NUMERICAL PROBLEMS ASSOCIATED WITH THE PRESENCE

OF CONTINUOUS SPECTRA

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ABSTRACT

The discretisation of non-compact operators leading to continuous spectra and resonant absorption is discussed from a physical point of view. Relations between discrete "continua" and validity limits in evolution codes are revealed. In particular, it is demonstrated that spectral pollution might be an unpleasant problem in multidimensional evolution codes. Several open questions concerning present-day computational models are put forward.

1. INTRODUCTION

Operators with continuous spectra are quite common in plasma physics. Three well-known examples are the Vlasov-operator,[1],[2] the operator describing the interaction of laser light with cold nonuniform plasma[3-6] and the ideal MHD-operator.[7-9] These continua arise from singularities of the operator and are associated with singular eigenfunctions which have a meaning in the distributional sense.[5] There is a close connection between the singularities and what is usually called "collisionless" dissipation, Landau-damping or resonant absorption.

"The existence of singular eigenfunctions is a sure indication that some physics is left out. In the real world almost nothing is either zero or infinite. Such a result can only come from a bad estimate" as J. Greene[9] formulates it. We can, in fact, remove the singularities from all the three examples mentioned by introducing collisions (dissipation). Alternatively, finite temperature effects (dispersion) remove the singularity in the last two cases.[3],[10] The price to pay is a substantial complication of the mathematical model; usually a differential equation of higher order is obtained.

One might opt for the simplest analytical model, and therefore be willing to cope with singularities and to treat them numerically in an appropriate way. The motivation could also be more subtle. Realising that for meaningful physical parameters the dissipative effects in the complete model are often too small to smear out the singularity over many grid-points, one would like to devise methods which do not depend on smoothing at all or work with a minimum of it.

In this paper we present the technical aspects of finite element approximations to the ideal MHD-operator in the context of eigenvalue problems (MHD stability), and initial and boundary value problems (Alfvén wave heating). We are lucky that the circumstances allowed or even pushed us to investigate the properties of the same operator in

different contexts. The resulting knowledge is evidently highly specialised and its details are therefore not of direct use for most of the readers. We are, however, convinced that a case study like this can best demonstrate the numerical problems associated with the presence of continuous spectra. We also feel that it could and should stimulate a critical discussion of "ad hoc" numerical methods extensively used by the community for a variety of physical problems.

The plan of the paper is as follows. In chapter 2 the basic physics of our stability and wave studies is presented. We explain in simple terms the origin of continuous spectra and their connection with resonant absorption. In chapter 3 the numerical results are described. First we present polluted and unpolluted discrete "continua". We then investigate the question whether a discrete "continuum" may approximate the physics inherent to a real continuum. We find certain validity bounds. In the concluding chapter 4 we formulate some questions, connected with the existence of continua, to which we do not know the answers.

2. THE PHYSICS

2.1 MHD-wave excitation

We consider the excitation of small amplitude waves in a perfectly conducting cylindrical plasma. Specifically, we imagine the plasma to be surrounded by a vacuum region, an infinitely-thin current-carrying antenna, a second vacuum region and finally by a perfectly conducting shell. We are interested in the power emitted by the antenna.

Making use of the cylindrical symmetry of both the geometry and the equilibrium, one can look for plasma displacements $\vec{\xi}(r, \theta, z, t)$ of the form $\vec{\xi}(r,t) \exp(im\theta + ikz)$. Here r, θ and z are the cylindrical coordinates, and m and k are the poloidal and the longitudinal wavenumbers, respectively. The equation of motion for the plasma displace-

ment has the form

$$\rho_0 \frac{\partial^2 \vec{\xi}}{\partial t^2} = \vec{F}(\vec{\xi}) \ . \tag{1}$$

It describes the plasma response to the exciting antenna which acts on the plasma through appropriate boundary conditions.[11] The force $\vec{F}$ is the usual ideal MHD-operator in the cylindrical geometry and $\rho_0(r)$ is the mass density.

We introduce a discretised form of Eq. (1) already at this point because it allows us to present some parts of the physics in a very short way. To be definite, imagine that Eq. (1) is discretised by means of finite elements defined on a spatial grid consisting of N intervals. The equation may then be written as

$$B_{ij} \frac{d^2 x_j}{dt^2} = A_{ij} x_j + S_i(t), \quad i = 1, "3N", \tag{2}$$

where x_i are the "3N" nodal points of $\vec{\xi}$ and $s_i(t)$ are the components of the pump vector imposed by the antenna. The notation "3N" means approximately 3N, the precise number of the nodal points depending on the discretisation method used. There is a sum over double indices.

Without going through the detailed theory[11] we can guess the form of the power emitted by the antenna by constructing an energy conservation law from Eq. (2):

$$\frac{d}{dt} \frac{1}{2} \left[\frac{dx_i}{dt} B_{ij} \frac{dx_j}{dt} - x_i A_{ij} x_j \right] = \frac{dx_i}{dt} S_i \equiv P. \tag{3}$$

Here we have made use of the symmetry of the matrices $\vec{A}$ and $\vec{B}$.[12] The first term in the bracket represents the kinetic plasma energy and the

second term the plasma and a part of the vacuum potential energy; hence the right-hand side of the equation represents more or less the power emitted by the antenna.

2.2 Continuous spectra

The continuum-engendering character of $\vec{F}$ can best be seen in an alternative form of Eq. (1). If we assume a time dependence $\exp(-i\omega t)$ Eq. (1) may be written[7] as

$$
\left.
\begin{aligned}
D\frac{d}{dr}\left(r\xi_r\right) &= C_1\,r\,\xi_r - r\,C_2\,P \\
D\frac{d}{dr}\,P &= C_3\,\xi_r - C_1\,P
\end{aligned}
\right\}, \tag{4}
$$

where P is the total perturbed pressure which can be expressed in terms of $\vec{\xi}$. For reasonable equilibrium quantities $\rho_0(r)$, $p_0(r)$ and $\vec{B}_0(r) = (0, B_{\theta 0}, B_{Z0})$ (density, pressure and magnetic field), the coefficients D, C_1, C_2 and C_3 are analytic functions of $r > 0$. The coefficient D has the structure

$$
D = \left(\omega^2 - \omega_A^2(r)\right)\left(\omega^2 - \omega_S^2(r)\right), \tag{5}
$$

where

$$
\omega_A^2 = \left(\frac{m}{r}B_{\theta 0} + k\,B_{Z0}\right)^2 / \rho_0, \tag{6}
$$

and

$$\omega_S^2 = \omega_A^2 \, \gamma p_o \, / \, (\gamma p_o + \vec{B}_o^2) . \tag{7}$$

Here γ is the adiabaticity index.

Let us, for a moment, interpret Eq. (4) as an eigenvalue problem for the frequency ω (MHD stability). Also, let us assume that we find an eigenfrequency satisfying D = 0 somewhere within the plasma. From the form of Eq. (4) it is then straightforward to see that the associated eigenfunction must be singular at this place.

Each frequency ω satisfying D = 0 somewhere within the plasma is, in fact, an eigenvalue[8] and belongs either to the Alfvén continuum if $\omega = \omega_A(r)$ or to the slow wave continuum if $\omega = \omega_S(r)$.

The physical reason for, say, the Alfvén continuum is easy to understand. Equation (6) is the dispersion relation in the WKB sense for the shear Alfvén wave in a diffuse cylindrical plasma. The phase velocity depends on the position r. A possible "eigenmotion" at the frequency ω is therefore a wave which is confined to a narrow region around the so-called resonant surface r_s, where $\omega = \omega_A(r_s)$. Conversely, for each r_s within the plasma, a wave must exist whose frequency is given by $\omega = \omega_A(r_s)$. The shear Alfvén waves have therefore a continuous spectrum.

2.3 Resonant absorption

Imagine now that such a system is to be excited with a given pump frequency ω_p within the range of the continuum, starting at the time t = 0. Initially, a broad band of frequencies is excited; but as time progresses the bandwidth tends to zero and yet infinitely many modes in the continuum remain in resonance with the pump and grow in amplitude. The system therefore, "absorbs" energy at a constant rate by increasing the energy content of an ever diminishing thin layer around the resonant surface at r_s. Obviously, this is an unphysical behaviour which we could describe as a resonant accumulation of energy. The

inclusion of any physical dissipation mechanism, however small, will prevent the system from evolving so far. It will attain a stationary state where the dissipation in the neighbourhood of the resonant surface just balances the energy inflow from the pump.

The important point now is that the absorbed energy depends on neither the specific dissipation mechanism nor its quantitative value. This is one of the characteristic features of resonant absorption.

3. THE NUMERICS

3.1 The discrete "continuum"

The continuum character of the Alfvén and slow wave spectra is lost when the Eqs. (1) or (4) are discretised in space. If we use Eq. (2), discrete "continua" are obtained. The question is now under which conditions the numerical system is able to describe the plasma response, for instance in the Alfvén range of frequency, correctly. In other words we could ask: How continuous is a discrete "continuum"?

We are able to give a quantitative answer to this question in the case of an unpolluted spectrum in the next two subsections. The problems concerning polluted spectra have not yet been studied in detail neither by physicists nor by mathematicians. In the third subsection we will present certain qualitative aspects of polluted spectra.

In this paper we do not discuss the origin of pollution and methods to avoid it; we just note that certain methods lead to a pollution and others do not. Details on polluting and non-polluting methods applied to the MHD-problem, Eq. (1) in cylindrical geometry, can be found in the references 12 - 15.

In the context of this paper it is sufficient to note the typical effect of the pollution in an example, Fig. 1. The spectra have been obtained for a currentless plasma cylinder, having a density $\rho_0(r) = (1 - 0.9r^2/a^2)\, \rho_0(0)$, which is imbedded in a constant magnetic field B_{Z0}. The frequencies ω are given in dimensionless units $C_A(r=0)/a$, where $C_A(r=0)$ is the Alfvén velocity on the axis and a is the plasma radius. The gas pressure is zero, the conducting wall is at 1.5a and the wavenumbers are m=1 and k=0.5/a.

The exact analytical spectrum is shown on the leftmost axis. For graphical reasons a logarithmic scale for $\omega - \omega_A(r=0)$ has been used. The Alfvén continuum extends up to $\omega - \omega_A(0) = \omega_A(1) - \omega_A(0) = 2.5^{1/2} - .25^{1/2} = 1.08$ and is followed by the lowest fast magnetosonic modes F_1, F_2, and F_3. The next axis shows the Alfvén frequencies, Eq. (6), evaluated at the location of the 21 equidistant spatial grid points r_i, used for the discretisation of the problem. The two axes on the right show numerical spectra. The unpolluted spectrum was obtained by means of the method described in Ref. 12. The polluted spectrum results from the most natural finite element approximation.[14]

Most strikingly, the pollution may push the "continuum" frequencies beyond the physical boundary $\omega - \omega_A(0) = 1.08$. It may even push them above the fast modes; see e.g. the polluting Alfvén mode A_{20}. At about half of the Alfvén modes only fall into the frequency band of the physical continuum. The frequencies near to $\omega_A(0)$ are badly represented: the lowest mode A_1 appears with a frequency corresponding to roughly $\omega_A(r_9)$ which is near to the unpolluted A_9.

In contrast to this, in the unpolluted case the frequencies in the "continuum" lie near the frequencies at the spatial grid points $\omega_A(r_i)$. Therefore, the density of the spatial grid at some place r can directly be related to the density in frequency at $\omega = \omega_A(r)$. If at some place r the width of the grid is Δr then the distance $\Delta\omega$ between the adjacent frequencies of the "continuum" is

$$\Delta\omega = \frac{d\omega_A}{dr}\,\Delta r \; . \tag{8}$$

3.2 Resonant accumulation of energy

We can investigate the properties of a "continuum" by exciting the discretised system, Eq. (2), with a sinusoidal signal $s_i(t)$ $\propto$ $\sin\omega_p t$, and using a pump frequency ω_p lying in the range of the Alfvén continuum, Eq. (6). A convenient quantity to evidence the response of the system is the power, Eq. (3), flowing from the antenna into the plasma. In the case of resonant accumulation, its value averaged over an oscillation period, $\bar{p}$, should be independent of time.[16,17] In other words, the mean energy E contained in the plasma should grow linearly with time as $\bar{p}t$.

The numerical results obtained with an equidistant mesh consisting of 80 intervals and a pollution-free method are presented in Fig. 2. The runs shown concern a typical tokamak equilibrium given by $B_{Zo} = B_{Zo}(0)$, $1/r$ d/dr $rB_{\theta o}$ = j_Z = $.6(1-r^2/a^2)^2$ $B_{Zo}(0)/a$ and $\rho_0 = (1 - .99\ r^2/a^2)\ \rho_0(0)$. The antenna and conducting shell radii are 1.2a and 1.5a, respectively. The helical antenna currents are characterised by m=1, k=.6/a and $I=aB_{Zo}/\mu_0$, where I is the total current of a given polarity.[11] The average power per unit length of the machine $\bar{p}$ is measured in units of $aC_A(0)B_{Zo}(0)/\mu_0$. The unit of time is $a/C_A(0)$. The energy per unit length E is measured, therefore, in $a^2 B_{Zo}/\mu_0$. Two pump frequencies have been chosen. The first frequency ω_{p1} lies between two eigenfrequencies of the discrete "continuum", the second one ω_{p2}, on the other hand, is equal to an eigenfrequency. We find that the energy grows linearly with time as long as t < 2 $\pi/\Delta\omega$ where $\Delta\omega$ is the difference between adjacent eigenvalues in the region of the pump frequency. If t > 2 $\pi/\Delta\omega$ the energy content in the system starts to decrease again when pumped with ω_{p1} whereas it starts to grow quicker than linearly when pumped with the eigenfrequency ω_{p2}.

The interpretation of this result is straightforward. At finite times t the system does not see a pump having precisely the frequency ω_p but a pump having a width $\Delta\omega_p$ around ω_p of the order of 2 π/t (uncertainty relation). In other words, at time t we act upon a system of harmonic oscillators (our discrete "continuum") by a force with a

continuous spectrum.[18] As long as $t < 2 \, \pi/\Delta\omega$ at least two oscillators are in resonance. From Fig. 2 we conclude, therefore, that two modes (oscillators) are sufficient to approximate a continuous spectrum.

For times $t > 2 \, \pi/\Delta\omega$ the spectrum appears as discrete. The result $E \propto t^2$ is obtained when a single undamped oscillator is excited at its resonant frequency, its amplitude growing like $t \, \sin\omega_{p2}t$. If, on the other hand, none of the undamped oscillators is in resonance with the pump the average energy transfer has to be zero for $t \to \infty$: the energy swings forth and back at certain beat frequencies between the antenna and the system, consistent with the curve ω_{p1} in Fig. 2.

3.3 Resonant absorption

There is another way to show that the excitation of two modes belonging to the discrete "continuum" is sufficient to make it look continuous. The idea is to change the resonant accumulation into a resonant absorption by introducing a small artifical damping term into Eq. (2). We may then look for stationary states behaving as $\exp(i\omega_p t)$. The problem is considerably simplified and consists of the solution of the linear system

$$\left(-\omega_p^2 + 2i\nu\omega_p\right) B_{ij} x_j = A_{ij} x_j + S_i \, , \qquad (9)$$

for $x \epsilon \mathbb{C}$. In this case the time averaged power is given by $\mathrm{Im}\omega_p x_i s_i/2$.[11] Here ν denotes the small ($\nu \ll \omega_p$) artificial damping rate. Note that x_i and s_i have not the same meaning as in Eq. (2). Here they are amplitudes of a harmonic time dependence $\exp(i\omega_p t)$ which has been separated out in Eq. (9).

The numerical problem we study now resembles to a system of coupled oscillators with different real eigenfrequencies but a common damping coefficient ν. Imagine now that such a system is to be excited

with a given pump frequency ω_p such that $\omega_i < \omega_p < \omega_{i+1}$, where ω_i and ω_{i+1} denote two adjacent eigenfrequenies of the system.

Let us first discuss the case where $\nu \ll \omega_{i+1} - \omega_i = \Delta\omega$. If ω_p is chosen near enough to the eigenfrequency ω_i, i.e.
$\omega_p - \omega_i \ll \nu$, the oscillator which has ω_i is resonantly excited and the dissipated energy is proportional to $1/\nu$. If, on the other hand, ω_p lies in between ω_i and ω_{i+1}, say $\omega_p = (\omega_i+\omega_{i+1})/2$, none of the oscillators is in resonance and a negligible amount of energy proportional to ν is dissipated. These two situations have obviously nothing to do with the excitation of a continuous spectrum, in contrary, the eigenfrequencies of the system behave as real discrete eigenfrequencies.

The story is quite different in the opposite limit where $\nu \gg \Delta\omega$. In this case the resonancies at adjacent eigenfrequencies overlap and many oscillators respond simultaneously to the pump: a "continuum" is excited and "resonant absorption" takes place. In certain limits of ν the amount of dissipated energy is independent of ν.

This behaviour is evidenced in Fig. 3. The calculations concern the same equilibrium as used for Fig. 2. The radial mesh and the pump frequencies are also the same as in Fig. 2. We find that the absorbed power is more or less independent of ν for $\nu > \nu_{lim} \equiv \Delta\omega$, demonstrating once again that two modes make up a continuum.

3.4 Pollution is bad; but is it dangerous ?

In Fig. 1 we have remarked that one half of the 20 available Alfvén frequencies have been pushed from the range of the physical continuum. This is one possible manifestation of the spectral pollution.

There are two consequencies to this. First of all, the density in frequency space of the "continuum" modes is certainly smaller in the polluted than in the unpolluted case. We therefore expect ν_{lim} to be greater accordingly. That this is indeed true is demonstrated in

Fig. 3, where the run with ω_{p2} has been repeated using the same standard finite elements as in Fig. 1. In the example presented ν_{lim} is 3 times greater than in the unpolluted case. This means that for a given accuracy the pollution-free method needs merely 1/3 of the spatial grid points required by the polluting method.

The second and quite frightening consequence of the pollution is the existence of spurious modes (A_{20} in Fig. 1) among real physical modes (F_1, F_2 etc.). These spurious modes do not disappear when the number of grid points is increased; on the contrary, new such modes may be created at increasingly-higher frequencies.[14] The question is how the system responds when excited on such frequencies.

The answer concerning the spectrum in Fig. 1 is depicted in Fig. 4. We show the average power $\bar{p}$ delivered by an antenna of the radius 1.2a, obtained with two different damping coefficients $\nu = 0.15$ and 0.015. Here single modes are excited; hence the absorption is proportional to $1/\nu$ at resonance. We find that the mode A_{20} is not as easily accessible as the fast modes but responds quite distinctly in the weakly-damped case.

We conclude that pollution is bad; but is it, in general, in any numerical and physical context dangerous? It is certainly not! Convergence studies will always reveal the nature, physical or numerical, of a given motion. Physical modes are approximately invariant when the grid size is changed in contrast to spurious modes which move in frequency.[14] Also we have found that modes in the neighbourhood of F_2, for instance, are less accessible as the number of grid points is increased. They become increasingly more titillant.[21] Note also that the mode A_{19}, which is near to F_1 in Fig. 1, does not show up in Fig. 4. To make it apparent an even lower damping coefficient would have to be chosen.

4. OPEN QUESTIONS

In multidimensional codes, where often only very limited conver-
gence studies are thought to be justifiable, the polluting spurious
modes could sometimes play nasty roles. The coarser the grids are the
easier it is to excite them and the more they look physical. It is,
however, an open question how this kind of numerical defect would
manifest itself in the context of a code including all kinds of addi-
tional physics such as dissipation, dispersion or nonlinearities.

From the studies with a resistive compressional MHD-stability
code we know[19] that resistivities of the order of those observed in
tokamaks are by far too small to make the numerical problem of pollu-
tion disappear. On the other hand, we know from the studies into
EM-wave-plasma-interaction[20] that the dispersion may replace the pro-
blem of pollution by a simple and manifest resolution problem.

What do the eigenfunctions associated with polluting eigenvalues
represent? Are they needed to approximate a reasonable physics? It
seems to us that the truncated system of eigenfunctions, not including
the polluting (titillant[21]) ones, should be approximately complete in
some sense. This is an open question for which the mathematicians
should find an answer.

There is another open question concerning evolution codes con-
nected with the discreteness of continua. We have demonstrated in
Fig. 2 that the discreteness in frequency leads to limits in time when
the code results are valid. Obviously, the discreteness in frequency
may be smeared out by physical damping mechanisms, and the time limits
may therefore disappear. We have, however, just remarked[19] that toka-
mak resistivities, for instance, are very small. Tremendously fine
grids would, in fact, be needed to make the time limits disappear. Are
the codes which are used for the modeling of present day machines free
of such time limits? Have ever strange recurrencies been observed? A
well-documented example of such a recurrence is presented in Ref. 22.

The catalogue of questions put forward by us is the product of a certain professional deformation which one could call the "MHD-stability syndrome". In spite of this our questions might be pertinent.

Acknowledgements

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FIGURE CAPTIONS

Fig. 1. From the right to the left are shown typical polluted and
         unpolluted spectra ω_i, together with the Alfvén frequen-
         cies ω_A at the spatial gridpoints r_i, in comparison with
         the exact analytic spectrum. Alfvén modes (A) are shown with
         circles, fast magnetosonic modes (F) with crosses.

Fig. 2. Energy per unit length E versus time. The insert shows where
         the pump frequencies ω_{p1} and ω_{p2} lie in the "continuous"
         spectrum.

Fig. 3. Power per unit length $\bar{p}$ versus the artificial damping rate
         ν. The pump frequencies ω_{p1} and ω_{p2} are the same as in
         Fig. 2. The "polluted" result has been obtained with
         standard finite elements.

Fig. 4. Power per unit length $\bar{p}$ versus the pump frequency ω for two
         different artificial damping rates: $\nu = 0.15$ (-----) and
         $\nu = 0.015$ (_____). A_{20} shows the response of a spurious
         Alfvén mode. Without a convergence study it is not easy to
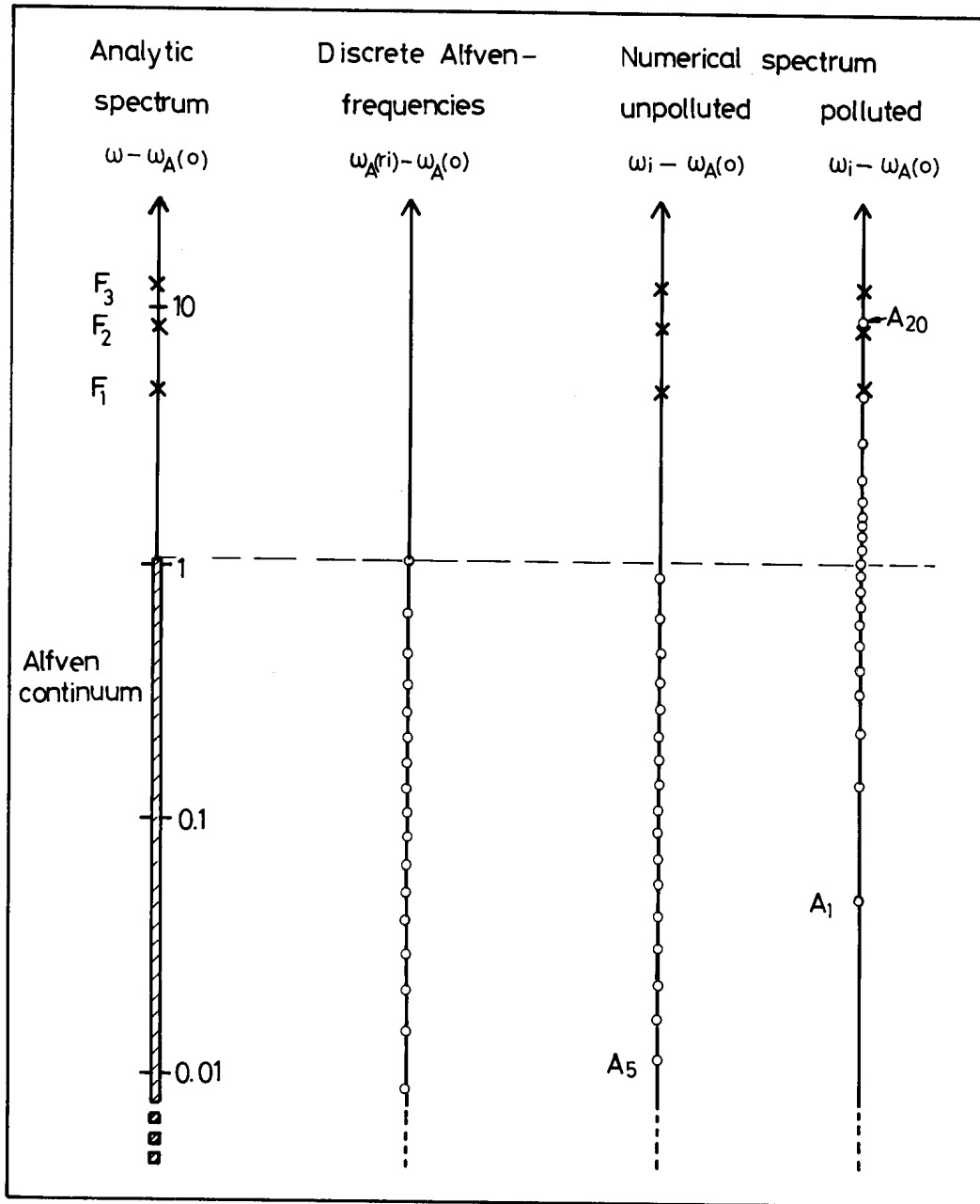   distinguish it from the response at the frequencies of real
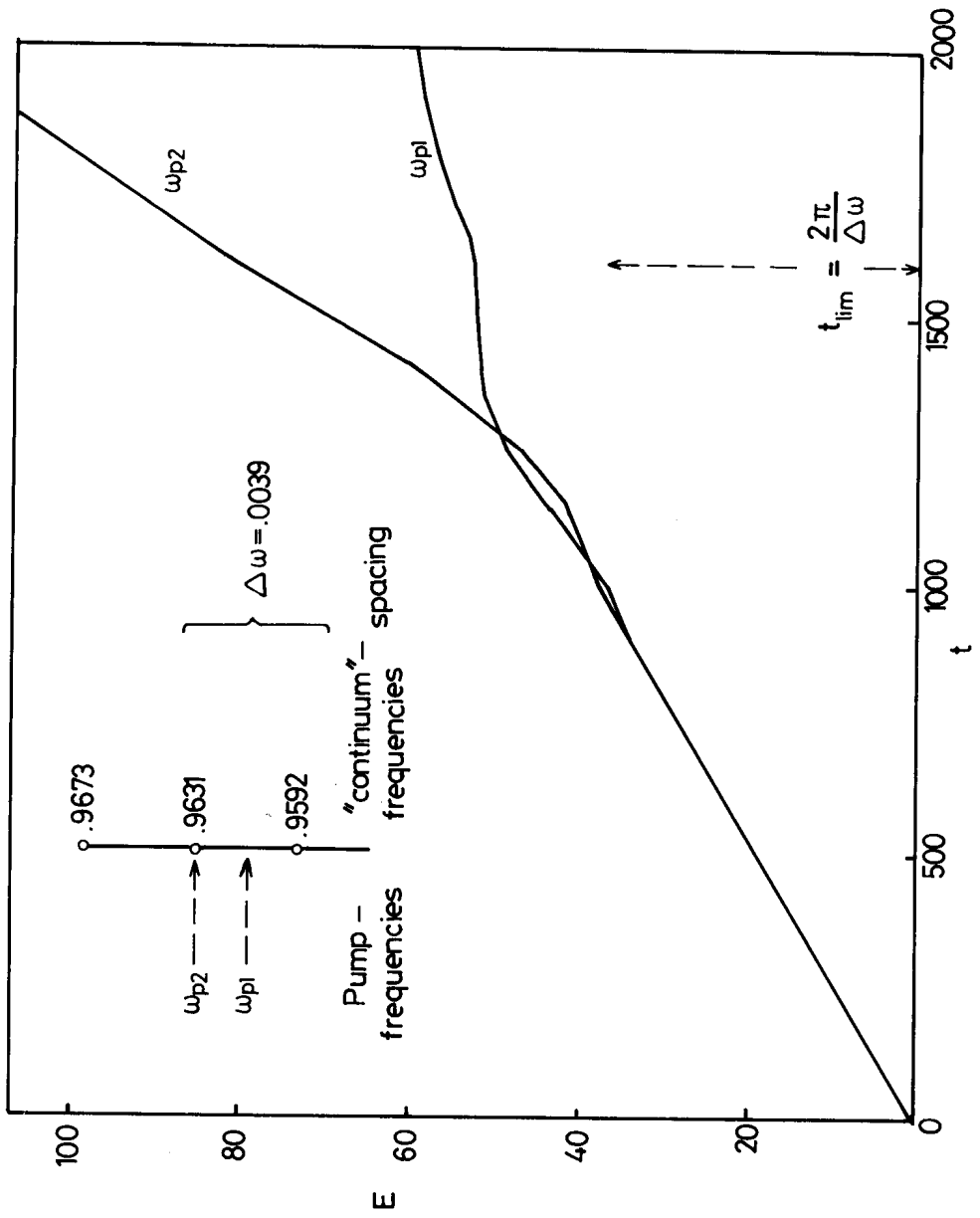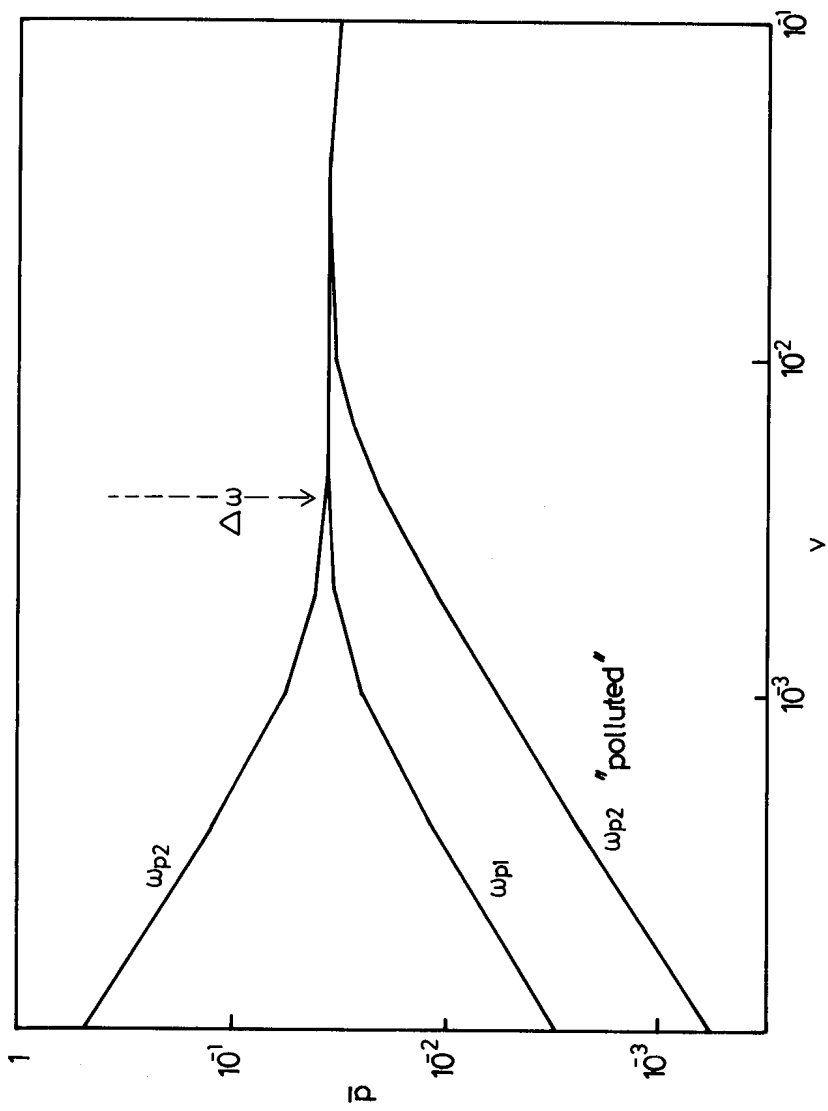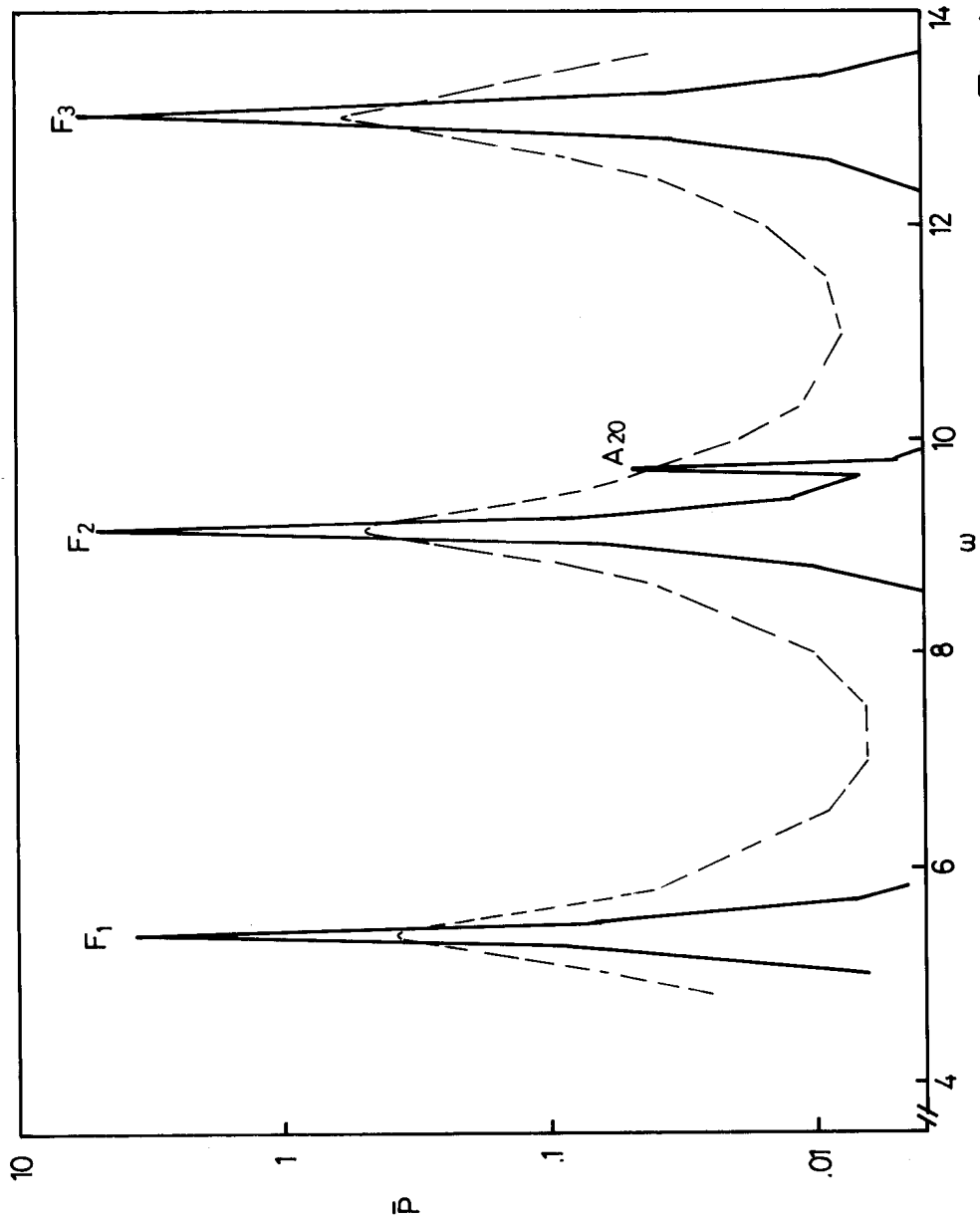   fast magnetosonic modes (F_1, F_2, F_3).

Fig. 1

Fig. 2

Fig.3

Fig. 4