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Systematic Methods for Calculation of the Dielectric Properties of Arbitrary Plasmas

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A new approach to the calculation of the dispersion integrals involved in determining the dielectric properties of arbitrary plasmas is developed. Rather than relying on ad hoc approximation methods, the dispersion integrals for an arbitrary distribution function with continuous derivative are systematically expanded in terms of a set of orthogonal functions for which the corresponding dispersion functions are known. Realizations of this general approach are discussed for unmagnetized plasmas and generalizations to treat relativistic and magnetized plasmas are also outlined. The method developed here enables the dispersion integrals for an arbitrary distribution to be calculated both systematically and efficiently for either real or complex arguments. © 1990 Academic Press, Inc.

1. INTRODUCTION

The dielectric properties of a plasma determine the dispersion, absorption, and mode conversion of the waves it supports, and hence are of central importance in all problems concerning wave propagation and absorption. In connection with laboratory experiments and astrophysical observations, it is often necessary to calculate the dielectric properties of actual observed plasmas, rather than analytically tractable idealized ones. Hence, the principal purposes of this paper are to develop a systematic approach to the calculation of the dielectric properties of nonrelativistic unmagnetized plasmas having arbitrary velocity distribution functions and to indicate how these results can be generalized to treat relativistic and magnetized plasmas.

General analytic treatments express the dielectric tensor of a plasma in terms of integrals over the plasma velocity distribution and their analytic continuations in the complex plane, but do not answer the question of how to calculate the dispersion in a practical way. The relevant velocity-space integrals contain singularities, are only analytically tractable in special cases, and are extremely time consuming to perform numerically. Furthermore, a case-by-case treatment of the analytic properties of the analytically-continued velocity distribution in the complex plane is required if those roots of the wave-dispersion equation (which involves the plasma dielectric tensor) corresponding to damped or growing waves are to be treated correctly by either numerical or analytic means. A further reason that

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knowledge of the analytic properties is necessary is that the analytic continuations of the velocity-space integrals, rather than the integrals themselves, define the dispersion functions in the lower half of the complex plane. Together, these limitations pose a formidable barrier to the use of the general formulas in practice. Indeed, Batchelor *et al.* [1], for example, found the numerical evaluation of the dispersion integrals to be the limiting factor in their numerical investigations of the dispersion of cyclotron waves.

In addition to general treatments of the dielectric properties of plasmas, a number of more specific analyses have been carried out. In these analyses the plasma velocity distribution function is restricted to a particular form for which the dispersion functions can be obtained analytically. Examples from the latter category include the well-known analytic expressions for the dielectric properties of unmagnetized Maxwellian plasmas [2] and analytic forms for the dispersion functions of unmagnetized Lorentzian, generalized-Lorentzian, and piecewise-continuous velocity distributions (e.g., [3–5], and the references cited therein). While these analyses permit rapid computation of wave dispersion using analytic expressions for the dispersion integrals, their lack of generality is a serious limitation. Many authors have attempted to circumvent this disadvantage by approximating a velocity distribution of interest by an ad hoc superposition of distributions (most often Maxwellians) for which the dispersion functions are known. This method is widely used but is unsatisfactory in that the parameters of the component distributions must be adjusted by hand until a reasonable fit is obtained.

What is developed in this paper is a systematic method of decomposing an arbitrary distribution into a linear combination of orthogonal functions for which the corresponding dispersion functions are known and whose analytic properties are well understood. Using this method, evaluation of the wave dispersion is accelerated and it is straightforward to extend the dispersion functions to the complex plane in order to treat damped or growing waves. No such decomposition of the dispersion functions appears to have been previously undertaken.

The structure of this paper is as follows: In Section 2 the method of decomposing the distribution function and constructing the corresponding dispersion function is described. The results of Section 2 are applied to a nonrelativistic unmagnetized plasma in Section 3, in which three realizations of the basic scheme are developed. Numerical results are discussed in Section 4, while Section 5 outlines how the method developed in Section 2 can be generalized to treat relativistic and magnetized plasmas.

2. General Theory

In this section we develop a systematic approach to the calculation of the dispersion integrals for a nonrelativistic unmagnetized plasma having an arbitrary distribution function.

2.1. *Dielectric Tensors and Dispersion Integrals*

The dielectric tensor of a single-species, nonrelativistic unmagnetized plasma is given by

$$\varepsilon_{ij} = \delta_{ij} + \frac{\omega_p^2}{\omega^2} \int d^3\mathbf{v} \frac{v_i}{\omega - \mathbf{k}\cdot\mathbf{v}} \{(\omega - \mathbf{k}\cdot\mathbf{v})\,\delta_{sj} + k_s v_j\} \frac{\partial f(\mathbf{v})}{\partial v_s}, \tag{1}$$

for $\operatorname{Im}\omega < 0$, where $\mathbf{k}$, ω, ω_p, $\mathbf{v}$ and f are the wave vector, wave frequency, plasma frequency, particle velocity, and velocity distribution, respectively; the analytic continuation of (1) defines the dielectric tensor if $\operatorname{Im}\omega > 0$. The singular integrals in (1) can be written in the form

$$D(z) = \int_{-\infty}^{\infty} dx \frac{g(x)}{x - z}, \tag{2}$$

where x is proportional to v and $g(x)$ involves the derivative of the velocity distribution function [6]. The remainder of this section is devoted to describing the systematic evaluation of the dispersion function $D(z)$, which is defined by (2) if $\operatorname{Im} z > 0$ (with the contour chosen to pass above the pole), and by the analytic continuation of (2) if $\operatorname{Im} z \leqslant 0$.

2.2. *Systematic Decomposition of Dispersion Integrals*

The systematic procedure proposed here for decomposing dispersion integrals of the form (2) is as follows:

Step 1. Choose an interval I (possibly infinite) outside which the function $g(x)$ is negligible. On physical grounds such an interval must exist because the distribution function and its derivative must vanish at large velocities. Next, choose a complete set of basis functions $\{u_n(x)\}$, $n = 0, 1, \ldots$, orthogonal with respect to some weight function $w(x)$ on the interval I; i.e., with

$$\int u_m(x)\, u_n(x)\, w(x) = h_m\, \delta_{mn}, \tag{3}$$

where the h_m are normalization constants. The integration in (3), and henceforth, extends over the chosen interval I. Use of a complete set of functions guarantees that any continuous function can be approximated to arbitrary accuracy by this method. The appearance of the weight function $w(x)$ is significant because it can be used to factor out the dominant variations in $g(x)$ by writing $g(x) = b(x)\, w(x)$, where $b(x)$ is relatively slowly varying. Examples of this aspect of the analysis are given in Section 3.

Step 2. Decompose $g(x)$ in terms of the chosen weighted orthogonal functions, to give

$$g(x) = \sum_{n=0}^{\infty} a_n u_n(x)\, w(x), \tag{4}$$

with the weight function appearing explicitly and

$$a_n = h_n^{-1} \int dx\, g(x)\, u_n(x). \tag{5}$$

Step 3. Introduce the dispersion functions $D_n(z)$, defined by

$$D_n(z) = \int dx\, \frac{u_n(x)\, w(x)}{x - z}. \tag{6}$$

The overall dispersion function $D(z)$ is then given by

$$D(z) = \sum_{n=0}^{\infty} a_n D_n(z). \tag{7}$$

Note that the weight function $w(x)$ appears in (6), rather than (5), owing to the form of the expansion in (4), in which $w(x)$ occurs explicitly.

Two key requirements must be made of the foregoing procedure before the expression (7) can be deemed to be useful; namely, the dispersion functions $D_n(z)$ must have clearly known analytic properties and must be of a form which can be evaluated efficiently. Typically, this involves finding a stable recursion relation for $D_n(z)$.

Estimates of the accuracy of the method described here can be made by noting that, for $\operatorname{Im} z > 0$, $D(z)$ comprises a contribution from the residue of the integral (2) in the complex plane, and a remainder. Of these contributions, the contribution from the residue $D_{\text{res}}(z)$ is the more sensitive to inaccuracies in the approximation of $g(x)$. We note that $D_{\text{res}}(z) = 2\pi i g(z)$ for $\operatorname{Im} z > 0$ and, hence, the fractional error in approximating $D_{\text{res}}(z)$ using a finite number of terms in (7) is the same as that of the corresponding orthogonal-function decomposition of $g(z)$, for which standard formulas exist. When $\operatorname{Im} z < 0$, $D(z)$ is defined by the analytic continuation of (2), rather than by the integral (2) itself. In this case, similar estimates of the error incurred in truncating the sum in (7) to a finite number of terms follow from the analytic continuation of this sum.

3. Nonrelativistic Unmagnetized Plasmas

Here, we present realizations of the scheme described in Section 2 for three sets of orthogonal functions, Hermite, Legendre, and Chebyshev polynomials. Other decompositions are also possible, but will not be developed explicitly in this work. As mentioned earlier, a major advantage of being able to choose from a variety of orthogonal functions is that this flexibility permits one to select the set of functions best suited to exploit the qualitative form of the distribution and, hence, of $g(x)$ (e.g., asymptotically Gaussian in form; zero outside some range; etc.), thereby speeding numerical calculations and providing for a more compact expression of the dispersion functions.

3.1. *Hermite Decomposition*

If the plasma velocity distribution function is asymptotically Maxwellian, $g(x)$ is of the form $g(x) = b(x) \exp(-x^2)/\pi^{1/2}$, where $b(x)$ is relatively slowly varying. This leads us to use the weight function $w(x) = \exp(-x^2)/\pi^{1/2}$, with the Hermite polynomials $H_n(x)$ as orthogonal functions on the interval $(-\infty, \infty)$.

The dispersion function corresponding to $(-1)^{n+1} H_{n+1}(x)$ is

$$D_{n+1}(z) = \frac{1}{\pi^{1/2}} \int dx \frac{(-1)^{n+1} H_{n+1}(x) e^{-x^2}}{x - z} \tag{8}$$

$$= -2z\, D_n(z) - 2n\, D_{n-1}(z), \tag{9}$$

where the recursion relation $H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$ has been used to obtain (9). Together with the specific relations

$$D_0(z) = Z(z), \tag{10}$$

$$D_1(z) = Z'(z), \tag{11}$$

(9) provides the necessary recursion relation for $D_n(z)$, where Z is the standard plasma dispersion function [2]. The formula $Z'(z) = -2 - 2zZ(z)$ enables one to show that the derivatives $Z^{(n)}(z)$ of the Z-function satisfy the same recursion relation as the functions $D_n(z)$; hence one can make the identification $D_n(z) = Z^{(n)}(z)$. The final result for $D(z)$ is, thus,

$$D(z) = \sum_{n=0}^{\infty} (-1)^n a_n Z^{(n)}(z), \tag{12}$$

where the coefficients a_n are given by

$$a_n = \frac{1}{2^n n!\, \pi^{1/2}} \int_{-\infty}^{\infty} dx\, g(x)\, H_n(x). \tag{13}$$

The integrations in (13) need be done only once for any given distribution function and, hence, need not be optimized for speed because the vast bulk of computational time is typically expended in subsequent multiple evaluations of the dispersion. We note that the analytical and recursive-stability properties of functions closely related to $Z^{(n)}(z)$ have been explored by Gautschi [7, 8], who also obtained an efficient algorithm for evaluating $Z(z)$ in the complex plane [9, 10]. The relationship of Gautschi's results to the calculation of $Z^{(n)}(z)$ is summarized in the Appendix.

Although the sum (12) is guaranteed to converge to $D(z)$ by the completeness of the Hermite polynomials, a warning is in order regarding the possibility of catastrophic cancellation when (12) is evaluated numerically. A simple, but highly demanding, example illustrates this point in a case for which the dispersion function is known exactly. We consider an expansion of the integral

$$D(z) = \frac{1}{\pi^{1/2}} \int dx \, \frac{e^{-(x-x_0)^2}}{x-z} \tag{14}$$

about the origin, where the integrand becomes exponentially small as x_0 is increased. The integrand in (14) is asymptotically Gaussian and can be decomposed into Hermite polynomials, with coefficients $a_n = x_0^n/n!$. This yields

$$D(z) = \sum_{n=0}^{\infty} (-x_0)^n \, Z^{(n)}(z)/n!, \tag{15}$$

$$= Z(z - x_0), \tag{16}$$

which could, of course, have been obtained directly in this particular case. It is important to note a loss of accuracy in the numerical evaluation of (15), which manifests itself for large x_0: the Hermite polynomials are unbounded and catastrophic cancellation can occur for some values of z if x_0 is large, despite the formal convergence of the sum. More generally, this problem can be mitigated by expanding about the centroid of $g(x)$, rather than a poorly chosen point at which $g(x)$ is exponentially small, as in the case leading to (15). A more representative example might involve $g(x)$ being of the form $g(x) = p_n(x) \exp(-x^2)/\pi^{1/2}$, where $p_n(x)$ is an nth-degree polynomial; in this case complete convergence is attained with just n terms of the Hermite decomposition and cancellation problems are considerably reduced. Numerical examples of Hermite decomposition are presented in Section 4.

3.2. *Legendre Decomposition*

If the function $g(x)$ in (2) is negligible outside some finite range, which we shall choose to be $(-1, 1)$ without loss of generality, then an expansion in Legendre polynomials $P_n(x)$ is possible, with a weight function of unity. These functions form a complete orthogonal set. In this case we have

$$u_n(x) = P_n(x), \tag{17}$$

$$a_n = \left(n + \frac{1}{2}\right) \int_{-1}^{1} dx \, g(x) \, P_n(x), \tag{18}$$

$$D_n(z) = -2Q_n(z), \tag{19}$$

where $Q_n(z)$ is a Legendre function of the second kind. Methods for calculating $P_n(z)$ and $Q_n(z)$ have been described by Gautschi [7] and Stegun [11]. The use of Legendre decomposition is helpful in avoiding catastrophic cancellation such as that described in Section 3.1, because the Legendre polynomials are bounded on the interval $(-1, 1)$. In this decomposition a branch cut appears when the Legendre functions $Q_n(z)$ are extended to the complex plane; an appropriate definition of the branch is necessary, but corresponds directly to making an appropriate choice of the branch of log $[(z-1)/(z+1)]$ [3].

3.3. *Chebyshev Decomposition*

Similar results to those of Section 3.2 can be obtained using Chebyshev polynomials of the second kind $U_n(x)$ as orthogonal functions on the interval $(-1, 1)$ with the weight function $(1-x^2)^{1/2}$. This choice is useful for treating plasmas having distribution functions which vanish at the ends of the interval (e.g., physically, when the particle velocity equals the speed of light) and leads to

$$u_n(x) = U_n(x), \tag{20}$$

$$a_n = (2/\pi) \int_{-1}^{1} dx\, g(x)\, U_n(x), \tag{21}$$

$$D_n(z) = -\pi[T_{n+1}(z) - i(1-z^2)^{1/2}\, U_n(z)], \tag{22}$$

where $T_{n+1}(z)$ is a Chebyshev polynomial of the first kind. The polynomial nature of $T_{n+1}(z)$ and $U_n(z)$ makes the analytic properties of $D_n(z)$ especially simple in this case.

4. Numerical Examples of Hermite Decomposition

In this section two numerical examples of Hermite decomposition are presented to illustrate the methods developed in this work.

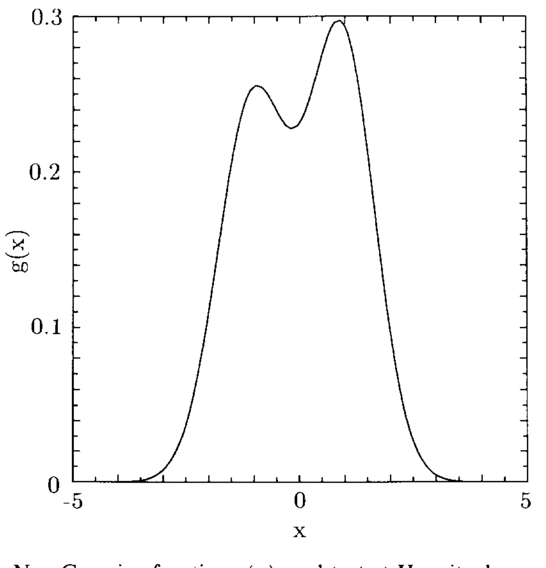

FIG. 1. Non-Gaussian function $g(x)$ used to test Hermite decomposition.

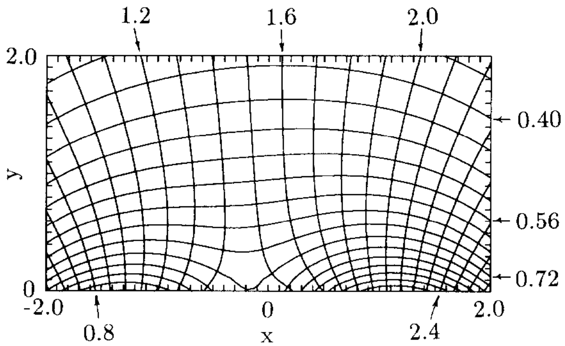

FIG. 2. Modulus-argument diagram of the dispersion function $D(z)$ corresponding to the function $g(x)$ shown in Fig. 1, with $z = x + iy$, $-2.0 \leqslant x \leqslant 2.0$, and $0 \leqslant y \leqslant 2.0$. Labels with arrows indicate modulus contours at 0.40, 0.56, and 0.72. Similarly, argument contours are labelled at 0.8, 1.2, 1.6, 2.0, and 2.4 radians.

The first example is essentially the one discussed at the end of Section 3.1, in which we set $x_0 = 1$ to give $g(x) = \pi^{-1/2} \exp[-(x-1)^2]$. Here, the approximate dispersion function obtained by Hermite decomposition is compared with the exact one, which is given by (16) with $x_0 = 1$. The exact function, $Z(z-1)$, is evaluated using Gautschi's algorithm [9, 10], which has an accuracy of $\lesssim 10^{-10}$ in the upper half of the complex plane. If we denote the Nth order approximation to $Z(z-1)$ by $Z_N(z-1)$, and the maximum fractional error in the upper half plane by $\varepsilon_N = |[Z_N(z-1) - Z(z-1)]/Z(z-1)|_{\max}$, then the results of this comparison are $\varepsilon_4 = 0.44$, $\varepsilon_8 = 3.0 \times 10^{-2}$, $\varepsilon_{12} = 8.5 \times 10^{-4}$, and $\varepsilon_{16} = 1.36 \times 10^{-5}$. Rapid convergence to the exact result is evident as the order of the approximation is increased.

For the second example we choose a more complicated distribution, given by

$$g(x) = \frac{1}{\pi^{1/2}} [0.4e^{-(x-1)^2} + 0.1e^{-(x-0.8)^2} + 0.15e^{-(x+0.4)^2} + 0.35e^{-(x+1.2)^2}],$$

as shown in Fig. 1. The choice of a superposition of Gaussian functions renders the exact dispersion integrals tractable, while nonetheless providing an example of a highly non-Maxwellian $g(x)$. A modulus-argument diagram of the dispersion function $D(z)$ is shown in Fig. 2. The maximum fractional error of the 16-term Hermite approximation in the upper half-plane is $\varepsilon_{16} = 1.4 \times 10^{-4}$.

5. RELATIVISTIC AND MAGNETIZED PLASMAS

Thus far, we have considered only unmagnetized nonrelativistic plasmas; however, it is quite possible to extend the methods described here to treat relativistic and magnetized plasmas. In this section we briefly outline some such extensions.

5.1. Unmagnetized Relativistic Plasmas

The dielectric properties of unmagnetized relativistic plasmas can be written in terms of integrals of the form

$$\int_{-1}^{1} dx \frac{g(x)}{x-z}, \tag{23}$$

with $g(\pm 1)=0$ and x equal to the velocity in units of c [12]. A Legendre decomposition of (23), as in Section 3.2, is clearly possible. Alternatively, an expression of (23) in Chebyshev polynomials of the second kind $U_n(x)$ can be undertaken, as in Section 3.3, by writing $g(x)=b(x)(1-x^2)^{1/2}$. In the latter case, the weight function $w(x)=(1-x^2)^{1/2}$ qualitatively embodies the physical requirement $g(\pm 1)=0$.

5.2. Magnetized Nonrelativistic Plasmas

Nonrelativistic magnetized plasmas can be treated by the methods described in Sections 2 and 3, since their dispersive properties can be expressed in terms of integrals of the form

$$\int_{-\infty}^{\infty} \frac{dx}{x-z} \int_{0}^{\infty} dy\, h(x, y), \tag{24}$$

where x and y are the dimensionless momentum components parallel and perpendicular to the ambient magnetic field, respectively, and $h(x, y)$ involves products of Bessel functions and derivatives of the momentum distribution function [6]. The integral (24) is of the form (2) with $g(x)=\int_0^\infty dy\, h(x, y)$, where $g(x)$ is the Bessel-function-weighted reduced distribution. In the case of distributions separable in x and y (which correspond to $v_\parallel$ and $v_\perp$, physically), the integral over y need be done only once for all x. More generally, $g(x)$ must first be numerically evaluated over the range of x of interest, and then the methods of Sections 2 and 3 can be used to treat the remaining singular integral over x. This compares with the alternative of evaluating both integrals directly by numerical means, with the consequent loss of knowledge about the analytic properties of the resulting dispersion functions and their correct continuation into the complex plane.

Two complications enter the analysis for magnetized plasmas: First, one set of integrals of the form (24) must be evaluated for each relevant harmonic of the cyclotron frequency. Second, and more importantly, $\int dy\, h(x, y)$ is a function of the wave properties in the magnetized-plasma case and hence the coefficients a_n in (7) must be re-evaluated for each new set of wave parameters. This point dictates that greater attention be paid to optimizing the speed of calculation of a_n when treating magnetized plasmas. Nonetheless, the methods developed here reduce each integral from a two-dimensional singular form whose analytic properties are unknown to a set of one-dimensional nonsingular integrals (to determine the a_n) which correspond to dispersion functions whose analytic properties are understood.

5.3. *Magnetized Relativistic Plasmas*

Relativistic magnetized plasmas can be treated relatively easily by the methods described above when determining the dispersive properties of waves propagating perpendicular to the magnetic field. In this case the dispersion integrals are of the form

$$\int_0^\infty \frac{dx}{x-z} \int_{-1}^1 dy\, g(x, y) \tag{25}$$

with x and y being proportional to the kinetic energy and the pitch angle of the particles, respectively [6]. The x integral then extends from 0 to ∞ and it may thus be appropriate to choose Laguerre polynomials as orthogonal functions.

Dispersion functions for waves propagating at an arbitrary angle to the field in a relativistic magnetized plasma can also be cast into the form considered in this paper. Usually, these functions are written in terms of integrals of the form

$$\int_{-\infty}^\infty dx \int_0^\infty dy \frac{g(x, y)}{\gamma - \alpha x - \beta}, \tag{26}$$

with $\gamma = (1 + x^2 + y^2)^{1/2}$, where x and y are the dimensionless parallel and perpendicular momentum components, respectively, and α and β are constants [6]. By changing variables from x and y to ones (V and μ here) tied to the resonance ellipses of cyclotron maser theory (26) can be rewritten in the form

$$\int_0^1 \frac{dV}{V - V_0} \int_{-1}^1 d\mu h(V, \mu), \tag{27}$$

with

$$x/\gamma = U - V(1 - e^2)^{1/2} \mu, \tag{28a}$$

$$y/\gamma = V(1 - \mu^2)^{1/2}, \tag{28b}$$

where V_0, U, and e are constants [6, 13]. As in the case of nonrelativistic magnetized plasmas, one set of such integrals must be evaluated for each set of wave parameters and for each harmonic.

6. Summary

A general procedure for systematic calculation of the dispersive properties of plasmas has been developed. This general scheme has been illustrated for unmagnetized plasmas with three concrete realizations based on Hermite, Legendre, and Chebyshev polynomials, and extensions of these methods to treat relativistic and magnetized plasmas have been outlined. Numerical examples of Hermite decomposition show that this method is capable of yielding accurate results for the dispersion integrals for both real and complex arguments.

The expansion method developed here should be of considerable use in calculating the dielectric properties of plasmas in a wide variety of situations, particularly in the automated calculation of the dielectric properties of plasmas observed in astrophysical situations and the laboratory. The main features of this work are: (i) A systematic alternative to ad hoc approximation of the plasma dispersion integrals has been obtained, based on orthogonal-function expansion of the integrands. (ii) The weight function for the orthogonal functions can be used to advantage by factoring out the dominant variations in the dispersion integrands. (iii) Use of orthogonal-function expansion enables one to use dispersion functions which can be evaluated rapidly and which have known analytic properties in the complex plane. Knowledge of the analytic properties of the dispersion integrals is essential if the dispersion of damped or growing waves is to be treated correctly; such waves are extremely difficult to treat if the integrals are performed directly because analytic continuation to the lower half plane is required, a region in which the integrals no longer define the dispersion functions.

APPENDIX: Calculation of $Z^{(n)}(u)$

This appendix contains a brief description of how to calculate the dispersion functions $Z^{(n)}(z)$; for further details, the reader should consult Refs. [7–10].

The Z-function is related to the complex complementary error function by

$$Z(u) = i\pi^{1/2} e^{-u^2} \operatorname{erfc}(-iu). \tag{A1}$$

The nth derivative and nth integral of the right-hand side of (A1) are interrelated by

$$\frac{d^n}{du^n} e^{-u^2} \operatorname{erfc}(-iu) = (2i)^n\, n!\, e^{-u^2} I^n \operatorname{erfc}(-iu), \tag{A2}$$

where I^n denotes the nth integral. Hence, we have

$$Z^{(n)}(u) = i\pi^{1/2} (2i)^n\, n!\, e^{-u^2} I^n \operatorname{erfc}(-iu). \tag{A3}$$

Gautschi [7] described calculation of $I^n \operatorname{erfc}(-iu)$ by recursion. Computation of $Z(u)$ for u in the first quadrant was also discussed by Gautschi [9, 10], with Z being used to normalize the recursive series for $Z^{(n)}$. Extension of these results to other quadrants is attained by use of the symmetry relations [14]

$$Z^{(n)}(u) = (-1)^{n+1} [Z^{(n)}(-u^*)]^*, \tag{A4}$$

$$Z^{(n)}(u^*) = Z^{(n)}(u)^* + 2i\pi^{1/2}(-1)^n [e^{-u^2} H_n(u)]^*, \tag{A5}$$

which generalize the corresponding known results for $Z(u)$ [2].

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