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Automation of the Derivation of Dispersion Relations: II. Higher Order Dielectric Functions in Hot Plasmas*

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Symbol manipulation by computer was used to carry out the analytic operations leading to the evaluation of higher-order dielectric functions connected with electrostatic modes in hot plasmas. Application was made to mode–mode coupling between amplifying waves in a beam–plasma system. The basic input data were the Vlasov–Poisson equations. A perturbation calculation was carried out to fourth order in terms of an unspecified zeroth order distribution function. The analytic results were then converted automatically to FORTRAN statements in terms of the plasma dispersion function. The third-order dielectric function was evaluated numerically for the purpose of comparison with the experimental results of Carr *et al.* on mode–mode mixing.

PL/1–FORMAC was the programming medium used for the symbol manipulation.

1. INTRODUCTION

Mode mixing via nonlinear processes is a well-known phenomenon in plasma physics [2]. One approach to its theoretical treatment is a perturbative expansion of the Vlasov equations in powers of the electric field strength. This paper describes a method for automating this type of perturbative expansion; we have carried it out to fourth order. Further, we discuss the generation of a program for numerical evaluation of these results. The specific impetus for these calculations was the results of Carr *et al.* [1] on mode coupling in an unstable medium. Fig. 1 shows the essential result of this experiment. It is to be noted that the amplitudes of the generated sidebands appear to decrease logarithmically with the order of the sideband. One purpose of this work was to investigate whether or not this behavior could be attributed to some dominant contribution in each of the odd-order dielectric functions even though the experiment involves magnetized plasma behaving quite nonlinearly. At the same time we developed (to the extent discussed below) an automatic programming system to expedite calculations of this nature.

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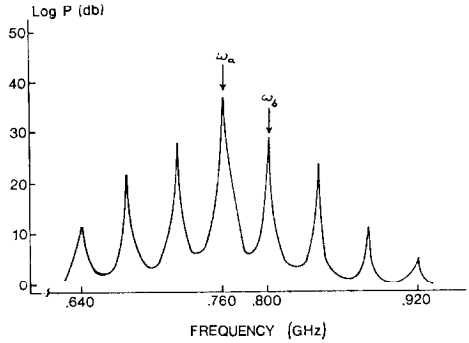

FIG. 1. Experimental results on wave-wave mixing.

The symbol manipulation programs carry out the following analytic steps:

(1) Perturbation expansion of the Vlasov–Poisson equations both in implicit and explicit form.

(2) Conversion of integrals over the velocities into appropriate combinations of plasma dispersion functions by use of integration by parts and partial fraction expansion.

(3) The generation of a FORTRAN code for the numerical evaluation of frequently occurring expressions.

In the next section we briefly delineate the problem in physical and mathematical terms. The symbolic programs for carrying out the perturbation expansion are discussed in Section 3. The analytic results obtained by symbolic manipulation are discussed in Section 4. We present the solutions in a form in which no specification of the zeroth order distribution function is made at this point; in this sense the results are general. In Section 5, we describe the conversion of the symbolic output into FORTRAN statements and the numerical evaluation of the third-order dielectric function. The basic programs were written to have a wider range of applicability than merely the specific problem treated here. These programs include ORDERS [3], which performs ordering of differential equations, and REPLACE, which substitutes lower-order results for higher-order equations. The programming medium used for the symbolic manipulation was PL/1–FORMAC [4].

2. DESCRIPTION OF PROBLEM

We consider a hot plasma (single species) occupying a semi-infinite region of space. There is a beam of electrons entering the plasma. In a limited region of space about the nearer boundary the plasma (and beam) electrons are modulated

in density and/or velocity by an external source so as to excite electrostatic waves. This modulation has Fourier components at (at least) two different frequencies, which correspond to amplifying modes in the system. The system is immersed in a strong unidirectional, uniform magnetic field.

The Vlasov equations for a one-dimensional collisionless electron plasma provide an adequate description of this model in which the positive charges are considered to form an immobile background with density n_0. The relevant equations are [3] (in original form):

$$\frac{\partial E}{\partial x} = \int f \, dv \tag{1}$$

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + E \frac{\partial f_0}{\partial v} = -\beta E \frac{\partial f}{\partial v}. \tag{2}$$

We apply the Laplace transform in space and Fourier analyze in time to obtain

$$+ik\tilde{E} = \int \tilde{f} \, dv + E_B(\omega) \tag{1'}$$

$$-i(\omega - kv)\tilde{f}(\omega, k) + \tilde{E} \frac{\partial f_0}{\partial v} = v f_B(\omega, v) - \beta \iint \tilde{E}(\omega_1, k_1) \frac{\partial \tilde{f}}{\partial v} (\omega - \omega_1, k - k_1, v) \, d\omega_1 \, dk_1 \tag{2'}$$

wherein v is the velocity variable parallel to magnetic field, f_0 is the part of the distribution function that is independent of time, $f = f(x, v, t)$ is the rest of the distribution function, and $E = E(x, t)$ is the self-consistent electric field. The quantities marked with a subscript B represent the Fourier transform of the boundary values and the twiddles indicate the double transform. For simplicity we have written the equations in terms of reduced variables in which the Debye wavelength, the plasma frequency ω_p, and the electron thermal velocity V_{th} are all unity. The electric field is measured in units of $m\omega_p V_{th}/e$, wherein m and e are the electron mass and charge, respectively. The distribution functions are measured in units of the average density divided by the thermal velocity. Finally, we have introduced a formal ordering parameter β, whose actual value is 1. As discussed in further detail below, the function f_0 is a prescribed function while the first-order electric field denotes the linear response of the medium to the excitation.

We assume that the electric field E, and the distribution function f, each can be expanded in a power series in β, thus

$$E = \sum_1^\infty \beta^n E(n) \tag{3}$$

$$f = \sum_1^\infty \beta^n f(n). \tag{4}$$

The boundary terms contain first-order terms. Inserting these expansions into Vlasov set ((1′) and (2′)), we are led to the following equations for the terms of different orders of coupling

$$ik\tilde{E}(n) = \int \tilde{f}(n)\, dv + \delta_{n,1}E_B \tag{5}$$

$$-i(\omega - kv)\,\tilde{f}(n) + \tilde{E}(n)\,\frac{\partial f_0}{\partial v}$$

$$= vf_B\delta_{n,1} - \iint \sum_{\delta=1}^{n} \frac{\partial \tilde{f}}{\partial v}\,(s, \omega', k', v)\, E(n - s, \omega - \omega', k - k')\, d\omega'\, dk'. \tag{6}$$

The first-order electric field is a functional of the boundary values f_B and E_B, which are to be specified; this first-order field is the *linear* response of the medium to the modulation and can be written as

$$E(1) = \sum_{l} E_{10}(\omega_m(l)) \exp[i(k_m x - \omega_m t)]. \tag{7}$$

The values of ω_m in our particular application in which there are two modulating signals are $\pm\omega_a$ and $\pm\omega_b$. The (complex) values of k_m are determined by the solution of the dispersion relation

$$1 - \frac{\omega_p^2}{k^2} \int \frac{1}{v - \omega/k}\,\frac{\partial f_0}{\partial v}\, dv = 0.$$

In the actual calculation we performed we took f_B to be zero and $E_B \neq 0$. The results of the calculation are then a prediction of the value of $E(n)$ in terms of the lowest-order distribution function f_0, and the parameters of the excitation such as the ω_m's and the $E_{10}(\omega_m)$'s.

3. Automated Perturbation Expansion

In this section we shall discuss the two programs ORDER and REPLACE, which carry out the perturbation expansion of the Vlasov–Poisson equations. The programs that convert the symbolic results into FORTRAN statements are discussed briefly in Section 5.

The program ORDERS [3] accepts as data (differential) equations and information indicating the ordering (or orderings) of parameters and dependent variables in these equations. Its operation is then as follows: (a) It forms an expansion of the dependent variables in powers of the ordering parameter; (b) It

segregates the results according to powers of the ordering parameter; and (c) Under user control, it carries out the transformations

$$\frac{\partial}{\partial t} \to -i\omega; \qquad \frac{\partial}{\partial x} \to ik.$$

In performing the transformations just mentioned, products of dependent variables are transformed according to the usual convolution rule

$$a(x, t) \cdot b(x, t) \to \iint \tilde{a}(\omega_1, k_1)\, \tilde{b}(\omega - \omega_1, k - k_1)\, d\omega_1\, dk_1 .$$

In the internal (that is, within the program) representation of the integrals over k_1 and ω_1 is implicit. Further details can be found in the first paper of this series.

The ordering operation is actually rather trivial in this case and we have presented the results for different orders in Eqs. (5) and (6). However, these equations give the results in implicit rather than explicit form. The next step, performed by REPLACE, proved to be more difficult. This was the substitution of the lower-order results into the higher-order equations in order to make these latter results explicit functions of ω and k.

Prior to substitution into the nth order terms, it is necessary to solve the nth order results for $E(N)$ and $F(N)$. As a result one finds that E and F of order N can be expressed as a sum of nonlinear terms, each of which has one factor $F(I)$ and a factor $E(J)$ where $I + J = N$. The process of substitution is somewhat more complicated than the mere replacement of one expression by another since the correct frequency and wavenumber dependence of the terms must be maintained. (One must remember that $E(J)$ and $F(I)$ in turn consist of contributions from lower-order terms.) We have used the following method on a term by term basis:

(1) A table was made of the order in the perturbation expansion of F and of E in each term.

(2) Prior to any substitutions, the frequency and wavenumber variables in each term are changed to an appropriate sum of such terms. If the term is of order N and consists of the product of a term of F of order $N1$ and a term in E of order $N - N1$, then the frequency argument of F is made SUMW(1, $N1$) and that of E is made SUMW($N1 + 1$, N). Here $\text{SUMW}(J, L) = \sum_{i=J}^{L} \omega_i$, which may be a single term or several. It is understood that $\sum_1^N \omega_i = \omega$, where ω is the frequency argument of $F(N)$ and of $E(N)$.

(3) At the time of substitution of a term of order M (such as has been just described) into a term of order $N > M$, two possibilities occur for the form of the term in which substitutions are to be made.

It is of the form $F.(\mathrm{SUMW}(1, M)) * E.(\mathrm{SUMW}(M + 1, N))$ and we are substituting for F. No change need be made.

It is of the form $F.(\mathrm{SUMW}(1, N - M), N - M) * E.(\mathrm{SUMW}(N - M + 1, N), M)$ and we are substituting for E. In this case we must augment the frequency and wavenumber arguments of the *explicit* form of E. $(\mathrm{SUMW}(1, M), M)$ by $N - M$ before substituting. In other words, in the term being substituted, any frequency argument such as $W(I)$ would become $W(I + N - M)$ just prior to substitution.

An example will serve to illustrate this. The fourth-order distribution function contains a term proportional to $E(2)(\partial f/\partial v)(2)$ where the numbers denote the order of the term. More explicitly, this term can be written as $E(\mathrm{SUMW}(3, 4), 2)(\partial f/\partial v)(\mathrm{SUMW}(1, 2), 2)$. The second-order electric field itself consists of terms that depend on $W(1)$ and $W(2)$. Before substituting these terms for $E(2)$ the frequency arguments $W(1)$ and $W(2)$ must be changed to $W(3)$ and $W(4)$.

4. Symbolic Manipulation Analytic Results

The form of the symbolic output produced by the combined action of the programs ORDERS and REPLACE is illustrated by the following term in the third-order distribution function

$$
\begin{aligned}
\text{'TERMS}(1, 1, 3) = {} & \mathrm{EPS.}\,(\mathrm{SUMW.}\,(2, 3), K.\,(2, 3)) ** (-1) * K.\,(2, 3) ** (-1) \\
& * \mathrm{EMO.}\,(\mathrm{SUMW.}\,(3, 3)) * \mathrm{DV.}\,(-\mathrm{EMO.}\,(\mathrm{SUMW.}\,(1, 1)) \\
& * \mathrm{DV.}\,(F00.\,(\mathrm{NULL}, V, 0), V) * (-V * K.\,(1, 1) * \#I \\
& + \mathrm{SUMW.}\,(1, 1) * \#I) ** (-1), V) * \mathrm{DV.}\,(-\mathrm{EMO.} \\
& (\mathrm{SUMW.}\,(2, 2)) * \mathrm{DV.}\,(F00.\,(\mathrm{NULL}, V004, 0), V004) \\
& * (-V004 * K.\,(2, 2) * \#I + \mathrm{SUMW.}\,(2, 2) * \#I) \\
& ** (-1), V004) * \mathrm{SUM.}\,(V004) * (-V004 * K.\,(2, 3) * \#I \\
& + \mathrm{SUMW.}\,(2, 3) * \#I) ** (-1) * (-V * K.\,(1, 3) * \#I \\
& + \mathrm{SUMW.}\,(1, 3) * \#I) ** (-1) * \#I'. \qquad (8)
\end{aligned}
$$

The conventions and symbols used in this result are the subject of this section. First the indices on the left-hand sides represent the term number, variable number, and order of approximation respectively, so that the *term* above is the first term of the first dependent variable (f is the distribution function) in the third order.

The quantities $\mathrm{SUMW.}\,(I, J)$ and $K.\,(L, M)$ represent $\sum_{i=I}^{J} \omega_i$ and $\sum_{i=L}^{M} k_i$, respectively. Throughout we use the convention that the sum of all frequencies

from the first to the Nth is ω; a similar convention for the wavenumber holds. In the Nth order there are N summations over the possible frequencies of modulation; these are implicit in the equation above. If we adhere to the example given in Section 2 in which there are two modulation frequencies ω_a and ω_b, then each of the ω_i's range over the four values ω_a, $-\omega_a$, ω_b, $-\omega_b$. The formulas are general enough to take into account any finite number of discrete modulating frequencies; one need only extend the summations in the obvious way. The function denoted by EPS is the first-order permittivity of plasma and beam and is given by the familiar expression

$$1 + \frac{\omega_p^2}{k^2} \int_{-\infty}^{+\infty} \frac{1}{(\omega/k) - v} \frac{\partial f_0}{\partial v}\, dv. \tag{9}$$

The distribution function f_0 that we used was

$$f_0 = \frac{\exp(-v^2)}{\pi^{1/2}} + \omega_B{}^2 \delta(v - v_B) \tag{10}$$

wherein the $\omega_B{}^2$ and v_B characterize the beam density and beam velocity. Also $\#I$ is the FORMAC representation of the imaginary unit and $F00 = f_0$ is the zeroth order distribution function. The EMO represent the first-order electric field Fourier transforms corresponding to those given in Eq. (7).

Finally two special conventions must be explained. The presence of a factor of the form SUM. (variable) as in SUM. ($V004$) indicates that there is an integration over the variable $V004$ such that all terms dependent on $V004$ are in the integrand of that integration which runs from minus infinity to plus infinity. The function DV indicates that a derivative of its first argument with respect to its second argument is to be taken. This was used instead of the ordinary FORMAC DERIV function since the actual process of differentiation was to be deferred as, in fact, the subsequent processing of these terms involved integration by parts prior to substitution of the form of the distribution function.

5. Symbol Manipulation and Numerical Evaluation

We have employed the techniques of symbolic manipulation further to convert the results presented in the last section into the form of FORTRAN statements. The integrals over the velocity variables were transformed into algebraic combinations of the plasma dispersion functions [5] and beam contributions following an expansion into partial fractions. For example, Fig. 2 lists the FORTRAN-deck produced for the evaluation of int 2 defined below in Eq. (18).

```
      TERM(1) = WB2*(-XARG(1) + VB)**(-3 )*(-XARG(2) + VB)**(-1 )*2.
      TERM(2) = WB2*(-XARG(1) + VB)**(-2 )*(-XARG(2) + VB)**(-2 )
      TERM(3) = XARG(1)*ZFC (XARG(1))*(XARG(1)-XARG(2))**(-2 )*2.
      TERM(4) = XARG(1)*(XARG(1)-XARG(2))**(-1 )*4.
      TERM(5) = -XARG(2)*ZFC (XARG(2))*(XARG(1)-XARG(2))**(-2 )*2.
      TERM(6) = -ZFC (XARG(1))*(XARG(1)-XARG(2))**(-1 )*2.
      TERM(7) = XARG(1)**2*ZFC (XARG(1))*(XARG(1)-XARG(2))**(-1 )*4.
      NTOTAL=  7
      SUM=0
      DO100I=1,NTOTAL
  100 SUM=SUM+ TERM(I)
      INT2 =SUM
```

FIG. 2. FORTRAN statements produced for the evaluation of INT2 (versus Eq. (29)).

The actual computations carried out were limited to the evaluation of the first sidebands (upper and lower) as determined by the third order dielectric function. The results are tabulated in Table I in which we show the variation of the amplitudes of the upper and lower sidebands as a function of one modulating frequency while the other one is held at 0.97 of the plasma frequency. The quantity listed is the ratio of $(eE^{(3)}/m\omega_p V_{th})$ to the appropriate product of (three) first-order fields.

TABLE I

Relative Magnitudes of Third-Order Fields for $\omega_B/\omega_p = 0.1$ and $V_B/V_{th} = 5.0$

$\omega_m(a)/\omega_p$	$E^{(3)}(2\omega_a - \omega_b)$	$E^{(3)}(2\omega_b - \omega_a)$
0.88	2.10	2.23
0.90	2.06	2.31
0.92	2.01	2.37
0.94	1.96	2.32
0.96	1.93	2.14

The actual fields are to be determined by means of inverse Fourier (ω) and Laplace (k) transformations. The integrals over the frequency variables are trivial because of the presumed sharpness (δ-function) of the modulation. The integrals over the wavenumber variables involve the residue calculus.

We can write the form of the third-order terms as

$$E_3(x, t) = \sum_{\omega_m^{(1)}} \sum_{\omega_m^{(2)}} \sum_{\omega_m^{(3)}} \iiint dk_1\, dk_2\, dk_3\, F(k_1, k_2, k_3)$$
$$\cdot \exp[i(k_m^{(1)} + k_m^{(2)} + k_m^{(3)}) \cdot x - i(\omega_m^{(1)} + \omega_m^{(2)} + \omega_m^{(3)})\, t]$$
$$\cdot \prod_{i=1}^{3} E_M(k_m(i), \omega_m(i)) \tag{11}$$

wherein $F(k_1, k_2, k_3)$ is given in detail by Eqs. (13)–(22) below and where E_M denotes the quantity given by Eq. (7) (the Fourier transform of the first-order field) with the obvious difference that its ω-dependent δ-functions have been integrated out. Inspection of the terms indicates that the poles of Laplace transforms occur at the positions where the plasma–beam dispersion function vanishes.

There are, potentially, two distinct types of contribution; the first occurs at the poles of the dielectric functions explicitly indicated in the formulas by the ϵ functions and the second occurs at the poles of the function E_M. These latter functions, it may be recalled, represent the transform of the linear response of the system to the modulation. In the calculation presented here, therefore the second group of terms might be described as the linear response of the system to combination frequencies while the first group represents the driven response to the first-order fields.

The experimental results of Carr *et al.* indicate that the base waves were close to saturation levels before the sidebands appeared above noise level, indicating that the response at these sideband frequencies was driven by the main waves.

Furthermore, while it is theoretically possible to assume that the base waves possess lower growth rates than the sideband waves, in the actual experiments trapping and other nonlinear effects would manifest themselves before the fast growth rate could make up for the low initial level. In addition, the amplified noise at the sideband frequencies would complicate the interpretation of the experiments. Therefore, we used only the poles of the E_M functions.

In any event, granted the assumptions stated above, the electric fields in third order will depend only on the first-order electric field strengths. The analytic results obtained by means of the ORDERS and the REPLACE programs can now be converted into a FORTRAN program for the numerical evaluation of the dielectric functions. The zeroth order distribution appropriate to the beam–plasma system under discussion is given by

$$f_0 = \frac{e^{-v^2}}{\pi^{1/2}} + \frac{n_B}{n_p}\,\delta(v - v_B) \tag{12}$$

where v_B is the beam velocity, and n_p and n_B are the plasma and beam number density, respectively. Consequently, the order dielectric functions for this system are combinations of rational functions and plasma dispersion functions.

We shall give an outline of this conversion. First, recall that the derivatives were not carried out explicitly. There are then three terms in F that we must calculate

$$\text{term}(1) = c(1) * \text{int } 2(\phi_{13}, \phi_{11}) * \text{int } 2(\phi_{23}, \phi_{22}) \tag{13}$$

$$\text{term}(2) = c(2) * \text{int } 3(\phi_{13}, \phi_{12}, \phi_{11}) \tag{14}$$

$$\text{term}(3) = c(3) * \text{int } 2(\phi_{13}, \phi_{12}) * \text{int } 2(\phi_{12}, \phi_{11}) \tag{15}$$

in which we have used quantities defined as follows

$$\phi_{ij} = \sum_{l=i}^{j} \omega_m(l) \Big/ \sum_{l=i}^{j} k_m(l) \tag{16}$$

$$\epsilon_{ij} = \epsilon \left(\sum_{l=i}^{j} \omega_m(l), \sum_{l=i}^{j} k_m(l) \right) \tag{17}$$

$$\text{int } 2(a, b) = \int_{-\infty}^{+\infty} \frac{1}{v - a} \frac{\partial}{\partial v} \left(\frac{1}{v - b} \frac{\partial f_0}{\partial v} \right) dv \tag{18}$$

$$\text{int } 3(a, b, c) = \int_{-\infty}^{+\infty} \frac{1}{v - a} \frac{\partial}{\partial v} \left(\frac{1}{v - b} \frac{\partial}{\partial v} \left(\frac{1}{v - c} \frac{\partial f_0}{\partial v} \right) \right) dv \tag{19}$$

$$\frac{1}{c(1)} = k_{11} k_{22} k_{13} k_{23} \epsilon_{13} \epsilon_{23} \tag{20}$$

$$\frac{1}{c(2)} = k_{11} k_{12} \epsilon_{13} k_{13}^2 \tag{21}$$

$$\frac{1}{c(3)} = \epsilon_{12} \epsilon_{13} k_{13}^2 k_{12}^2 \,. \tag{22}$$

Each of the integrals given above was translated into a FORTRAN subroutine in the following steps using FORMAC:

(i) Integration by parts was carried out to the point at which the f_0 function was no longer differentiated.

(ii) The zeroth order distribution function was, as given in Eq. (22), substituted for f_0.

(iii) The δ-function terms were evaluated easily and the other terms were expanded in partial functions.

(iv) Finally, the terms still to be integrated were converted to various combinations of the plasma dispersion function and its derivatives. Use of the functional equation $Z'(z) = -2(zZ(z) + 1)$ was made an option.

In connection with the strictly numerical evaluation (i.e., the FORTRAN program) the following problem arose. In making the partial fraction expansions the possibility that quantities having distinct symbolic names could have identical numerical values was not taken into account. Since

$$\frac{1}{v - a} \frac{1}{v - b} \xrightarrow{b \to a} \frac{\partial}{\partial a} \frac{1}{v - a} \,,$$

provision for this eventuality was made.

We carried out numerical differentiation in the program by allowing each $\omega_m(l)$ to be replaced by $\omega_m(l) + l \cdot 10^{-6}$, $l = 1, 2, 3$.

6. Summary and Conclusions

We have described a group of symbol manipulation programs that start with the differential equations governing a physical system (in this case the Poisson–Vlasov set) and eventually produce portions of the computer code needed for the evaluation of higher order effects.

It was stated that the original goal was to isolate, if possible, the dominant contributions to the wave–wave mixing process. However, the numerical values obtained in third-order for field amplitudes of the first upper and lower sidebands resulted from cancellations between numbers of larger magnitude.

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References

1. W. Carr, D. Boyd, H. Liu, G. Schmidt, and M. Seidl, *Phys. Rev. Letters* **28** (1972), 662.
2. R. Z. Sagdeev and A. A. Galeev, "Non-Linear Plasma Theory," Benjamin, New York, 1969.
3. B. Rosen, *J. Comp. Phys.* **15** (1974), 98–115.
4. R. Tobey *et al.*, PL/1-FORMAC Interpreter Users Reference Manual, SHARE. Contributed Program Library (SHARE 360.D-03.3.004).
5. B. D. Fried and S. D. Conte, "The Plasma Dispersion Function," Academic Press, New York, 1961.