PROBLEM OF THE MOST EFFECTIVE PLASMA DISPERSION FUNCTION EVALUATION

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The principal question of the fastest plasma dispersion function evaluation in the most "expensive" presently region R in both the complex region and the real axis was investigated with usage of additional computer memory and somewhat modification of the well-known algorithm 380, most effective in present. It was shown that the minimal time for evaluation of that function in the complex region R is about 1.5 times for computation of the single exponential function and in the real region R about the time for evaluation of the single exponent. Usage of present algorithm, and a negligible additional computer memory allow perform twice faster calculations in the complex plane and ten times faster on the real axis in comparison with algorithm 380.

PACS: 52.27.Ny

INTRODUCTION

The special function

$$w(z)=\exp(-z^2)\left[1+2i/\sqrt{\pi}\int_0^z \exp(t^2)dt\right]$$

of a complex variable $z = x + iy$ is well-known as the complex error function or as Fadeeva function. This function occurs in many branches of physics and mathematics. However, the mainstream of our interest is usage of this function in the region of plasma physics, because its computation is a necessary ground of the ion cyclotron resonance wave analysis in the laboratory fusion plasmas. The nonrelativistic plasma dispersion function, $Z(z)$, that describes the absorption and dispersion properties of plasma particles along the magnetic field, is related to the function $w(z)$ as $Z(z) = i\sqrt{\pi}w(z)$. In this reason, it is also named by the plasma dispersion function.

To solve the wave boundary value problems it is necessary evaluating this function only for real argument while resolving of the time initial value problems of Cauchy type requires estimating this function in the entire complex plane. Routinely, in plasma wave applications the function $w(z)$ is evaluated massively, therefore the efficiency of involved numerical algorithm is of primary importance.

There are many methods evaluating this function from tables [1, 2] to modern software [3-5]. All these methods can be divided in two main trends in accordance with the calculation purpose. There are some applications, where accuracy of calculation is more important that computation time and the wide applications that require evaluation of this function massively. We will consider the second type–the trend connected with the efficiency of calculations with a reasonable, previously specified, high enough accuracy.

At present time the algorithm 380 of Gautschi & Poppe & Wijers [3, 4] is the most successful, and most of the program libraries contain this one. Jacobi's continued fraction

$$w(z)=\frac{1}{z-}\,\frac{1/2}{z-}\,\frac{1}{z-}\,\frac{3/2}{z-}\dots$$

has been proved to provide the fast evaluation of the complex error function by means of this method for large absolute *z*-values (Region Q, Fiqure). The same continued fraction in combination with the Taylor expansion along a negative direction of the imaginary axis has been exploited for moderate absolute *z*-values (Region R, Fig.1). The Taylor expansion at the zero point

$$w(z)=\exp(-z^2)\left(1+\frac{2i}{\sqrt{\pi}}\sum_{n=0}^{+\infty}\frac{z^{2n+1}}{(2n+1)\,n\,!}\right)$$

has been used for small absolute *z*-values (Region S, see Figure). This method provides the accuracy up to 14 significant digits and the average computational time of the single function value approximately equals to 10 times for the single computation of exponential function. As it follows from see Figure, from the standpoint of the computational time this method is most cheap (10…20 Arbitrary Units) in the regions S and Q and most expensive (30…70 Arbitrary Units) in the Region R. Here appears an interesting question about the extreme speed of calculations in the most expensive region R .

The main purpose of the present work is an attempt to clarify the issue of maximum possible efficiency to evaluate this function in the most problematic region R as in complex plane so on the real axis.

1. COMPUTATIONAL PROCEDURE

1.1. ALGORITHM 380

For evaluation of the complex error function $w(z)$ at thepoint z of the region R it was suggested to use a truncated Taylor expansion of this function at the point $z_0 = z + ih$ [3],

$$w(z) = \sum_{n=0}^{N} \frac{w^{(n)}(z+ih)}{n!}(-ih)^n \ , \qquad (1)$$

where $h > 0$ was previously chosen. To speed up the convergence of the series was used the introduction of the functions $w_n(z) = d_n \big/ (2i)^n$, where d_n are the coefficients for the series (1).

The recurrence for these functions could be as follows

$$W_{k+1} - \frac{iz_0}{k+1} W_k - \frac{1}{2(k+1)} W_{k-1} = 0, k = 1,2,3 \ldots$$

Hence the start function, $w_{-1}(z) = 2/\sqrt{\pi}\ w_n(z)$, is related to the derivatives $w^{(n)}(z)$ as

$$w^{(n)}(z) = (2i)^n n!\, w_n(z), \qquad n = 0,1,2, \ldots.$$

So, the expression (1) can be written in the form

$$w(z) = \sum_{n=0}^{N} (2h)^n \ w_n(z+ih). \qquad (2)$$

A ratio of two successive functions $r_{n-1} = w_n(z+ih)/w_{n-1}(z+ih)$ can be developed into the continued fraction

$$r_{n-1} = \frac{1/2}{h - iz + (n+1) r_n}. \qquad n = 0, 1, 2, \ldots \qquad (3)$$

In principle, this fraction may be used to calculate the sum (2) by two ways. The method [3] uses the fact that at the one end of this continued fraction (with the ratios of these functions with higher subscripts) these ratios rather quickly are tending to zero, if point $z_0 = z + ih$ is not close to abscissa axis. For this reason, this continued fraction can be truncated for the some finite value of the index $n = \nu > N$, and the last ratio can be put to zero $(r_\nu = 0)$. All ratios r_n $(n = \nu - 1, \ldots 1, 0, -1)$ can be calculated in accordance with (3). It can be shown that the sum in (2) can be recursively $(n = N, N-1 \ldots, 0)$ calculated through

$$s_{n-1} = r_{n-1}\left[(2h)^n + s_n\right], \qquad (4)$$

where $s_N = 0$ and $w(z) = 2/\sqrt{\pi} \cdot s_{-1}$. It is obviously that the expansion (1) is performed strictly along the imaginary axis in the negative direction, i.e. in the direction in which the inaccuracies, associated rounding errors, are not accumulating, since homogeneous and inhomogeneous solutions of the differential equation for the function $w(z)$ behave as $\exp\left[(\mathrm{Im}\, z)^2\right]$ and are mutually subtracted, providing the condition $w(z) \to 0$ when $\mathrm{Im}\, z \to +\infty$. The choice of h affects both the convergence of the fraction (3) so and the convergence of the expansion (2). In fact, large values of h give rise to fast convergence of fraction (3), but slow convergence in (2), while small values of h yield slow convergence of (3), but fast convergence in (2). A good choice of h is therefore one which strikes a balance between these two opposing effects. This compromise value, corresponding to accuracy up to 10 significant digits, is $h = 1.6$ (Gautschi) and for accuracy up to 14 significant digits is $h = 1.88$ (Poppe&Wijers). In this algorithm, such a compromise in the choice of h corresponds to the optimum efficiency of the function evaluation and, consequently, the issue of the further algorithm improvement seems totally exhausted.

1.2. MODIFICATION IN ALGORITHM 380

However, the expansions (1, 2) can be performed not only strictly along the imaginary axis, but along the somewhat direction to real axis as well. In general case of expansion the step is $h = i(z - z_0)$ and for real axis $h = i(x - x_0)$. Instead the expansion (1), which is performed strictly along the imaginary axis, we can also use a more general expansion,

$$w(z) = \sum_{n=0}^{N} \frac{w^{(n)}(z_0)}{n!}(z - z_0)^n \ . \qquad (5)$$

Applying this formula to the region R, we receive

$$w(z) = \sum_{n=0}^{N} \frac{w^{(n)}(x_0)}{n!}(x - x_0)^n$$

and, instead the Gautschi functions $w_n(z)$, introduce a set of the functions $\varphi_n(z)$, related to the derivatives $w^{(n)}(z)$ by means of relations

$$w^{(n)}(z) = (2e^{-\varphi})^n n!\, \varphi_n(z) \ , \ (n = 0, 1, 2, \ \ldots \ ). \qquad (6)$$

Here φ is related to $z - z_0$ in (5) as $z - z_0 = a e^{i\varphi}$ ($a = \sqrt{(x - x_0)^2}$). It is easy to see that for $\varphi = -\pi/2$ it is true $\varphi_n(z) = w_n(z)$ and, consequently, the functions $\varphi_n(z)$ generalize the functions $w_n(z)$ to the case of arbitrary expansion angle in expressions (1, 2). The expansion (5) has then the form

$$w(x) = \sum_{n=0}^{N} \varphi_n(x_0)(2a)^n . \qquad (7)$$

These functions satisfy to the recursive relation of 2[nd] order

$$\varphi_{n+1}(x_0) + \frac{x_0 e^{i\varphi}}{n+1}\varphi_n(x_0) + \frac{e^{2i\varphi}}{2(n+1)}\varphi_{n-1}(x_0) = 0,$$
$n = 0,\ 1, 2,\ \dots,$

where there are true relations $\varphi_0(x_0) = w(x_0)$ and $\varphi_{-1} = -i2e^{-i\varphi}/\sqrt{\pi}$. A ratio of two those successive functions $r_{n-1}^{\varphi} = \varphi_n(x_0)/\varphi_{n-1}(x_0)$ can be developed into recursive relation of the type (3)

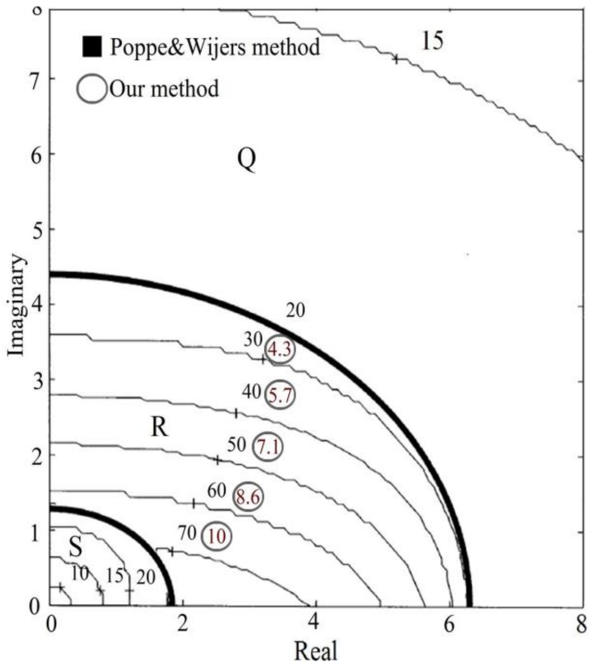
$$\cdots r_n^{\varphi} = -\frac{e^{i\varphi}}{n+1}\left[z_0 + \frac{1/2\, e^{i\varphi}}{r_{n-1}^{\varphi}}\right]\cdots \quad n = 0, 1, 2, \dots \quad (8)$$

If one assumes that the value of the function $\varphi_0(x_0) = w(x_0)$ is known, it will be also known the ratio $r_{-1}^{\varphi} = \varphi_0(x_0)/\varphi_{-1}$. On the base the recursive relation (8) can be evaluated r_n^{φ} with indexes $n = 0, 1, \dots, N-1$, respectively. Then using the recursion of type (4), namely

$$s_{n-1} = r_{n-1}^{\varphi}\left[(2a)^n + s_n\right], \quad (9)$$

for $(n = N, N-1\dots,0)$ with first $s_N = 0$, and last $w(x) = \varphi_{-1}\cdot s_{-1}$, can be calculated the sum (7) on the prescription of [3].

So this algorithm has some advantages in comparison with algorithm 380. As for defining of the maximum deviation angle, the test calculations have showed that it should not significantly differ from the angle $-\pi/2$.These features give possibilities in reducing numbers of term in the sum (7).



Computational time for evaluation of complex error function by Poppe&Wijers method and by our modificated method

This strategy is as follows. The region R is covered by a grid with the variable step, a. The step size is chosen inversely proportional to the cost of computing time for evaluation of the function, $w(z)$, presented in see Fig.ure. For example, for area of R below the line with the number 70 a step is 20/70, where the number 20 corresponds to the region Q. Previously, the values of function $w(z)$ are calculated in knots of the grid, for example, on the base the method [6] with accuracy higher than 14 significant digits. Although this method is twice less effective than Gauschi-Poppe-Wijers method, nevertheless it can be used for calculating $w(z)$ with more high accuracy. Thus when the point z will belong somewhat a quadrilateral in the region R (near the upper boundary instead of a quadrangle may be a trigon), in this case the point, corresponding to the nearest vertex of one of the two upper corners of this quadrangle, is selected as an expansion point z_0 (near an upper boundary it will be the upper vertex of a trigon). Then for estimation of $w(z)$ the expansion (7) is performed using, respectively, the recursion (9) instead of the recursive relation (4). Obviously, that a decrease of the grid size will lead to a reduction of the expansion (5) and, consequently, for a given accuracy of calculations will improve the speed of calculations.

It should also be noted that this approach is rather similar to the ideology of cellular telephony, when the grid nodes as would replace the antennas of mobile communication.

The some disadvantage of this algorithm is fact that somewhat array of storage must be provided to hold the values of function $w(z)$ at the knots of the grid. However, the preservation of a two-dimensional array, even large enough, is not a big problem in the time of rapid progress in technology of information storage.

2. PERFORMANCE CHARASTERISTICS AND TESTS

Fortunately, this approach can be utilized for estimation of the maximum possible efficiency to compute this function. Really, if one reduces the step of grid, a, the series (7) will converge faster and therefore the number of terms of the series can also be reduced. This process can continue until the series (7) will consist of only four members that corresponds to the value $a = 2.5\cdot 10^{-4}$. Calculations shown that for the grid of that size the speed of calculations for this function in region R of the complex region will be near seven times greater than the calculation using the algorithm 380. Note however, that in this case array of storage about 4GB must be provided to hold the values of function at the knots of the grid. Of course, at present time it is rather a big memory. But for the grid with $a = 0.125$ the series (7) will consist of 13 terms, the speed of calculations will be twice faster than by means of the algorithm 380 and the storage about 15KB must be reserved to hold the function values. Obviously, it is a negligible memory.

Figure represents a computational time for calculating a complex error function in the region R of complex plane.

For the case of evaluation of the function $w(z)$ by means of this method in region R on the real axis only the estimates of the same type shown that the speed of calculations with the step $a = 2.5 \cdot 10^{-4}$ will be near ten times faster than calculations on the base algorithm 380. In this case a negligible array of storage about 80 KB must be provided to hold the values of function at the knots of the grid. It is rather important to solve efficiently the wave boundary value problems.

CONCLUSIONS

1. The question of the maximally possible acceleration of the complex error function evaluation in the region R has been resolved with usage of some additional computer memory and somewhat modification of the algorithm 380.
2. The minimal time for evaluation of the complex error function in the complex region of R is about 1.5 times for computation of the single exponential function plus an array of storage about 4 GB must be provided to hold the values of function at the knots of the grid. The same time for calculations on the real axis in the region R is about the time for evaluation of the single exponent plus the storage about 60 KB must be reserved to hold the function values.
3. Usage of present algorithm, and a negligible additional computer memory allow perform twice faster calculations of $w(z)$ in the complex plane and ten times faster on the real axis in comparison with algorithm 380.

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Article received 15.10.2014

ПРОБЛЕМА НАИБОЛЕЕ ЭФФЕКТИВНОГО ВЫЧИСЛЕНИЯ ПЛАЗМЕННОЙ ДИСПЕРСИОННОЙ ФУНКЦИИ

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Принципиальный вопрос о времени наиболее быстрого вычисления плазменной дисперсионной функции в наиболее "дорогой" по времени в настоящее время области *R* для случаев комплексного и реального аргумента исследовался с использованием дополнительной компьютерной памяти и некоторой модификации наиболее эффективного на сегодня алгоритма 380. Показано, что для комплексного аргумента минимальное время для вычисления этой функции может быть примерно в 1.5 раза выше времени вычисления одной экспоненциальной функции и для действительного аргумента примерно соответствует времени вычисления одной экспоненты. Использование данного алгоритма и небольшой дополнительной компьютерной памяти позволяет вычислять $w(z)$ в два раза быстрее в комплексной плоскости и в десять раз быстрее на реальной оси в сравнении с алгоритмом 380.

ПРОБЛЕМА НАЙБІЛЬШ ЕФЕКТИВНОГО ОБЧИСЛЕННЯ ПЛАЗМОВОЇ ДИСПЕРСІЙНОЇ ФУНКЦІЇ

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Принципове питання про час найбільш швидкого обчислення плазмової дисперсійної функції в найбільш "дорогій" за часом нині області R для випадків комплексного і реального аргументу досліджувався з використанням додаткової комп'ютерної пам'яті і деякої модифікації найбільш ефективного на сьогодні алгоритму 380. Показано, що для комплексного аргументу мінімальний час для обчислення цієї функції може бути приблизно в 1.5 рази вище часу обчислення однієї експонентної функції і для дійсного аргументу приблизно відповідає часу обчислення однієї експоненти. Використання даного алгоритму і невеликої додаткової комп'ютерної пам'яті дозволяє обчислювати $w(z)$ в два рази швидше в комплексній площині і в десять разів швидше на реальній осі в порівнянні з алгоритмом 380.