problem definite we restrict ourselves to the eigenvalue problems of second-order, self-adjoint differential equations, although our method clearly has much wider application. The results could readily be duplicated in a particular case by following the procedure outlined in this paper.

We proceed in the usual way, and approximate to the differential equation by a difference equation on a finite grid of points of mesh length h. As we increase the number of points in the grid and let $h \to 0$, we expect the eigenvalues of this difference equation to tend to the eigenvalues of the differential equation. We can write this as

$$\lim_{h\to 0} \lambda_p(h) = \lambda_p$$

for the pth eigenvalue. We also ask that the components of the pth eigenvector of the difference equation tend to the values of the pth eigenfunction evaluated at the ordinate points $x = ih$. That is

$$\lim_{h\to 0} \phi_p(x = ih, h) = \phi_p(x),$$

where here we regard x as a fixed ordinate point and i (an integer) and h as variables, and where we set

$$\phi_p(\bar{x}, h) = \phi_p(\bar{x}) \neq 0$$

for all h and fixed $\bar{x}$ to make definite the scaling of the eigenvectors.

† The argument in sections 1–3 follows closely that of Fox (**1**), 332–42.

This behaviour is certainly guaranteed if we can form the expansions

$$\lambda(h) = \sum_{m=0}^{\infty} \frac{h^m}{m!} \frac{d^m\lambda(0)}{dh^m} \tag{1}$$

and
$$\phi(x = jh, h) = \sum_{m=0}^{\infty} \frac{h^m}{m!}\left\{ \sum_{r+s=m} (j-i)^s \frac{m!}{s!\,r!} \frac{\partial^m\phi(x = ih, 0)}{\partial x^s \partial h^r}\right\}. \tag{2}$$

In all subsequent discussion we will write

$$\frac{\partial^m\phi(x = ih, 0)}{\partial x^s \partial h^r} = \frac{d^s}{dx^s}\left\{\frac{\partial^r\phi(x = ih, 0)}{\partial h^r}\right\} = \frac{d^s}{dx^s}\frac{\partial^r\phi(x)}{\partial h^r}$$

to emphasize that the coefficients of h^m in (2) are functions of x alone. Note that we could just as well have written (2) as

$$\phi(x = ih, h) = \sum_{m=0}^{\infty} \frac{h^m}{m!}\phi_m(x = ih).$$

However, convergence of this expansion gives to ϕ_m the meaning $\partial^m\phi/\partial h^m$; and our notation anticipates this result.

The most general differential equation of the type we consider can be written, after suitable transformation, in the form

$$\frac{d^2\phi}{dx^2} + r(x)\{\lambda - q(x)\}\phi = 0. \tag{3}$$

Together with (3) we consider the class of boundary conditions

$$A_0\phi(0) + B_0\frac{d\phi(0)}{dx} = 0 \tag{4}$$

and
$$A_1\phi(1) + B_1\frac{d\phi(1)}{dx} = 0 \tag{5}$$

given at the ends of the interval $(0, 1)$. We put $r(x) = 1$ in our subsequent calculations as this simplifies the arithmetic—it is not difficult to return to the more general case.

2. Approximation of the boundary conditions

We first consider what restrictions central difference approximations to (4) and (5) place on the expansion (2). The simplest representation of (4) is

$$A_0\phi(0, h) + \frac{B_0}{2h}\{\phi(h, h) - \phi(-h, h)\} = 0. \tag{6}$$

This must be an identity in h. Therefore, when (2) is substituted in (6), the coefficients of powers of h must vanish. This leads to a series of

relations, the first few of which are

$$h^0\colon\ A_0\phi(0)+B_0\frac{d\phi(0)}{dx}=0, \tag{7}$$

$$h^1\colon\ A_0\frac{\partial\phi(0)}{\partial h}+B_0\frac{d}{dx}\frac{\partial\phi(0)}{\partial h}=0, \tag{8}$$

$$h^2\colon\ A_0\frac{\partial^2\phi(0)}{\partial h^2}+B_0\left\{\frac{d}{dx}\frac{\partial^2\phi(0)}{\partial h^2}+\frac{1}{3}\frac{d^3\phi(0)}{dx^3}\right\}=0. \tag{9}$$

It is to be noted that the first two relations are similar to the given boundary condition (4); but that this is no longer true for the third. If we take a more accurate representation of (4)—ignoring fifth differences—we get

$$A_0\phi(0,h)+\frac{B_0}{12h}\{-\phi(2h,h)+8\phi(h,h)-8\phi(-h,h)+\phi(-2h,h)\}=0. \tag{10}$$

This fails to reproduce the boundary condition in the coefficient of h^4 giving

$$h^4\colon\ A_0\frac{\partial^4\phi(0)}{\partial h^4}+B_0\left\{\frac{d}{dx}\frac{\partial^4\phi(0)}{\partial h^4}-\frac{4}{5}\frac{d^5\phi(0)}{dx^5}\right\}=0. \tag{11}$$

In general our ability to reproduce the given boundary condition in the coefficient of h^m depends on the accuracy of our difference approximations. It would seem from the above examples that central difference formulae including differences up to the $(2m-1)$th fail in the coefficient of h^{2m}.

3. Formal recurrence for the solution of the difference equation

The simplest difference equation approximating to (3) is obtained by setting

$$h^2\frac{d^2}{dx^2}=\delta^2,$$

and ignoring the higher order differences. This gives the equation

$$\phi((i+1)h,h)-2\phi(ih,h)+\phi((i-1)h,h)+h^2(\lambda(h)-q(ih))\phi(ih,h)=0, \tag{12}$$

which can be written as the matrix eigenvalue problem

$$\{A+h^2\lambda(h)I\}\boldsymbol{\varphi}=0.$$

If the boundary condition (6) has been used, then the matrix A is

$$\begin{bmatrix} -2-h^2q(0)+2hA_0/B_0 & 2 & & \\ 1 & -2-h^2q(h) & 1 & \dots \\ & 1 & & \\ & \dots & & \\ & \dots & & \end{bmatrix},$$

The eigenvector $\boldsymbol{\varphi}$ has the components $\phi_i=\phi(ih,h)$.

Substituting (1) and (2) into (12) and writing $ih = x$ to indicate an arbitrary ordinate point we get, on equating to zero the coefficients of powers of h, the series of equations the first few members of which are given below:

$$h^2\colon \left\{\frac{d^2}{dx^2}+(\lambda-q(x))\right\}\phi = 0, \tag{13}$$

$$h^3\colon \left\{\frac{d^2}{dx^2}+(\lambda-q(x))\right\}\frac{\partial\phi}{\partial h} = -\frac{d\lambda}{dh}\phi(x), \tag{14}$$

$$h^4\colon \left\{\frac{d^2}{dx^2}+(\lambda-q(x))\right\}\frac{\partial^2\phi}{\partial h^2} = -\frac{d^2\lambda}{dh^2}\phi(x)-2\frac{d\lambda}{dh}\frac{\partial\phi(x)}{\partial h}-\frac{1}{6}\frac{d^4\phi(x)}{dx^4}, \tag{15}$$

$$h^5\colon \left\{\frac{d^2}{dx^2}+(\lambda-q(x))\right\}\frac{\partial^3\phi}{\partial h^3} = -\frac{d^3\lambda}{dh^3}\phi(x)-3\frac{d^2\lambda}{dh^2}\frac{\partial\phi(x)}{\partial h}- -3\frac{d\lambda}{dh}\frac{\partial^2\phi(x)}{\partial h^2}-\frac{1}{2}\frac{d^4}{dx^4}\frac{\partial\phi(x)}{\partial h}, \tag{16}$$

$$h^6\colon \left\{\frac{d^2}{dx^2}+(\lambda-q(x))\right\}\frac{\partial^4\phi}{\partial h^4} = -\frac{d^4\lambda}{dh^4}\phi(x)-4\frac{d^3\lambda}{dh^3}\frac{\partial\phi(x)}{\partial h}- -6\frac{d^2\lambda}{dh^2}\frac{\partial^2\phi(x)}{\partial h^2}-4\frac{d\lambda}{dh}\frac{\partial^3\phi(x)}{\partial h^3}-\frac{d^4}{dx^4}\frac{\partial^2\phi(x)}{\partial h^2}-\frac{1}{15}\frac{d^6\phi(x)}{dx^6}. \tag{17}$$

The general equation is

$$h^{m+2}\colon \left\{\frac{d^2}{dx^2}+(\lambda-q(x))\right\}\frac{\partial^m\phi}{\partial h^m} = V_m(x), \tag{18}$$

where
$$V_m(x) = -\sum_{p=0}^{m-1}\frac{m!}{p!(m-p)!}\frac{d^{m-p}\lambda}{dh^{m-p}}\frac{\partial^p\phi}{\partial h^p}- -2\sum_{r=2}^{[\frac{1}{2}(m+2)]}\frac{d^{2r}}{dx^{2r}}\frac{\partial^{m+2-2r}\phi}{\partial h^{m+2-2r}}\frac{m!}{2r!(m+2-2r)!}.$$

We see that (13) is the original differential equation (3), and that in all subsequent equations we regain the left-hand side of (3) operating on $\partial^m\phi(x)/\partial h^m$; but now forcing terms appear on the right.

4. Solution of this recurrence

We now discuss the way in which the terms in expansions (1) and (2) are determined by the manner in which they appear in the above equations. In equation (14) we know that $\partial\phi(x)/\partial h$ always satisfies the same boundary conditions as the eigenfunction $\phi(x)$ of the original equation. Therefore the corresponding λ is again an eigenvalue; and, for a solution to be

possible, the right-hand side must be orthogonal to $\phi(x)$ over the range $(0, 1)$ of x. That is

$$\int_0^1 \frac{d\lambda}{dh}\phi^2\,dx = 0,$$

whence

$$\frac{d\lambda}{dh} = 0.$$

We thus regain the original equation, and hence $\partial\phi(x)/\partial h$ is $\phi(x)$ apart from a numerical factor. This factor is zero for we agreed to fix $\phi(x = \bar{x}, h)$ as a constant (non-zero and independent of h) for all h, and hence $\partial^m\phi(x = \bar{x})/\partial h^m = 0$ $(m \geqslant 1)$.

The general equation (18) not only has the right-hand side non-zero, but also satisfies the inhomogeneous boundary conditions

$$A_0\frac{\partial^m\phi(0)}{\partial h^m} + B_0\frac{d}{dx}\frac{\partial^m\phi(0)}{\partial h^m} = G_m(0),$$

and

$$A_1\frac{\partial^m\phi(1)}{\partial h^m} + B_1\frac{d}{dx}\frac{\partial^m\phi(1)}{\partial h^m} = H_m(1).$$

The condition that (18) has a solution can be expressed in the form (see (**2**) 214–16)

$$\int_0^1 V_m\left(\frac{d^m\lambda}{dh^m}, x\right)\phi(x)\,dx = \frac{G_m(0)\{d\phi(0)/dx\}}{A_0} - \frac{H_m(1)\{d\phi(1)/dx\}}{A_1}. \tag{19}$$

Applying (19) to equation (15) we get

$$G_2(0) = -\frac{B_0}{3}\frac{d^3\phi(0)}{dx^3},$$

$$H_2(0) = -\frac{B_1}{3}\frac{d^3\phi(1)}{dx^3},$$

and

$$\frac{d^2\lambda}{dh^2}\int_0^1 \phi^2\,dx = \frac{B_0}{3A_0}\frac{d^3\phi(0)}{dx^3}\frac{d\phi(0)}{dx} - \frac{B_1}{3A_1}\frac{d^3\phi(1)}{dx^3}\frac{d\phi(1)}{dx} - \frac{1}{6}\int_0^1 \frac{d^4\phi}{dx^4}\phi\,dx.$$

This simplifies to

$$\frac{d^2\lambda}{dh^2} = \left\{\frac{1}{3}\frac{d^3\phi(1)}{dx^3}\phi(1) - \frac{1}{3}\frac{d^3\phi(0)}{dx^3}\phi(0) - \frac{1}{6}\int_0^1 \frac{d^4\phi}{dx^4}\phi\,dx\right\}\Big/\int_0^1 \phi^2\,dx. \tag{20}$$

Equation (19) can always be solved for $d^m\lambda/dh^m$ because we can assume that, at this stage, all other terms and their derivatives with respect to x are known quantities. The solution of (18) is determinate to within an arbitrary multiple of the original eigenfunction ϕ. This is fixed by the condition $\partial^m\phi(\bar{x})/\partial h^m = 0$.

We now show that $\partial^m\phi/\partial h^m$ and $d^m\lambda/dh^m$ are uniquely determined by the condition that (18) should have a solution satisfying the imposed boundary conditions together with the condition $\partial^m\phi(\bar{x})/\partial h^m = 0$.

We prove this by induction. It certainly holds for $m = 2$ for, if we denote the difference between two solutions satisfying the above conditions by $\Delta(\partial^2\phi/\partial h^2)$, we have the following differential equation satisfied

$$\left\{\frac{d^2}{dx^2}+(\lambda-q)\right\}\Delta\frac{\partial^2\phi}{\partial h^2} = -\left(\Delta\frac{d^2\lambda}{dh^2}\right)\phi,$$

also the original boundary conditions (4) and (5), and the adjoined condition $\Delta(\partial^2\phi(\bar{x})/\partial h^2) = 0$, whence

$$\Delta\frac{d^2\lambda}{dh^2} = 0, \quad \text{and} \quad \Delta\frac{\partial^2\phi(x)}{\partial h^2} \equiv 0.$$

Now if we assume that the result is true for $\partial^i\phi/\partial h^i$ $(i < m)$, we can repeat the above argument exactly for $\partial^m\phi/\partial h^m$ and $d^m\lambda/dh^m$, and hence the uniqueness follows.

5. Convergence of the formal series

We can now establish the convergence of expansions (1) and (2) under the assumption that $q(x)$ is a regular function with a non-zero radius of convergence ρ about every point x in $(0, 1)$. We know from standard theorems that ϕ and $\partial^m\phi/\partial h^m$ are regular functions with the same radius of convergence as $q(x)$. Let the minimum value of ρ for x in $(0, 1)$ be not less than $\bar{\rho}$.

We have the estimate

$$\left|\frac{d^p}{dx^p}\frac{\partial^q\phi}{\partial h^q}\right| \leqslant \frac{p!}{\bar{\rho}^p}K,$$

where K is independent of p, q, and x and is bounded in $(0, 1)$ since $\partial^q\phi/\partial h^q$ has no singularities in this range, and vanishes at $x = \bar{x}$.

We can now form an expansion which dominates (2). We have that the modulus of the mth term in (2) is less than

$$|j-i|^m\frac{h^m}{m!}\frac{m!\,K}{\bar{\rho}^m}\sum_{p=0}^{m}\frac{1}{(m-p)!}\frac{\bar{\rho}^{m-p}}{|j-i|^{m-p}} < |j-i|^m\frac{h^m}{\bar{\rho}^m}K\sum_{p=0}^{\infty}\frac{1}{p!}\frac{\bar{\rho}^p}{|j-i|^p}$$

$$= |j-i|^m\frac{h^m}{\bar{\rho}^m}K\exp\left\{\frac{\bar{\rho}}{|j-i|}\right\}.$$

The series

$$\sum_{m=0}^{\infty}|j-i|^m\frac{h^m}{\bar{\rho}^m}K\exp\left\{\frac{\bar{\rho}}{|j-i|}\right\}$$

converges for $|j-i|h < \bar{\rho}$.

We proceed to prove similarly the convergence of (1). To estimate $|d^m\lambda/dh^m|$ we evaluate (18) at $x = \bar{x}$. We know that the left-hand side

is bounded—in fact $\partial^m\phi(\bar{x})/\partial h^m = 0$, and we can take $(d^2/dx^2)(\partial^m\phi(\bar{x})/\partial h^m)$ into the second sum on the right. Writing $K_1 = K/\phi(\bar{x})$ we have, since all terms in the first sum vanish except $(d^m\lambda/dh^m)\phi(\bar{x})$,

$$\left|\frac{d^m\lambda}{dh^m}\right| \leqslant \sum_{p=1}^{[\frac{1}{2}(m+2)]} \frac{(2p)!}{\bar{\rho}^{2p}} K_1 \frac{m!}{(2p)!\,(m+2-2p)!} = \frac{2K_1 m!}{\bar{\rho}^{m+2}} \sum_{p=1}^{[\frac{1}{2}(m+2)]} \frac{\bar{\rho}^{(m+2-2p)}}{(m+2-2p)!}$$

$$< \frac{2K_1 m!}{\bar{\rho}^{m+2}} \begin{cases} \sinh\bar{\rho}: & m \text{ odd} \\ \cosh\bar{\rho}: & m \text{ even,} \end{cases}$$

and hence

$$< \frac{2K_1 m!}{\bar{\rho}^{m+2}} \cosh\bar{\rho}.$$

The series

$$\sum_{m=0}^{\infty} \frac{2K_1 \cosh\bar{\rho}}{\bar{\rho}^2} \frac{h^m}{\bar{\rho}^m},$$

which dominates the series (1) for $\lambda(h)$, converges for $h < \bar{\rho}$. We have thus proved that expansions (1) and (2) exist, and that they satisfy (12) for $h < \bar{\rho}$.

6. Proof of the 'deferred approach to the limit'

The result that forms the basis of Richardson's technique of deferred approach to the limit can now be deduced.

If central difference formulae are used to approximate to the boundary conditions (4) and (5) of the differential equation (3), then all odd derivatives of ϕ and λ with respect to h are identically zero. To prove this we need the following results.

(1) *The inhomogeneous terms in the boundary conditions on*

$$\{\partial^{2m+1}\phi(x)\}/(\partial h^{2m+1})$$

involve odd derivatives with respect to x of odd derivatives with respect to h of degree less than $2m+1$.

This follows because (*a*) the $1/h$ term multiplying the difference operator means that derivatives of total order $2m+2$ are involved; and (*b*) the coefficient of $\phi(x,h)$ is the negative of the coefficient of $\phi(-x,h)$ in the central difference expansion of $d\phi/dx$ about $x = 0$, and a similar result holds about $x = 1$. Thus the even derivatives with respect to x cancel.

(2) *The forcing term on the right-hand side of the differential equation for $\{\partial^{2m+1}\phi(x)\}/(\partial h^{2m+1})$ consists of odd derivatives of λ (ϕ) times even derivatives of ϕ (λ)—the derivatives being taken with respect to h, and even derivatives with respect to x of odd derivatives of ϕ with respect to h.*

With this information we can form an induction.

If we assume that odd derivatives of ϕ and λ with respect to h of order up to $2m-1$ vanish, then $\partial^{2m+1}\phi/\partial h^{2m+1}$ must satisfy the boundary conditions exactly ($G_{2m+1} = H_{2m+1} = 0$); and the right-hand side of the

differential equation must be equal to $-(d^{2m+1}\lambda/dh^{2m+1})\phi$. We have already proved that $\partial\phi(x)/\partial h = d\lambda/dh = 0$; and, as the circumstances here are exactly similar, our result is established.

This vanishing of the odd derivatives of ϕ and λ with respect to h does not occur in general if forward or backward differences are used to approximate to the boundary conditions. For instance, if we approximate to the condition $d\phi(0)/dx = 0$ by the difference relation $\Delta\phi(0,h) = 0$, the boundary condition on $\partial\phi/\partial h$ is

$$\frac{d}{dx}\frac{\partial\phi(0)}{\partial h} = -\frac{1}{2}\frac{d^2\phi(0)}{dx^2};$$

and we have $G_1 \neq 0$. This leads to a non-trivial relation for $d\lambda/dh$; and hence we get h-extrapolation only.

7. h^2-Extrapolation of the eigenvalues

Our equation (20) can be used as the basis for a method of obtaining h^2-extrapolation of the eigenvalues. We have

$$\frac{d^2\lambda}{dh^2} = \left\{-\frac{1}{3}\frac{d^3\phi(0)}{dx^3}\phi(0)+\frac{1}{3}\frac{d^3\phi(1)}{dx^3}\phi(1)-\frac{1}{6}\int_0^1 \frac{d^4\phi}{dx^4}\phi\,dx\right\}\Big/\int_0^1 \phi^2\,dx.$$

But
$$\frac{d^3\phi}{dx^3} = -(\lambda-q)\frac{d\phi}{dx}+q'\phi,$$

also
$$\frac{d^4\phi}{dx^4} = (\lambda-q)^2\phi+2q'\frac{d\phi}{dx}+q''\phi,$$

and
$$\int_0^1 \phi\left\{2q'\frac{d\phi}{dx}+q''\phi\right\}dx = q'\phi^2\Big|_0^1,$$

so that (20) involves only quantities which lie in the range $(0,1)$, and which are known to within $O(h^2)$ when the simple difference equation (12) has been solved. Thus the error in using the results of (12) and, say, the trapezoidal rule to evaluate $h^2/2!\times(20)$ is $O(h^4)$; and we have an h^2-extrapolation.

There is a very close relationship between formula (20) and the difference correction given by Fox (**1**). We show this for the case when boundary conditions of the form (6) have been used; and we restrict our attention to the integral terms of (20).

The difference correction $\Delta\lambda$, with boundary terms suitably interpreted, to be applied to the eigenvalues of (12) is just $-h^2/2!\times(20)$ evaluated by the trapezoidal rule with error $O(h^4)$.

We use the fact that

$$h^4\frac{d^4\phi(x=ih)}{dx^4}=\delta^4\phi(ih)-\tfrac{1}{6}h^6\frac{d^6\phi(ih)}{dx^6}+O(h^8).$$

Applying the trapezoidal rule to (20) we get

$$-\frac{h^2}{2!}\frac{d^2\lambda}{dh^2}=\sum_{i=0}^{m}{}^{*}\phi(ih)\left\{\frac{h^{-2}}{12}\delta^4\phi(ih)\right\}\Big/\sum_{i=0}^{m}{}^{*}\{\phi(ih)\}^2+\text{boundary terms}+O(h^4).$$

We use the notation $\sum^*$ to indicate that we take $\frac{1}{2}$ the first and last members of the sum.

The difference correction is given by

$$\Delta\lambda=\frac{\boldsymbol{\varphi}^{*\prime}C\boldsymbol{\varphi}}{\boldsymbol{\varphi}^{*\prime}\boldsymbol{\varphi}}+\text{boundary terms},$$

where $\boldsymbol{\varphi}$ and $\boldsymbol{\varphi}^*$ are the right and left eigenvectors of (12) respectively, and C is the correction matrix. Here C is the matrix representing the operation $(h^{-2}/12)\delta^4$ on $\boldsymbol{\varphi}$. We see from the matrix form of (12) that, if $\phi_0^*=\frac{1}{2}\phi_0$, then $\phi_i^*=\phi_i$ $(i=1,\ldots,m-1)$, and $\phi_m^*=\frac{1}{2}\phi_m$. This establishes the required result. The role of the boundary values in difference correction is discussed in section 9.

8. h^2-Extrapolation of the eigenvectors

We can obtain an h^2-extrapolation of the eigenvector by solving (15) numerically. In doing this we must use $\partial^2\phi(\bar{x})/\partial h^2=0$ as one of our boundary conditions to avoid trouble from the eigensolution of the homogeneous equation. For example, if we assume that difference conditions of the form (6) have been used, and that we may fix the scale by setting $\bar{x}=0$, $\phi(0,h)=1$ (say), then we get a marching problem for $\partial^2\phi(x)/\partial h^2$ with the initial conditions

$$(a)\quad \frac{\partial^2\phi(0)}{\partial h^2}=0,\quad\text{and}$$

$$(b)\quad \frac{d}{dx}\left(\frac{\partial^2\phi(0)}{\partial h^2}\right)=-\frac{1}{3}\frac{d^3\phi(0)}{dx^3},$$

and the terminal condition (which gives a numerical check)

$$A_1\frac{\partial^2\phi(1)}{\partial h^2}+B_1\left\{\frac{d}{dx}\frac{\partial^2\phi(1)}{\partial h^2}+\frac{1}{3}\frac{d^3\phi(1)}{dx^3}\right\}=0.$$

In practice one would probably need to repeat the computations at least once using the improved value at each stage to reduce the residual error. If the marching problem is unstable we could solve (15) as a two-point boundary problem using one or other of the initial conditions as a check. If the original boundary condition is $\phi(0)=0$, then we must have $\bar{x}\neq 0$, and we get two two-point boundary value problems. The

condition that $(d/dx)\{\partial^2\phi(x)/\partial h^2\}$ be continuous at $x = \bar{x}$ supplies the check.

We could now proceed to obtain an h^4-improvement using equation (17) provided we have worked to $O(h^4)$ in solving for $d^2\lambda/dh^2$ and $\partial^2\phi(x)/\partial h^2$.

As a numerical example consider the equation

$$\frac{d^2\phi}{dx^2}+(\lambda-x)\phi = 0 \tag{21}$$

with the boundary conditions

$$\phi(0)+\frac{d\phi(0)}{dx} = 0$$

and

$$\phi(1)+2\frac{d\phi(1)}{dx} = 0.$$

We give below the result of the numerical computation of the first eigenvalue; formula (20) was used to compute $d^2\lambda/dh^2$.

h	$\lambda(h)$	$d^2\lambda/dh^2$	improved λ
0·1	−0·82621	−0·040	−0·82601

The correct value to six places of decimals is −0·825980.

As a check on the numerical solution of (15) we used inverse interpolation to determine $d^2\lambda/dh^2$ such that the terminal boundary condition was satisfied. This gave $d^2\lambda/dh^2 = -0{\cdot}041$ for $h = 0{\cdot}2$.

9. A method of difference correction

The process outlined in section 8 suffers from the important disadvantage that the correction terms are defined by differential equations. The numerical solution of these (and the construction of the terms appearing in them) provides another source of error; and a revision procedure involving all terms previously calculated is necessary when proceeding to a higher order of accuracy. Our work does, however, suggest a modification of the difference correction method described in (**1**), and we give a sketch of this below.

The exact eigenfunction $\phi(x)$ satisfies the difference equation

$$h^{-2}\delta^2\phi_i+(\lambda-q_i)\phi_i = h^{-2}\{\tfrac{1}{12}\delta^4-\tfrac{1}{90}\delta^6+\ldots\}\phi_i$$

at the ordinate point ih.

We write the approximation given by equation (12) as

$$h^{-2}\delta^2\bar{\phi}_i+(\bar{\lambda}-q_i)\bar{\phi}_i = 0;$$

and

$$\phi_i = \bar{\phi}_i+h^2C_i,$$

$$\lambda = \bar{\lambda}+h^2\mu,$$

using the results of section 6.

Now h^2C_i and $h^2\mu$ are given by the difference equation

$$h^{-2}\delta^2\{h^2C_i\}+(\bar{\lambda}-q_i)\{h^2C_i\} = -h^2\mu\bar{\phi}_i-h^2\mu h^2C_i+ \\ +h^{-2}\{\tfrac{1}{12}\delta^4-\tfrac{1}{90}\delta^6+\ldots\}\bar{\phi}_i+h^{-2}\{\tfrac{1}{12}\delta^4-\tfrac{1}{90}\delta^6+\ldots\}h^2C_i.$$

We define $h^2\bar{C}_i$ by the equation

$$h^{-2}\delta^2\{h^2\bar{C}_i\}+(\bar{\lambda}-q_i)\{h^2\bar{C}_i\} = -h^2\bar{\mu}\bar{\phi}_i+h^{-2}\{\tfrac{1}{12}\delta^4-\tfrac{1}{90}\delta^6+\ldots\}\bar{\phi}_i.$$

As the ignored terms are $O(h^4)$, we have that

$$h^2C_i = h^2\bar{C}_i+h^4D_i,$$

and

$$h^2\mu = h^2\bar{\mu}+h^4\nu,$$

where $h^2\bar{\mu}$ is defined by the usual orthogonality condition (that is the algebraic condition analogous to equation (19)).

Now h^4D_i, $h^4\nu$ satisfy the equation

$$h^{-2}\delta^2\{h^4D_i\}+(\bar{\lambda}-q_i)\{h^4D_i\} = -h^4\nu\bar{\phi}_i-h^2\bar{\mu}h^2\bar{C}_i-h^2\bar{\mu}h^4D_i-h^4\nu h^2\bar{C}_i- \\ -h^4\nu h^4D_i+h^{-2}\{\tfrac{1}{12}\delta^4-\tfrac{1}{90}\delta^6+\ldots\}h^2\bar{C}_i+h^{-2}\{\tfrac{1}{12}\delta^4-\tfrac{1}{90}\delta^6+\ldots\}h^4D_i.$$

Proceeding as before we define $h^4\bar{D}_i$ and $h^4\bar{\nu}$ by the equation

$$h^{-2}\delta^2\{h^4\bar{D}_i\}+(\bar{\lambda}-q_i)\{h^4\bar{D}_i\} = -h^4\bar{\nu}\bar{\phi}_i-h^2\bar{\mu}h^2\bar{C}_i+h^{-2}\{\tfrac{1}{12}\delta^4-\tfrac{1}{90}\delta^6+\ldots\}h^2\bar{C}_i,$$

ignoring terms which are $O(h^6)$.

This process can obviously be continued; and we have finally

$$\phi_i = \bar{\phi}_i+h^2\bar{C}_i+h^4\bar{D}_i+\ldots, \tag{22}$$

$$\lambda = \bar{\lambda}+h^2\bar{\mu}+h^4\bar{\nu}+\ldots. \tag{23}$$

It would be satisfying if at this stage we could make the identification

$$\bar{C}_i = \frac{1}{2!}\frac{\partial^2\phi(ih,h)}{\partial h^2}, \quad \text{and} \quad \bar{\mu} = \frac{1}{2!}\frac{d^2\lambda(h)}{dh^2},$$

and so on; but these relations do not hold. We can, however, say that (22) and (23) are asymptotic expansions in the sense that, if we truncate these expansions at their nth terms, the remainders will tend to zero like h^{2n}; for it can be shown that

$$|R_n(\phi)| \leqslant K_1\sum_{p=n}^{\infty}\frac{1}{2p!}\left|\frac{\partial^{2p}\phi(x,h)}{\partial h^{2p}}\right|h^{2p},$$

and

$$|R_n(\lambda)| \leqslant K_2\sum_{p=n}^{\infty}\frac{1}{2p!}\left|\frac{d^{2p}\lambda(h)}{dh^{2p}}\right|h^{2p},$$

where K_1 and K_2 are bounded for a fixed n.

Also, if the scale has been fixed by setting $\phi_\alpha = \bar{\phi}_\alpha$, $\alpha h = \bar{x}$, then we can adjoin the conditions

$$\bar{C}_\alpha = \bar{D}_\alpha = \ldots = 0,$$

as

$$\frac{\partial^{2n}\phi(\alpha h,h)}{\partial h^{2n}} = \frac{\partial^{2n}\phi(\alpha h,0)}{\partial h^{2n}} = 0 \qquad (n \geqslant 1).$$

Thus the procedure outlined in section 8 can be paralleled for the sequence of difference equations. The boundary conditions on the difference equations can be derived in the same way as we derived the equations themselves.

For example, we have that

$$A_0\phi_0+B_0h^{-1}\mu\delta\phi_0 = B_0h^{-1}\{\tfrac{1}{6}\mu\delta^3-\tfrac{1}{30}\mu\delta^3\ldots\}\phi_0,$$

and

$$A_0\bar{\phi}_0+B_0h^{-1}\mu\delta\bar{\phi}_0 = 0.$$

Hence,

$$A_0\{h^2C_0\}+B_0h^{-1}\mu\delta\{h^2C_0\} = B_0h^{-1}\{\tfrac{1}{6}\mu\delta^3-\tfrac{1}{30}\mu\delta^5+\ldots\}\bar{\phi}_0+$$
$$+B_0h^{-1}\{\tfrac{1}{6}\mu\delta^3-\tfrac{1}{30}\mu\delta^5+\ldots\}h^2C_0;$$

and

$$A_0\{h^2\bar{C}_0\}+B_0h^{-1}\mu\delta\{h^2\bar{C}_0\} = B_0h^{-1}\{\tfrac{1}{6}\mu\delta^3-\tfrac{1}{30}\mu\delta^5+\ldots\}\bar{\phi}_0\ldots.$$

All significant differences can be calculated provided we can extrapolate $\bar{\phi}_i$ far enough (see (**1**)).

10. Another application of our results

As a final example let us ask when the approximate difference equation is satisfied exactly by point values of the eigenfunctions of the differential equation. This means that $\partial^{2m}\phi(x)/\partial h^{2m} = 0$ for $m \geqslant 1$, which implies that (18) has a solution proportional to ϕ, so that the condition $\partial^{2m}\phi(\bar{x})/\partial h^{2m} = 0$ ensures its vanishing. This means that the orthogonality condition (19) must be trivially satisfied, and hence that $d^{2m}\lambda/dh^{2m}$ can be chosen to make $V_{2m}(x)$ vanish identically. Thus we get the differential equation

$$\frac{d^2\phi}{dx^2}+\lambda\phi = 0.$$

We have $G_{2m} = H_{2m} = 0$, which give as the possible boundary conditions $\phi = 0$, and $d\phi/dx = 0$.

In these cases it is possible to express $\lambda(h)$ in a closed form. We have

$$\frac{d^{2m}\lambda}{dh^{2m}} = -\frac{2\,.\,2m!}{(2m+2)!}(-1)^{m+1}\lambda^{m+1},$$

and

$$\lambda(h) = 2\sum_{m=0}^{\infty}\frac{(-1)^m}{(2m+2)!}\lambda^{m+1}h^{2m}$$
$$= \frac{2}{h^2}(1-\cos(\sqrt{\lambda}h))$$
$$= 4h^{-2}\sin^2\left(\frac{\sqrt{\lambda}h}{2}\right).$$

This result is readily verified. Equation (12) becomes

$$\phi_{i+1}-(2-h^2\lambda)\phi_i+\phi_{i-1} = 0.$$

This difference equation has the particular solutions $\phi_r = e^{ir\beta}$, $e^{-ir\beta}$, where β is defined by

$$(2-h^2\lambda) = 2\cos\beta, \quad \text{or} \quad \lambda = 4h^{-2}\sin^2\tfrac{1}{2}\beta.$$

From the boundary conditions we get the relations

$$(a) \quad \phi(0) = \phi(1) = 0: \quad \sin m\beta = 0 \quad (\beta = r\pi h),$$

$$(b) \quad \phi'(0) = \phi'(1) = 0: \quad \sin m\beta = 0 \quad (\beta = r\pi h),$$

$$(c) \quad \phi(0) = \phi'(1) = 0: \quad \cos m\beta = 0 \quad (\beta = \tfrac{1}{2}r\pi h),$$

where $1 \leqslant r \leqslant m$, and $h = 1/m$.

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