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Abstract

Finite difference and finite element approximations of eigenvalue problems, under certain circumstances exhibit spectral pollution, i.e. the appearance of eigenvalues that do not converge to the correct value when the mesh density is increased. In the present paper this phenomenon is investigated in a homogeneous case by means of discrete dispersion relations: the polluting modes belong to a branch of the dispersion relation that is strongly distorted by the discretization method employed, or to a new, spurious branch. The analysis is applied to finite difference methods and to finite element methods, and some indications about how to avoid polluting schemes are given.

1. Introduction

In the computation of the eigenvalues of the ideal linear magnetohydrodynamics equations for a homogeneous cylindrical plasma, using a linear finite element (FE) code, Appert et al. [1] found that the spectrum could not be well reproduced numerically: there were wrong eigenvalues, for any mesh density. As the number of intervals was increased, the eigenvalues, identified by the spatial behaviour of the eigenfunctions, converged to the true values, known analytically, but new eigenvalues appeared in the wrong place (Fig. 1). This phenomenon was called spectral pollution. In the last fifteen years it has been discussed extensively in the literature [2, 3 and references therein, 4, 5].

In fact, this kind of numerical instability is very common. And we should add that pollution is not always recognized as such, and it is treated as another numerical convergence problem, without giving it a specific name. For example, the well known 'odd-even' instability is a particular case of pollution. In this paper we limit ourselves to eigenvalue problems, although much of the analysis (and of the results) can be applied to more general cases. We gain some insight by studying equations that describe homogeneous models, that is, with constant coefficients in the differential equations. In this case there exists an analytical "dispersion relation" for the system, and we can test the behaviour of the numerical discretization by comparing the solutions of the analytical dispersion relation to those of the "discrete dispersion relation" as the mesh density increases.

To our knowledge, polluting modes have very short wavelengths, of the order of the mesh interval. In a system of differential equations with variable coefficients, these modes should be locally well described by a WKB approximation. Thus, the existence of pollution may be inferred from a local, constant-coefficient analysis.

Let us consider the following eigenvalue problem

$$L(\mathbf{u}) = \lambda \mathbf{u} \tag{1.1}$$

where L is a linear differential operator. For solutions of the form $\exp{(i\mathbf{k}\cdot\mathbf{x})}$, the "dispersion relation" (DR) takes the form $\lambda = \lambda(\mathbf{k})$, which is obtained explicitly from (1.1) by replacing the nabla operator by $i\mathbf{k}$.

The DR of the discretized system is similarly obtained by substituting solutions proportional to exp $(i\mathbf{k}\cdot\mathbf{x})$ and finding the zeros of the resulting

determinant. For a 1-D system with constant coefficients, in the case of only nearest neighbour coupling the matrix M representing the discretized Eq. (1.1) becomes block-tridiagonal:

where A_{-1} , A_0 and A_1 are square block matrices with some elements being linearly dependent on λ . Their dimension is the number of unknowns per mesh node, and their structure depends on the characteristics of the numerical method used. The discrete version of (1.1) is now $M \mathbf{u} = 0$. If we make the ansatz that the solutions behave as $\exp(i \mathbf{k} \mathbf{x})$, we arrive at the discrete DR:

$$\det [A_{-1} \exp(-i k h) + A_0 + A_1 \exp(i k h)] = 0$$
 (1.2)

where h is the mesh interval.

The extension of the analysis to higher dimensions is straightforward.

In a more general case the number of square matrices in a row of M is one plus the number of neighbours used; then, we have (with m neighbours on the left, and n on the right)

$$\det\left[\sum_{s=-m}^{n} A_{s} \exp(i k s h)\right] = 0$$
 (1.2')

In many cases Eq. (1.1) is the temporal Fourier transform of a partial differential equation in time and space, and the eigenvalue λ is connected with the eigenfrequency of oscillation, with an $\exp(i\omega t)$ dependence being assumed (e.g., in solid mechanics and ideal MHD the eigenvalue is the square of the eigenfrequency).

It is important to realize that the phenomenon of spectral pollution may have very different consequences depending on whether we are interested in the time evolution of a given initial condition or in the spectrum of a linear operator. Typically, very ill-represented eigenvalues only occur for numerical eigenmodes which are rapidly space-varying and show structure on the same scale as the mesh: kh = O(1) as $h \to 0$. In an initial value problem with a smooth initial

condition, the contribution of such components to the total solution vanishes as $h \to 0$ and the numerical solution therefore becomes increasingly accurate as h is decreased, because usually a slightly dissipative time integration scheme is chosen. However, in the case of a polluting numerical scheme, the <u>spectrum</u> may still contain spurious points in the region of interest (either in the vicinity of the exciting frequency in a driven problem or the unstable region $\omega^2 < 0$ in a stability problem). Thus, a given scheme may be unacceptable in a stability problem, if it gives wrong eigenvalues, and yet be very good for initial value problems, if the poorly represented part of the spectrum is irrelevant in this particular problem.

In the eigenvalue problems, pollution is marked by the appearance, in a fixed region of λ , of spurious solutions for k. These bad solutions are recognized by their lack of convergence as h is decreased. These concepts will be discussed later.

Although convenient, it might not be at all necessary to remove pollution. In effect, we could use a polluting method in a driven problem, and identify the purely numerical artifacts by their behaviour as a function of h [2]; or it could happen that the spurious modes are not excited by the source, or only very weakly, or that they are strongly damped.

In what follows, we present a test case, characterize pollution, and examine finite difference and finite element methods, providing some indications on how to avoid polluting schemes.

2. Basic test example

An example of a one dimensional system is the following [4]:

-a
$$u_1^*$$
 - $u_2' = \lambda u_1$
 $u_1' + d u_2 = \lambda u_2$ (2.1)

where prime denotes differentiation with respect to the independent variable x and $a \ge 0$ and d are constants. The eigenvalues are real because this system is self-adjoint.

Fourier transformation shows that there are two branches for the eigenvalues:

$$\frac{\lambda(\lambda-d)}{1+a(\lambda-d)} = k^2 \tag{2.2}$$

This is the "dispersion relation". If, furthermore, we introduce boundary conditions, k is fixed to a set of discrete values. For simplicity we consider (2.1) on the interval $0 \le x \le 1$ with the boundary conditions

$$\begin{array}{lll}
 u_1 = 0 & \text{at } x = 0 \\
 u_2 = 0 & \text{at } x = 1
 \end{array}$$
(2.3)

The eigenfunctions u_1 and u_2 are proportional to sine and cosine, respectively, of (n+1/2) π x, and k=(n+1/2) π , $n=1,2,\ldots$. For $d\geq 0$ one branch of the eigenvalue λ lies in the interval (d,∞) and the other branch in (0,d-1/a); for $d\leq 0$, the intervals are $(0,\infty)$ and (0,d-1/a). When $n\to\infty$, the second branch tends to $\lambda_\infty=d-1/a$ (accumulation point). In the case ad=1 this branch is reduced to a single, infinitely degenerated eigenvalue $\lambda=0$.

We have chosen the system (2.1) because, in its more general form (with variable coefficients) is very familiar to us, as it appears in MHD and electromagnetic problems; also, we believe that what can be learnt from it can be applied to other systems of equations.

The ideal MHD linear operator for a homogeneous plasma ($\mathbf{B_0} = B_0 \ \mathbf{z}$, zero pressure) can be written in the form (2.1) [4]. Assuming a exp(-i ω t + i k_y y + i k_z z) dependence, $k_y \neq 0$, and normalizing the Alfvén velocity to 1, we have $u_1 = -i\xi_x$, $u_2 = \xi_y$, $a = 1/k_y$, $d = k_y$, $\lambda = (\omega^2 - k_z^2)/k_y$. Then the spectrum is $\omega^2 = k_z^2$ (infinitely degenerated), the Alfvén continuum, and $\omega^2 = k_x^2 + k_y^2 + k_z^2$, the fast magneto-

sonic wave.

A related situation is the wave propagation in an unmagnetized, homogeneous plasma; it is also described by this system of equations. Taking k_z = 0, the equation for the z-component of the electric field is decoupled from the other two. The remaining two equations are of the form (2.1), using the same identifications as in the preceding paragraph, but with \boldsymbol{E} replacing ξ , and the plasma frequency ω_p replacing k_z . The degenerated branch is the electrostatic oscillations at $\omega=\omega_p$, and the other branch corresponds to the electromagnetic waves.

3. Diagnosis of pollution

We first consider a FD method to solve the system (2.1). The most straightforward approach, is to put u_1 and u_2 on the same grid, which gives the FD equations

$$\begin{array}{rcl} \lambda\,u_{1}^{i} \;+\; \frac{a}{h^{2}}\Big(u_{1}^{\,i\,+1} - 2\,u_{1}^{i} + u_{1}^{\,i\,-1}\Big) \;+\; \frac{u_{2}^{\,i\,+1} - \;u_{2}^{\,i\,-1}}{2\,h} \;=\; 0 \\ \\ & \frac{u_{1}^{\,i\,+1} - \;u_{1}^{\,i\,-1}}{2\,h} \;\;\; + \;\;\; (d-\lambda)\,u_{2}^{\,i} \;=\; 0 \end{array}$$

It is easy to see that, for an exp (ikx) dependence, the differential operators turn into numbers according to

$$\begin{array}{lll} d/dx & \to & G_1 \equiv & (1/2h) \left[\exp \left(ikh \right) - \exp(-ikh) \right] = (i/h) \sin kh \\ d^2/dx^2 & \to & G_2 \equiv & (1/h^2) \left[\exp \left(ikh \right) - 2 + \exp \left(-ikh \right) \right] = -(2/h^2) \left(1 - \cos kh \right) \end{array}$$

The DR is obtained from the determinant (1.2')

$$\begin{vmatrix} -a G_2 - \lambda_h & -G_1 \\ G_1 & d - \lambda_h \end{vmatrix} = 0$$
 (3.1)

where we use λ_h to emphasize that this is a discrete DR, whose solutions depend on the mesh interval, h. We then obtain,

$$(\lambda_h + a G_2) (\lambda_h - d) + (G_1)^2 = 0$$
 (3.2)

We can now examine some cases. For a = 0, the analytical DR (2.2) is

$$\lambda (\lambda - d) = k^2 \tag{3.3}$$

while (3.2) gives

$$\lambda_{h} \left(\lambda_{h} - d \right) = -(G_{1})^{2} \tag{3.4}$$

Shown in Fig. 2 is a plot of the right hand sides of (3.3) and (3.4), for k between 0 and $k_{max} = \pi/h$ (the shortest wavelength that can be present in the mesh is 2 h). The pollution is then readily observed: it occurs in the region near k_{max} , where these high wavenumber modes have low eigenvalues. In a driven problem, with λ given by the source, these modes appear as a ripple, with wavelength of the order of the mesh interval ($k \sim \pi/h$ - $[\lambda (\lambda-d)]^{1/2}$).

From this example we can put forward a first (numerical) characterization of pollution: when in a given range of eigenvalues λ there are wavelengths of the order of h, for h arbitrarily small, we <u>might</u> be in the presence of pollution. We qualify the statement because there could be a (nearly) horizontal branch of the DR, so the short wavelength modes could be real. This first description of pollution is valid when, for the true eigenvalues, $|\lambda| \to \infty$ as $|k| \to \infty$.

Let's now consider the case a > 0, d > 0, with $d-1/a \ge 0$. Then, (3.2) gives,

$$\left[\lambda_{h}-a\frac{2(1-\cos kh)}{h^2}\right](\lambda_{h}-d) = \left[\frac{\sin kh}{h}\right]^2$$
(3.5)

For small enough values of h (h² < 12 a/d), the two branches of the numerical DR give λ_h as monotonic functions of k, the plus branch going from $\lambda_{h+}(k=0)=d$ to $\lambda_{h+}(k_{max})=4$ a/h², and the minus branch going from $\lambda_{h-}(k=0)=0$ to $\lambda_{h-}(k_{max})=d$. In this case the pollution is clearly seen: the minus branch tends to the finite value d rather than to the finite value d - 1/a . This strongly changes the spectrum, as the gap ($\lambda_{\infty}=d$ -1/a , d) should be empty of eigenvalues, but it is filled by the λ_{-} branch.

With Eq. (3.5) we can qualitatively explain Fig. 1. The F label corresponds to λ_+ , and the A label to λ_- (we don't consider the S branch of the figure, as it corresponds to a nonzero pressure, and it is not described by (2.1)). We take $d=1/a=k_y$, h=L/N, where L is the dimension of the plasma and N the number of intervals, and $k=(n+1/2)\pi/L$. We plot in Fig. 3, as a function of N, the logarithm of $\omega_\pm{}^2=\lambda_\pm{}^n\,k_y+k_z{}^2$, with the values of $\lambda_+{}^n$ and $\lambda_-{}^n$ corresponding to n=1..N. To compare to Fig 1, we have to take into account that the shape of the "birth curves", the place where new modes appear, is strongly affected by the cylindrical geometry. In particular, since k_y is now m/r the "effective" k_y for the shortest-wavelength modes is proportional to 1/h near the axis; this shifts upwards the birth curve of λ_- , so it has now the same power dependence on N as the one for λ_+ .

If we were trying values of λ close to the accumulation point λ_{∞} , we would find, as it should be, values of k near k_{max} , both with polluting and with non-polluting methods. In this case, the easiest way to diagnose pollution is by tracking the new, short wavelength modes that appear when h is decreased: if the value λ_n at which a new mode appears does not tend towards λ_{∞} (that is, if $\lambda_n(h) - \lambda_{\infty}$ is not proportional to some positive power of h), there is pollution (clearly, the value of λ for fixed k will tend to λ_{∞}).

From this example we identify three steps that may be used to diagnose pollution:

- 1) Find the true accumulation points (if any) in the range of eigenvalues of interest.
- 2) Far from the accumulation points, numerical solutions with wavelengths of the order of the mesh interval indicate pollution.
- 3) When the eigenvalues of any fixed mode tend to an accumulation point (λ_{∞}) as h decreases, a more stringent test must be applied in the neighbourhood of λ_{∞} : if the new modes, which appear as the number of grid points increases, have eigenvalues that approach λ_{∞} the scheme is pollution-free.

This characterization of pollution is based on the dispersion relation alone; boundary conditions do not play any role in this analysis. It is possible that in a specific problem, the boundary conditions suppress the spurious modes that would appear with a given polluting numerical scheme. This scheme would then yield good solutions, although it should be used with caution, as it could be very sensitive to the boundary conditions.

4. Finite differences.

Now that we have characterized pollution, how can we avoid it?

Pollution is controlled by the high order spatial derivatives, which become the dominant terms as k becomes large. In the problem we are examining, there are two contributions to k^2 in the DR (see Eq. (3.2)): one from G_2 and one from $(G_1)^2$. The G_2 term gives a relatively good approximation to $-k^2$, as $G_2(k_{max}) = -4/h^2$, to compare with $-\pi^2/h^2$. In fact, the clearest way to see how well G_2 approximates $-k^2$ is to plot them versus k between 0 and k_{max} , and compare them (see Fig. 2). If we do now the same thing for $(G_1)^2$, we see that as $k{\to}k_{max}$, $(G_1)^2$ goes to zero. This is the feature that causes pollution.

One way to avoid pollution in this case is to use staggered meshes, i.e., to put u_1 on one grid (the integer grid) and u_2 on another (the half grid). The difference equations become

$$\lambda u_{1}^{i} + \frac{a}{h^{2}} \left(u_{1}^{i+1} - 2u_{1}^{i} + u_{1}^{i-1} \right) + \frac{u_{2}^{i+\frac{1}{2}} - u_{2}^{i-\frac{1}{2}}}{h} = 0$$

$$\frac{u_{1}^{i+1} - u_{1}^{i}}{h} + (d - \lambda) u_{2}^{i+\frac{1}{2}} = 0$$

In this way,

d/dx
$$\rightarrow$$
 H₁ \equiv (1/h) [exp (ikh/2) - exp(-ikh/2)] = (2 i/h) sin kh/2 d²/dx² \rightarrow G₂

and $(H_1)^2 = G_2$. The dispersion relation becomes

$$\frac{\lambda_{h} (\lambda_{h}-d)}{1 + a(\lambda_{h}-d)} = -G_{2} = \frac{2(1 - \cos kh)}{h^{2}}$$
(4.1)

which is a good, non-polluting approximation to (1.5), the exact dispersion relation (see Fig. 2).

This requirement, which could be called "consistent evaluation of the highest order terms", (in this case, that the first-derivative squared equals the second-derivative) seems to be necessary, but is not sufficient. In effect, another way to evaluate the derivatives consistently could have a second-derivative operator not describing correctly the shortest wavelength $kh = \pi$; for example, one involving

the nodes at $\pm m h$ (m>1) instead of those at $\pm h$. Then, there would be pollution in the sense discussed in Sect. 3 [with m=2, u₁ on the integer grid and u₂ in the staggered grid completely decouple from the opposite pair and we really have two uncoupled subproblems with half the mesh density; here "pollution" is nothing else than "aliasing"].

To make it clear that more than a consistent evaluation is needed, we consider this very simple case:

$$-i\frac{du}{dx} = \lambda u \tag{4.2}$$

With an exp (ikx) dependence, the DR is $\lambda = k$. A FD method, with the derivative operator as defined in Sect. 3, gives

$$\lambda_h = -i G_1 = (1/h) \sin kh$$
 (4.3)

which is clearly polluted, as for any finite value of λ there are two values of k, one approximating the true value, and the other being of the order 1/h. If we now evaluate the equation at mid-points, on a half-integer mesh, we have

$$(du/dx)^{i+1/2} = (u^{i+1} - u^i)/h$$

and evaluate ui+1/2 by

$$u^{i+1/2} = (u^{i+1} + u^i)/2$$

giving

$$\lambda_{h} = (2/h) \operatorname{tg}(kh/2)$$
 (4.4)

According to the definitions in Sect. 3 this is a non-polluted result.

Giving a general set of foolproof rules to avoid pollution seems rather impossible. What we present here is a method to analyze a given FD scheme and see whether it is polluting or not. We introduce first a set of derivative operators, and analyze the case of a single equation; we examine later the cases of two equations, and three or more equations.

4.1. Lowest order derivative operators

We present here the FD derivative operators that use the minimum number of nearest neighbours. Because we will apply them to a uniform grid, when acting on a Fourier component they become multiplicative factors.

Two different cases occur. One is when the equation is calculated on the opposite grid as that on which the function is defined. The lowest order numerical approximation of the differential operators d^n/dx^n , denoted by H_n , then become (h is the grid increment, and $\beta \equiv kh/2$):

$$\begin{split} H_0 &= \left[\exp(\ i \ \beta) + \exp(- i \ \beta) \right] / 2 = \cos \beta \\ H_1 &= \left[\exp(\ i \ \beta) - \exp(- i \ \beta) \right] / h = (2 \ i / h) \sin \beta \\ H_2 &= \left[\exp(3 \ i \ \beta) - \exp(\ i \ \beta) - \exp(- i \ \beta) + \exp(3 \ i \ \beta) \right] / 2 \, h^2 = (H_1)^2 \, H_0 \\ H_3 &= \left[\exp(3 \ i \ \beta) - 3 \exp(\ i \ \beta) + 3 \exp(- i \ \beta) - \exp(3 \ i \ \beta) \right] / h^3 = (H_1)^3 \end{split}$$

and, in general,

$$H_{2n} = (H_1)^{2n} H_0$$

 $H_{2n+1} = (H_1)^{2n+1}$

Similarly, when the equation is evaluated on the same grid points as the function itself, the discretized operators $d^n/dx^n\,,$ denoted by G_n , become

$$\begin{split} G_0 &= 1 \\ G_1 &= \left[\exp(\ 2\ i\ \beta) - \exp(-2\ i\ \beta) \right] / \ 2\ h = (i/h) \ sin \ 2\ \beta = H_1\ H_0 \\ G_2 &= \left[\exp(\ 2\ i\ \beta) - \ 2 + \exp(-2\ i\ \beta) \right] / \ h^2 = (2/h^2) \ (\cos\ 2\ \beta - 1) = (H_1\)^2 \end{split}$$

and, in general,

$$\begin{aligned} G_{2n} &= (H_1)^{2n} \\ G_{2n+1} &= (H_1)^{2n+1} H_0 \end{aligned}$$

4.2. Dispersion relation for one equation

Consider a single variable eigenvalue equation

$$\sum_{n=0}^{N} a_n \frac{d^n}{d x^n} u = \lambda u$$

with $a_N \neq 0$. The exact dispersion relation is

$$\lambda = \sum_{n=0}^{N} a_n (i \mathbf{k})^n$$
 (4.5)

When the equation is evaluated on grid points, we obtain

$$\lambda_{h} = \sum_{j=0}^{\lfloor N/2 \rfloor} a_{2j} (H_{1})^{2j} + a_{2j+1} (H_{1})^{2j+1} H_{0}$$
(4.6)

and, on half grid points, it gives

$$\lambda_h \; H_0 = \sum_{j=0}^{\left[N/2\right]} \; a_{2\,j} \, (H_1)^{2\,j} \; H_0 + a_{2\,j+1} \, (H_1)^{2\,j+1}$$

that is,

$$\lambda_{h} = \sum_{j=0}^{\lfloor N/2 \rfloor} a_{2j} (H_{1})^{2j} + a_{2j+1} (H_{1})^{2j+1} (H_{0})^{-1}$$
(4.7)

The powers of H_1 do not introduce spurious solutions, as H_1 is a reasonable approximation to (i k) in the range [-k_{max}, k_{max}], where k_{max} = π/h . More precisely, any polynomial $\mu = \sum b_j$ (i k)^j is well approximated in any finite range of μ by $\mu_a = \sum b_j$ (H_1)^j in the sense of

$$\lim_{h\to 0} \mu_a = \mu$$

The importance of this statement is that it helps to distinguish polluting from non-polluting approximations. Assume that we want to approximate the monomial $\mu=(ik)$ by $\mu_G=G_1$ or by $\mu_H=H_1$. At fixed k both approximations converge to the good values as $k\to 0$; in Fig. 4 we have plotted k, k and k for three values of k, and it is clear that both k and k tend to k. On the other hand, for a fixed value k, the solution k of k of k tends to the good solution k of k of k. But the equation k as two solutions, one which tends to k, and another of order 1/h; this second root causes pollution.

The multiplication of the odd terms by H_0 or $(H_0)^{\text{-}1}$ introduces a strong distortion in the range $~k_{\text{max}}$ /2 \leq |k| \leq k_{max} . The appearance of pollution

depends on the particular dispersion relation.

To decide which scheme to use, we should look at the highest derivative, N, and ensure that it is well represented in the dispersion relation, i. e., that it does not contain H_0 , and that it is larger, for $k \to k_{max}$ and $h \to 0$, than lower order derivatives. Also, H_0 should not be a common factor of all the terms in the DR, as the solution $H_0 = 0$ gives the polluting root $k = \pm k_{max}$.

As a consequence, if N is even, the equation should be computed at the grid points; in this way, the high-k end of the numerical dispersion relation (4.6) is dominated only by the Nth derivative. If there are only even derivatives, the choice of half-grid would yield the spurious root $H_0=0$; if there is at least one odd derivative, the dominant contribution in (4.7), for $|\,k\,|\,$ near k_{max} , would be from the $(H_0)^{\text{-}1}$ of the odd derivative.

Conversely, if N is odd, half-grid points should be used, to ensure that the high k end, which cannot be accurately approximated, gives numerically large eigenvalues that do not appear in any finite interval as $h \to 0$.

It might seem not evident that this rule gives good results when the leading coefficient a_N is very small. But we have to consider that the presence of the Nth derivative in the equation introduces a set of spatial lengths, (a_N / a_{N-1}) , $(a_N / a_{N-2})^{1/2}$, ..., and that the spectrum will be well represented only if the grid size is smaller than these scale lengths. Then the leading term in the DR is the Nth derivative, and it should be correctly approximated.

4.3. Dispersion relation for two equations

Consider now the system

$$\sum_{n=0}^{N} a_{n} \frac{d^{n}}{d x^{n}} u_{1} + \sum_{m=0}^{M} b_{m} \frac{d^{m}}{d x^{m}} u_{2} = \lambda u_{1}$$

$$\sum_{i=0}^{I} c_i \frac{d^i}{d x^i} u_1 + \sum_{j=0}^{J} d_j \frac{d^j}{d x^j} u_2 = \lambda u_2$$

with a_N , b_M , c_I , $d_J \neq 0$. The exact DR is given by the determinant

$$\left| \begin{array}{ccc} \displaystyle \sum_{n=0}^{N} \, a_n \, (\mathbf{i} \, \mathbf{k})^n - \lambda & & \displaystyle \sum_{m=0}^{M} \, b_m \, (\mathbf{i} \, \mathbf{k})^m \\ \\ \displaystyle \sum_{i=0}^{I} \, c_i \, (\mathbf{i} \, \mathbf{k})^i & & \displaystyle \sum_{j=0}^{J} \, d_j \, (\mathbf{i} \, \mathbf{k})^j - \lambda \end{array} \right| = 0$$

that is,

$$\lambda^2 - (A + D)\lambda + (AD - BC) = 0$$

where A, B, C and D are polynomials in (ik). As in the single equation case, to study pollution we need only to look at the high k limit. In general, to determine the leading term of the solutions of the DR ($\lambda = \alpha$ (ik) $^p + ...$, with $p \ge 0$ an integer or half integer and α a coefficient) only the leading term is necessary in each of the polynomials A, B, C and D, that is, a_N , b_M , c_I and d_J , unless there are some exact cancellations (for example, N = J, $a_N = -d_J$). Then, the method to avoid pollution is to obtain a good representation of these leading terms in λ .

In the discretization of the system of two equations, there is the choice of either defining both u_1 and u_2 on the same mesh, or to use staggered meshes. And then each equation can be computed on the mesh points or on the staggered mesh points; this gives a total of eight different possibilities.

To formalize these choices, we introduce some indices. Let v = 1,2 designate the equation and the function; let $g_v = f$,s indicate the mesh on which the function u_v is defined, f for the original mesh, s for the staggered mesh (shifted by h/2); and let $P_v = G$,H denote the point on which the equation v is computed, G for the original grid points, H for the half-grid (staggered) points. We choose to put the first function, u_1 , on the original grid, so $g_1 = f$, and the eight choices are labeled by the triplet (g_2, P_1, P_2) . The numerical operator D_n approximating the nth derivative of a function has now two indices: P_v and g_v , and we have,

$$D_n[G,f] = G_n$$
$$D_n[H,f] = H_n$$

from the preceding section, and

$$D_n[G,s] = H_n$$
$$D_n[H,s] = G_n$$

as it is straightforward to verify.

With this notation, the numerical DR is

$$\left| \begin{array}{ccc} \sum_{n=0}^{N} a_n D_n[P_1,f] - \lambda_h D_0[P_1,f] & \sum_{m=0}^{M} b_m D_m[P_1,g_2] \\ \\ \sum_{i=0}^{I} c_i D_i[P_2,f] & \sum_{j=0}^{J} d_j D_j[P_2,g_2] - \lambda_h D_0[P_2,g_2] \end{array} \right| = 0$$

As indicated before, only the high k limit needs to be considered. Thus, keeping only the leading terms (in the cases where exact cancellations occur more terms should be kept), we obtain

$$\begin{vmatrix} a_{N} D_{N}[P_{1},f] - \lambda_{h} D_{0}[P_{1},f] & b_{M} D_{M}[P_{1},g_{2}] \\ c_{I} D_{I}[P_{2},f] & d_{J} D_{J}[P_{2},g_{2}] - \lambda_{h} D_{0}[P_{2},g_{2}] \end{vmatrix} = 0$$
 (4.8)

We have to examine the eight possible choices and decide which one(s) to keep. The first thing to do is to exclude the choices that give a common factor H_0 in a row or in a column. We also have to exclude the choices in which non-leading terms in the equations become larger than the leading terms, for $k \to k_{max}$ and $h \to 0$. Then, we have to analyze the leading terms of the solutions λ_h of (4.8): they cannot contain H_0 to any positive power. The choices left, if any, are non-polluting.

For concreteness we give some explicit examples. Consider first the basic test case used in Sects. 2 and 3, Eq (2.1):

-a
$$u_1'' - u_2' = \lambda u_1$$

 $u_1' + d u_2 = \lambda u_2$

so N=2, M=1, I=1, J=0, a_2 = -a, b_1 = -1, c_1 = 1, d_0 = d. The leading terms of the solutions are λ_+ = -a (i k)² and λ_- = d- 1/a . Among the eight possible choices of discretization, only three combinations do not have a common factor H_0 ; these are (g_2,P_1,P_2) = (f,G,G), (s,G,H) and (f,H,H). The last choice can be excluded because it would give, for the first equation, a first derivative as H_1 and a second derivative as $(H_1)^2$ H_0 , and the first derivative term would be the leading term at high k. The λ_+ root is well represented, as its leading term of λ_{h+} is -a $(H_1)^2$ in the two cases left. The leading term of the λ_{h-} root is given by

$$\lambda_{h-} \approx d - \frac{1}{a} \frac{D_1[P_2, f] D_1[G, g_2]}{D_0[P_2, g_2] G_2}$$

For the case (f,G,G) we have

$$\lambda_{h-} \approx d - \frac{1}{a} \frac{G_1}{G_0} \frac{G_1}{G_2} = d - \frac{1}{a} (H_0)^2$$

which is a bad approximation, due to the $(H_0)^2$; so this scheme is polluting, as we already knew (cf Sect. 2). The case (s,G,H) gives

$$\lambda_{h-} \approx d - \frac{1}{a} \frac{H_1 H_1}{G_0 G_2} = d - \frac{1}{a}$$

and the DR is

$$\frac{\lambda_h(\lambda_h - d)}{1 + a(\lambda_h - d)} = -G_2$$

which is a good approximation. Thus, the non-polluting method in this case is to put the first function on the grid, the second on the staggered grid, compute the first equation on the grid points, and the second equation on the staggered grid points.

Consider now a second example:

-a
$$u_1'' - u_2' = \lambda u_1$$

 $u_1 + d u_2' = \lambda u_2$

N=2, M=1, I=0, J=1, a_2 = -a, b_1 = -1, c_0 = 1, d_1 = d. The leading terms of the solutions are λ_+ = -a (i k)² and λ_- = d (i k). The combinations (s,H,G) and (s,H,H) are excluded as they have the common factor H_0 . The cases (f,G,G) , (s,G,H) and (f,H,G) give the first derivative in the second equation as H_1H_0 , while the zeroth derivative is just 1, whereas in the case (H,H,f) the second derivative, in (H₁)² H₀ , is smaller than the first derivative, H₁. Thus we exclude all these cases. As in the first example, the λ_+ root is well represented, -a (H₁)² in the two cases left, (s,G,G) and (f,G,H). The other root is

$$\lambda_{h\text{-}} \approx d\,\frac{H_1}{H_0}$$

which is a good representation. In this case, we have two non-polluting schemes.

Although there is no guarantee that a non-polluting method can always be found using this set of compact operators, we have not found any counterexample.

4.4. Three and more equations, and other sets of derivative operators

In principle we can analyze the pollution of any FD scheme to solve a system of equations by checking the same features:

- i) No factorization in the discrete DR by H_0 or, in general, by a function of kh with a finite zero in $|Re(kh)| \le \pi$.
- ii) Leading terms in equations should be indeed larger than other terms, for $k\to k_{max}$ and $h\to 0.$
- iii) The leading terms in the solutions of the discrete DR should provide a good representation of the leading terms of the exact solutions. In the case of the "lowest order" operator set, they must not have positive powers of H_0 .

In practice, this last point may be the most difficult. One way to do it is to calculate the solution of the discrete DR for $k = k_{max}$ (sin $\beta = 1$) and small h. If there are no accumulation points in the analytic DR, all the solutions of a non-polluting discrete DR diverge as some negative power of h; if there are accumulation points, we should recover them in the limit $h \to 0$.

If another set of operators is used, the rules are the same. In fact, any derivative operator (including higher order approximations to D_n) can be written as a linear combination of the lowest order operators we have used here, although with coefficients that depend on h. For example, one could use a zeroth derivative of the form

$$\widetilde{G}_0 u^j = \frac{u^{j+1} + q u^j + u^{j-1}}{2 + q}$$

with $q \neq -2$, and q > 2 if we want it nonzero (when linear finite elements are used, q=4). Then,

$$\widetilde{G}_0 \; = \; G_0 + \frac{h^2}{q+2} \, G_2 \; = \; 1 \text{-} \, \frac{4}{q+2} \, \sin^2 \beta \; = \; \frac{q+2 \cos kh}{q+2}$$

The dispersion relation will in general contain this factor, or its inverse. If it appears multiplying positive powers of H₁, its effect is some "deformation" of the

DR, which in fact might improve the goodness of the approximation. However, if it is by itself the leading term, it causes pollution. In the first example of (4.3), Eq. (2.1), the second root would be given, with a (s,G,H) scheme, by

$$\lambda_{h\text{-}} \approx d - \frac{1}{a} \left(\widetilde{G}_0\right)^{\text{-}1}$$

which is d - (1/a) (q+2)/(q-2) at $k = k_{max}$, and the spectrum is significantly deformed. We should then add to "rule" iii), when using this operator set, "... nor leading terms in G_0 or $(G_0)^{-1}$."

5. Finite Elements

We now examine the FE method: we write the determinant (1.2) to obtain the discrete dispersion relation, and apply the rules we have used for the FD method. For methods with only one unknown per variable per node, the results are very similar to those obtained in FD.

Let's take first the basic test case, Eqs. (2.1). The DR (1.2), in the case of linear FE for u_1 and u_2 , is

$$\left(\lambda_{h} - a \frac{2(1 - \cos kh)}{h^{2}} \frac{3}{2 + \cos kh}\right) \left(\lambda_{h} - d\right) = \left[\frac{\sin kh}{h}\right]^{2} \left[\frac{3}{2 + \cos kh}\right]^{2}$$

that is,

$$\left(\lambda_h + a \frac{G_2}{\widetilde{G}_0}\right) \left(\lambda_h - d\right) = -\left(\frac{G_1}{\widetilde{G}_0}\right)^2$$

The comparison with (3.5) shows that it is equally polluted, as the factor 3/(2+cos kh) is not important (see Fig. 5).

The remedy offered by Appert et al. [7] is to use linear elements for u_1 , and piecewise constant elements for u_2 ; this gives

$$\frac{\lambda_h(\lambda_h - d)}{1 + a(\lambda_h - d)} = \frac{2(1 - \cos kh)}{h} \frac{3}{2 + \cos kh} = -\frac{G_2}{\widetilde{G}_0}$$

which is pollution-free (see Fig. 5). The limit values are

$$\begin{array}{lll} \lambda_{h+} \, (k=\!0) \; = \; d, & & \lambda_{h+} \, (k_{max} \,) \; \approx \; 12 \, a/h^2, \\ \\ \lambda_{h-} \, (k=\!0) \; = \; 0, & & \lambda_{h-} \, (k_{max} \,) \; \approx \; (d\text{-}1/a) \, (1\text{-}h^2/12a) \end{array}$$

thus the empty gap is indeed left empty by this discretization.

The case of Eq (4.2) is also instructive. Using continuous, piecewise linear elements for both the variable and the test functions, yields

$$\lambda_h = (1/h) \sin kh (2 + \cos kh)/3$$

which is polluted (compare to (4.3)). On the other hand, if discontinuous, piece-

wise constant elements are used for the test functions, the discrete DR becomes

$$\lambda = (2/h) \operatorname{tg} (kh/2)$$

which is unpolluted (identical to (4.4)).

The use of finite elements of order higher than one is sometimes just more convenient: it may give more precise results. And only equations up to second order can be solved with linear elements; we need higher order elements to solve higher order equations directly. Thus it is necessary to analyze the use of these elements.

Hermite elements (which have two unknowns per node) in the solution of (4.2) give rise to the equation

$$\begin{vmatrix} i G_1 h + \lambda_h h \left(G_0 + \frac{9}{70} G_2 h^2 \right) & -\frac{1}{10} \left(i G_2 h^2 + \frac{13}{21} \lambda_h h G_1 h \right) \\ \frac{1}{10} \left(i G_2 h^2 + \frac{13}{21} \lambda_h h G_1 h \right) & -\frac{i}{30} G_1 h - \frac{\lambda_h h}{140} \left(G_2 h^2 - \frac{2}{3} G_0 \right) \end{vmatrix} = 0$$

This equation, quadratic in λ_h , has two solutions: a good branch ($\lambda_h \approx k$), and a spurious branch ($\lambda_h \approx -7$ k). This is not what we usually consider as pollution, as this new mode appears at small values of k, with a long wavelength. But in fact the spurious solution still has very short wavelengths. What happens is that the short wavelength structure appears now inside the cells; the value of the solution at the nodes varies smoothly, but inside the cells it shows large amplitude ripples (analogous to a second Brillouin zone, in solid state physicists' language). The spectrum is wrong, and this phenomenon should be considered as pollution.

This is a general feature of the finite elements: as the number of unknowns per node is increased, additional branches appear. However, the situation is not hopeless, because these new branches may be relatively harmless. Let's consider the equation

$$-\mathbf{u}'' = \lambda \mathbf{u}$$

whose exact dispersion relation is $\lambda = k^2$. For linear elements, the discrete DR is

$$\lambda_h = -\frac{G_2}{\widetilde{G}_0} = \frac{4}{h^2} \, \frac{\sin^2 \beta}{1 - \frac{2}{3} \sin^2 \beta} \, .$$

On the other hand, for Hermite elements, the discrete DR becomes

$$\begin{vmatrix} -\frac{6}{5} G_2 h^2 - \lambda_h h^2 \left(G_0 + \frac{9}{70} G_2 h^2 \right) & \left(1 + \frac{13}{42} \lambda_h h^2 \right) \frac{G_1 h}{5} \\ -\left(1 + \frac{13}{42} \lambda_h h^2 \right) \frac{G_1 h}{5} & \frac{1}{10} \left(2 G_0 - \frac{G_2 h^2}{3} \right) + \frac{\lambda_h h^2}{140} \left(G_2 h^2 - \frac{2}{3} G_0 \right) \end{vmatrix} = 0$$

One of the solutions behaves as k^2 for small k, and at $k = \pi/h$ is (168/17) h^{-2} . This solution is the good one, corresponding to the exact eigenvalue. The other solution tends to $42 \ h^{-2}$ when $k \to 0$, and is $10 \ h^{-2}$ at $k = \pi/h$. This spurious solution gives only eigenvalues of the order of h^{-2} [8, p. 227]; this means that we need to take h such that $10 \ h^{-2}$ is (much) larger than the maximum eigenvalue we want to consider.

Thus in some cases the spurious branches are quite innocuous, but in other cases they produce pollution. In FD, it is sufficient to check the solutions at high k. For FE methods with more than one unknown per node per variable we have to determine the behaviour of the solutions also at small k, to see the location of the additional solutions; in fact, this means that we have to solve the dispersion relation for all the range of k, and check whether the spurious roots are proportional to some negative power of h, so that in the limit $h \to 0$ they do not have any finite value. If so, the scheme is pollution-free.

One way to avoid the issue of the spurious branches when solving systems of equations of order higher than two is to rewrite them as a system of second and first order equations, by introducing new variables; the additional equations do not involve the eigenvalue. Then it is possible to solve the system using only linear and piecewise constant elements, and the discrete dispersion relation will not be of higher order in λ than the exact dispersion relation. The analysis of the pollution at high k can be done following the rules given in the previous section. There is a strong similarity in the results, given the correspondence between choosing the grid points or half grid points and representing the function by linear or by piecewise constant finite elements, respectively, and between evaluating the equation at grid points or half grid points, and using a linear or a piecewise constant test function.

A method that has been successfully used, for self-adjoint systems of second and first order equations, is the "finite hybrid elements", introduced by Gruber [9] (see also [4]). The idea is to consider the vector components and its derivatives as distinct variables, and to choose the basis functions in such a way that each term in the weak form has the same functional dependence: in our case, constant over each cell.

This method also yields pollution-free schemes. To see that, we first consider the case of a single, second order equation:

$$au'' + bu' - \lambda u = 0$$

Multiplying by a test function v, taking the integral over the whole interval, and integrating the first term by parts we obtain the corresponding weak form (forgetting the surface terms that appear in the right hand side as source terms)

$$\int dx [-a v' u' + b v u' - \lambda v u] = 0$$
 (5.1)

In the finite hybrid element method two discretizations are used for the function u (similarly for v):

$$\begin{split} \hat{u} &= \sum u_i \; \sigma_i \qquad \qquad \text{(continuous, linear hat functions, with } \sigma_i \; (x_j) = \delta_{ij} \; \text{)} \\ \bar{u} &= \sum u_{i+1/2} \; c_{i+1/2} \; \quad \text{(discontinuous, piecewise constant} \; c_{i+1/2} \; (x) = 1 \; \text{if} \; \; x_i < x < x_{i+1} \; \text{)} \end{split}$$

The prescription [9] is to approximate all the terms in (5.1) by piecewise constants, i.e., use $\hat{\mathbf{u}}$ ($\hat{\mathbf{v}}$) when we need \mathbf{u}' (\mathbf{v}'), and $\bar{\mathbf{u}}$ ($\bar{\mathbf{v}}$) when we need \mathbf{u} (\mathbf{v}).

When both \hat{u} and \bar{u} are used, the relation between $u_{i+1/2}$ and u_i is given by imposing that the average of \hat{u} - \bar{u} should be zero on each interval; this gives

$$u_{i+1/2} = (u_i + u_{i+1})/2$$

A similar relation is imposed between $v_{i+1/2}$ and v_i when both \hat{v} and \bar{v} are used. Then, writing (5.1) as

$$\int dx \left[-a \widehat{v}' \widehat{u}' + b \overline{v} \widehat{u}' - \lambda \overline{v} \overline{u} \right] = 0$$

we obtain the Nth row of the stiffness matrix by taking the test function with v_j = δ_{jN} . The dispersion relation (1.2) is

$$aG_2 + bG_1 - \lambda_h H_0^2 = 0 (5.2)$$

(Integrating also the first-derivative term by parts gives the same result). As long as a is not zero, H_0 is not a factor. After division by H_0^2 , Eq. (5.2) shows that the finite hybrid elements do not introduce pollution; however, the eigenvalues corresponding to the fastest space-varying solutions (kh of order 1) are strongly overestimated.

If a is zero, only the piecewise constant representation of v is used in the integral (5.1); \hat{v} and v_j need not to be defined, and the rows of the stiffness matrix are obtained with $v_{j+1/2} = \delta_{jN}$. This yields the non-polluting result:

$$b H_1 - \lambda_h H_0 = 0 (5.3)$$

If the first-derivative term is integrated by parts, \bar{u} and u_j are not needed, and using only the $u_{i+1/2}$ we obtain, with $v_j = \delta_{jN}$, the same DR, Eq. (5.3).

The extension of the analysis to systems of more than one equation is straightforward, and follows the lines presented in the FD section. As an example, we discuss how the finite hybrid elements treat the system (2.1). There are now four different functions (trial functions u_1 and u_2 , test functions v_1 and v_2), each one with possibly two representations. We will see that now the integration by parts of first-derivative terms makes a difference if it allows a change of the basis elements, and that by the proper choice of element representations and a quadratic form a non-polluting scheme may be constructed.

It is clear that \hat{u}_1 , \bar{u}_1 , \hat{v}_1 , and \bar{v}_1 are needed, and so are \bar{u}_2 and \bar{v}_2 . There are four options left:

- 1) integrate only the first-derivative term in the first equation, not using the piecewise linear representations \hat{u}_2 and \hat{v}_2 ;
 - 2) integrate both first-derivative terms, and use only $\hat{\mathbf{v}}_2$;
 - 3) integrate none, and use only $\hat{\mathbf{u}}_2$;
 - 4) integrate only the term in the second equation, and use both $\hat{\mathbf{u}}_2$ and $\hat{\mathbf{v}}_2$.

The good variational form is obtained by choice 1 [9, 4] (in FD language, this amounts to defining u₂ and evaluating the second equation on the half grid).

This gives

$$\begin{vmatrix} -a G_2 - \lambda_h H_0^2 & -H_1 \\ H_1 & d - \lambda_h \end{vmatrix} = 0$$

which is a non-polluting dispersion relation.

But the finite hybrid element method is not inherently pollution-free, as shown by the other choices. With choice 2 we obtain

$$\begin{vmatrix} -a G_2 - \lambda_h H_0^2 & -G_1 \\ H_1 & (d - \lambda_h) H_0 \end{vmatrix} = 0$$

which has the polluting solution $H_0 = 0$, whereas with choice 3 we have

$$\begin{vmatrix} -a G_2 - \lambda_h H_0^2 & -H_1 \\ G_1 & (d - \lambda_h) H_0 \end{vmatrix} = 0$$

also with the $H_0 = 0$ polluting mode.

Choice 4 is even worse, as it gives

$$\begin{vmatrix} -a G_2 - \lambda_h H_0^2 & -G_1 \\ G_1 & (d - \lambda_h) H_0^2 \end{vmatrix} = 0$$

with the polluting solution $H_0 = 0$ twice.

There are no formal rules on the choice of the variational form to use to avoid pollution, but there are some empirical rules. One of them is [10]: translate, if possible, the hierarchy in differential operators to the basis elements. In our basic test case, the degree of the derivatives of u_1 is higher than those of u_2 , so the basis elements used for u_1 should be of higher order than those for u_2 ; similarly, the derivatives in the second equation are of lower degree than those in the first one, so the basis elements used for v_2 should be of lower order than those for v_1 . This rule picks choice 1 as the good one. Also, this choice preserves the self- adjointness of the original system, as the variational form is Hermitian (this is not unique of this choice, as option 4 yields also a Hermitian form).

6. Conclusion

We have presented an analysis of the pollution phenomenon, and shown for specific examples that pollution can be avoided. We have only considered linear differential equations, with constant coefficients, to be able to obtain a dispersion relation. While it is difficult, if not impossible, to give general rules to follow to avoid pollution, it is possible to analyze a given numerical scheme to see whether it is polluting, and then check whether this pollution is inconvenient for the problem at hand.

In the case of finite differences, this analysis is relatively straightforward: for one and two equations we can explore all the possibilities easily and select a non-polluting method; for three and more equations, an exhaustive search is too long to be done manually, and we will be constrained to limit the analysis to a few cases.

In the finite element method, the case of linear or piecewise-constant elements is similar to that of finite differences, and similar rules may be applied. Elements using more than one unknown per node per variable introduce additional branches in the dispersion relation, which cause pollution if they do not scale as some negative power of the mesh interval. A way to find a non-polluting method is to change the equations to a system of second and first order equations, and use then linear and piecewise constant elements, with a "standard" (conforming) representation or with a finite hybrid element method.

One point worth discussing some more is the "evilness" of pollution, and the use of polluting and non-polluting methods. As an example, we can compare (4.3) $\lambda = \sin(kh)/h$, and (4.4) $\lambda = (2/h)$ tg(kh/2) with the exact solution, $\lambda = k$. If we had to solve a time evolution problem, that is, Eq (4.2) with λ replaced by i d/dt = ω , the distortion of the DR would not raise any problem if the initial spectrum in k didn't have components larger than, say, k_{max} /2; that is, h should be smaller than 1/4 of the smallest wavelength of interest. If this is the case, both (4.3) and (4.4) are good, and pollution is not an issue. On the other hand, in a driven problem, where λ is fixed by the source, the existence of a spurious high-k branch will be very apparent, as the solutions will have a small scale ripple. Pollution can be equally disastrous when the eigenvalue spectrum is wanted (for example, in stability studies, where the lowest eigenvalue is desired); the spectrum associated with the spurious branch may completely mask the true spectrum. In these cases a non-polluting method is needed, and the kind of analysis presented in this paper may be very useful in finding one.

Acknowledgements

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Figure Captions

- Figure 1. MHD spectrum of a cylindrical homogenous magnetized plasma as a function of the number of intervals n. The analytic solution is given at the right hand side. (From [1]).
- Figure 2. Different FD approximations to the second derivative operator, as they appear in the paper. The horizontal axis is k. Curve (a) is the exact expression k^2 , the right hand side of Eqs. (2.2) and (3.3); curve (b) is the non-polluting approximation $-G_2$, the RHS of Eq. (4.1); curve (c) is the polluting approximation $-(G_1)^2$, the RHS of Eq. (3.4).
- Figure 3. Polluted spectrum of the test case (similar to Fig.1, but in slab geometry).
- Figure 4. Three plots of G_1 and H_1 (top and bottom panels, respectively) for three values of h: $h_1/h_2 = h_2/h_3 = 1.5$.
- Figure 5. Different FE approximations to k^2 . Curve (a) is the exact expression, k^2 ; curve (b) is the non-polluting approximation G_2/G_0 ; curve (c) is the polluting approximation $(G_1/G_0)^2$.

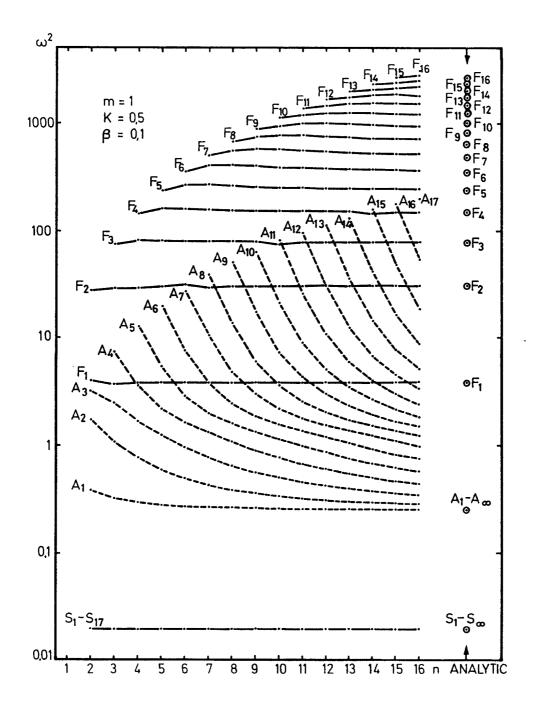


Figure 1

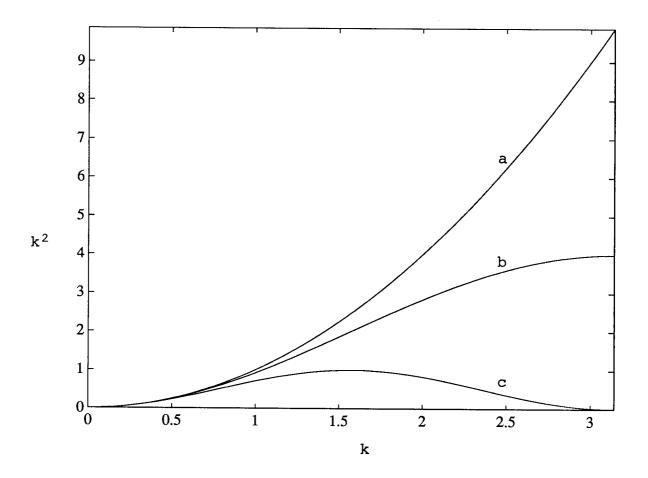


Figure 2

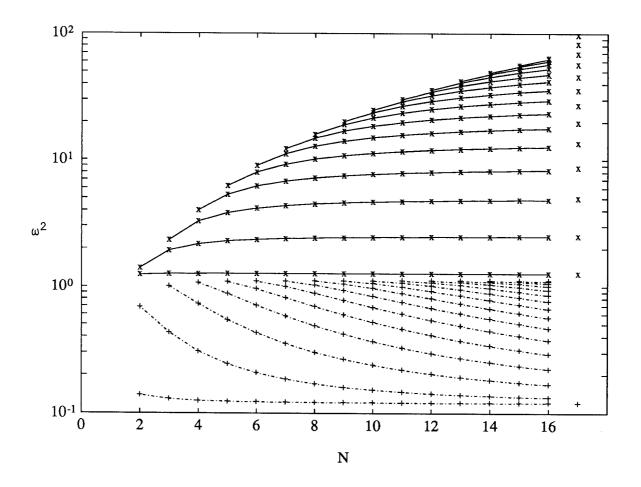
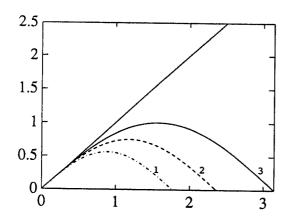


Figure 3



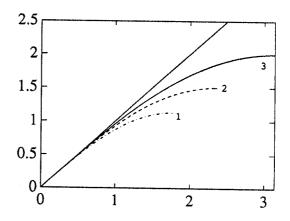


Figure 4

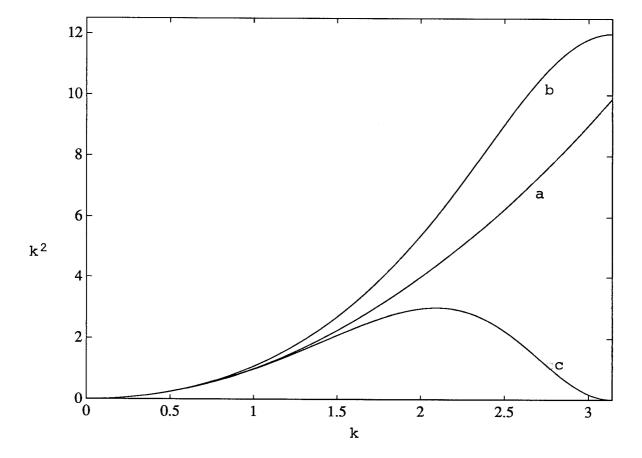


Figure 5