FAST COMPUTATION OF COMPLEX ERROR FUNCTION OF THE REAL ARGUMENT

S.V. Malko[1], S.S. Pavlov[2], K.K. Tretiak[2]

[1]Centro de Laseres Pulsados (CLPU), Salamanca, Spain;
[2]Institute of Plasma Physics of the NSC KIPT, Kharkov, Ukraine

A new efficient technique for evaluation of complex error function of the real argument on the base of the Euler-Maclaurin formula and a non-singular formula for the principal value of the Cauchy integral is given. . It is demonstrated that for the real values of argument, which are most "expensive" in the computational time, the new algorithm is almost two times faster than algorithm 680 with the same accuracy. The code was successfully implemented to ray tracing code that is used for application for investigation of ICR plasma heating in JET-type tokamaks.

PACS: 52.27.Ny

INTRODUCTION

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

is known as the complex error function or as Fadeeva function. The name "Fadeeva function" was probably introduced by Poppe and Wijers [1], since the function was firstly tabulated by Fadeeva and Terent'ev in 1954 [2]. This function appears in many areas of physics and mathematics in different forms. For example, considering such applications as plasma spectroscopy, nuclear physics, radiative heat transfer and nuclear magnetic resonance it is necessary efficient and accurate evaluation of this function. Depending on the problem there are two main trends of the evaluation techniques: high accuracy and computational time. We will consider applications when computational time is more important than accuracy.

Along with the applications, rather abundant are the methods evaluating this function, from tables [2, 3] to modern software [1, 4-7]. Still the main requirements are high efficiency or somewhat accuracy that should be investigated in the developing of any successful algorithm for the computation of this function.

For instance, this function is common in the theory of plasma waves, and its evaluation is a necessary ground of ion cyclotron wave analysis of the laboratory fusion plasmas. The nonrelativistic plasma dispersion function $Z(z)$, which describes the absorption and dispersion properties of plasmas along the magnetic field is related to the function $w(z)$ as $Z(z) = i\sqrt{\pi} w(z)$. For this reason the function $w(z)$ is named as well as the plasma dispersion function, which appears in all elements of the plasma dielectric tensor. As a rule, in plasma wave applications the function $w(z)$ is evaluated massively, therefore the efficiency of involved numerical algorithm is of primary importance. So, plasma applications can be related to the one of two main trends mentioned above: they are connected with the provision of high efficiency of calculations with a previously specified accuracy.

At present time, the most successful method of this trend is the method of Gautschi-Poppe-Wijers [1, 4]. The main idea of this method is to use the continued fractions. For example, the continued fraction of Jacobi

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

has been proved to provide the fast calculation of the complex error function by means of this method for large $-|z|$ values (Region Q, Fig. 1). For moderate $-|z|$ values (Region R, see Fig. 1) were used the same continued fractions in combination with the Taylor expansion in a special direction. For small $-|z|$ values (Region S, see Fig. 1) the Taylor expansion at the zero point

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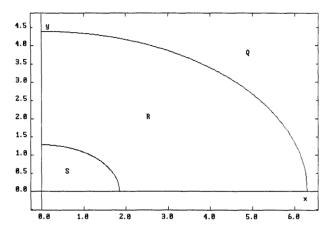
was used.

Fig. 1. Three regions of the first quadrant of a complex plane, where W(z) is calculated on the base three techniques

It worth to mention that it is enough to calculate this function in any quadrant due to its properties of symmetry.

This method provides the accuracy up to 14 significant digits and the average computation time of the single function value approximately equal to 10 times of the single computation of the exponential function. It worth to note, the computation time in this method is the most "expensive" on the real axis and near it in the Region R.

The main purpose of the present work is to increase the efficiency of calculation in the most important region R.

1. EVALUATION OF THE COMPLEX ERROR FUNCTION OF THE REAL ARGUMENT

In the theory of plasma waves, solving boundary value problems requires computation of complex error function only on the real axis, so it makes sense to consider this case separately. On the real axis this function can be defined by the means of the formula [8]

$$w(x) = \frac{1}{\pi i} \int_{-\infty}^{+\infty} \frac{e^{-t^2} dt}{t - x} . \qquad (1)$$

This function belongs to the class of analytic functions defined by Cauchy integral, with the integral density tending to 0 at infinity. In accordance with the formula of Plemelj-Sokhotskii real part of (1) equals to the density of the integral at the pole $t = x$ multiplied by πi i.e., e^{-x^2} and its imaginary part, named usually as the Dawson integral, equals to the principal value of this integral. In principle, for the $|x|$ values in the Region R, this principal value can be evaluated by means of the direct numerical integration on the base of the following integral form which is nonsingular on the real axis [9]:

$$\operatorname{Im} w(x) = iD(x) = \frac{1}{\pi i} P \int_{-\infty}^{+\infty} \frac{e^{-t^2}}{t-x} dt = \frac{1}{\pi i} \int_{-\infty}^{x} \frac{e^{-t^2} - e^{-(t-2x)^2}}{t-x} dt. \qquad (2)$$

The letter P denotes the principal value of the next integral. Since the numerator of the integrand in (2) is expressed in terms of exponentials, it can be estimated numerically up to the any required precision. Fortunately, the formulae (2) has an extra interesting property, which is manifested only in its use in conjunction with the famous Euler-Maclaurin formula

$$\int_a^b f(x)dx = h(y_1 + \dots + y_{n-1}) - \frac{B_1 h}{1!}\big[f(b) + f(a)\big] -$$

$$\sum_{m=1}^{+\infty} \frac{B_{2m} h^{2m}}{(2m)!} \Big[f^{(2m-1)}(b) - f^{(2m-1)}(a) \Big], \qquad (3)$$

$y_0 = f(a), y_1, y_2, \dots, y_{n-1}, y_n = f(b)$, are the values of function $f(x)$ in successive equally spaced points with the step h, and B_m are the Bernoulli coefficients. Let's apply the formula (3) to the right side of formula (2) by setting

$$\frac{1}{\pi i} \cdot \frac{e^{-t^2} - e^{-(t-2x)^2}}{t - x} = f(t). \qquad (4)$$

Then the Dawson integral can be presented as

$$\operatorname{Im} w(x) = \int_{-\infty}^{x} f(t)dt = h(y_1 + \dots + y_{n-1}) - \frac{B_1 h}{1!}\big[f(x) + f(-\infty)\big] -$$

$$\sum_{m=1}^{+\infty} \frac{B_{2m} h^{2m}}{(2m)!} \Big[f^{(2m-1)}(x) - f^{(2m-1)}(-\infty) \Big]. \qquad (5)$$

If we present function $w(x)$ as the expansion at the point $x = \infty$

$$w(x) = \frac{i}{\pi} \sum_{k=0}^{+\infty} \frac{\Gamma(k+1)}{x^{2k+1}} \qquad (6)$$

we can conclude the even properties of $f(t)$ with respect to the point x: $f(x - h) = f(x + h)$ for every $h > 0$. It's easy to see, that $f^{(2m-1)}(-\infty) = 0, (m = 1,2,3 \dots)$ and $f(-\infty) = 0$. Taking into account that $B_1 = -1/2$ and $f^{(2m-1)}(x) = 0$ we have

$$\operatorname{Im} w(x) = \frac{1}{\pi i} \int_{-\infty}^{x} \frac{e^{-t^2} - e^{-(t-2x)^2}}{t-x} dt = \frac{ih}{\pi}(y_1 + \dots + y_{n-1}) + \frac{ih}{\pi 2} y_n, \qquad (7)$$

where

$$y_{n-j} = f(x - jh) = \frac{e^{-(x-jh)^2}(1 - e^{-4xjh})}{jh}.$$

Since the limiting behavior of Bernoulli coefficients is $B_m = O(m!/(2\pi)^m)$, this formula is exact for some $h < 1$ rather close to 1. Direct calculations along the formula (7) show that the value $h = 0.5$ provides the accuracy up to 14 significant digits. This allows one performing computations about ten times faster in comparison with the direct numerical integration on the base the single nonsingular form (2).

2. COMPUTATIONAL PROCEDURE, TESTS

After transformation of the final expression (7) for evaluation of the Dawson integral in order to increase the efficiency of this algorithm we can have reduction of the calculation up to only three exponents: e^{-x^2}, $e^{-0.25}$, e^{x} and some additional power algebra. Numerical calculations have shown that efficiency of evaluation of the complex error function on the real axis is higher than algorithm of Gautschi-Poppe-Wijers (GPW).

From Table it follows that calculation of $w(x)$ for most "expensive" in computational time real values of argument from the region R demonstrates about twice higher efficiency in comparison with the algorithm [1, 4].

Comparison of computational times, which are required for estimation of function $w(x)$ in the points $x = 2,3,4,5,6$ from region R for our algorithm (the 2nd column) and the algorithm of GPW (the 3d column) with accuracy up to 14 significant digits

x-values of argument	Time of our computation	Time of GPW computation
2.0	5.4990999×10^{-2}	0.160976008
3.0	5.5991001×10^{-2}	0.154975995
4.0	5.3992003×10^{-2}	0.138979003
5.0	5.2992001×10^{-2}	0.123980999
6.0	5.3991001×10^{-2}	9.6986003×10^{-2}

3. JET-APPLICATION

The technique of the plasma dispersion function evaluation, presented above, was utilized to accelerate numerical calculations in the ray tracing code as an example of application in the field of nuclear fusion

[10]. This code was used for the theoretical investigation of ion cyclotron resonance frequency plasma heating in a tokamak of JET-type [11]. It was assumed that the antenna to excite the fast mode (FW) of the fast magnetosonic wave was located at the inner side of the plasma column. We investigated the scenario of plasma heating by means of FW excitation and its subsequent conversion to the ion Bernstein wave (IBW) in a plasma depth with subsequent IBW absorption in the central regions of the plasma column. This scenario is rather promising for high-power plasma heating in large size tokamaks because the RF energy is easily introduced into the FW and then fully absorbed by the IBW. The energy is easy injected into FW due to narrow area of FW opacity in the periphery of the plasma and then after conversion the entire energy is completely absorbed by the IBW which is linearly polarized and has a wavelength much smaller than that of fast wave. Note that direct excitation of IBW is currently the serious problem due to the wide opaque barrier on the periphery of the plasma column [12].

Ray tracing code allows a treatment of general tokamak magnetic field configurations with the poloidal divertor and realistic wall geometry on the base the equilibrium field data from the EFIT code [13]. In calculations was used cylindrical coordinate system $\vec{r} = \vec{r}(R, \varphi, Z)$.

The geometrical optics equations describing the propagation of rays in spatially non-uniform plasma are:

$$\frac{d\vec{r}}{dt} = \frac{\partial D / \partial \vec{k}}{\partial D / \partial \omega}, \quad \frac{d\vec{k}}{dt} = -\frac{\partial D / \partial \vec{r}}{\partial D / \partial \omega}, \qquad (8)$$

where $\vec{k}$ is the wave vector and $D = D(N_\perp, N_\parallel, \omega, \vec{r})$ is dispersion relation for waves. Here, $\vec{N} = c\vec{k}/\omega$ is refractive index, $\vec{N}_\parallel = (\vec{N} \cdot \vec{B})/B$ and $\vec{N}_\perp = \vec{N} - \vec{N}_\parallel$ are longitudinal component of the refractive index along the magnetic and the perpendicular field, respectively. In the region of ion cyclotron resonance frequency the dispersion relation for plasma waves contains the next components of the dielectric tensor

$$\varepsilon_1 = \varepsilon_1^c + \eta N_\perp^2, \quad \eta = -\sum_i \frac{3\omega_{pi}^2 \omega^2 v_{Ti}^2}{c^2(\omega^2 - \omega_{Bi}^2)(\omega^2 - 4\omega_{Bi}^2)}, \quad (9)$$

$$\varepsilon_1^c = 1 - \sum_i \frac{\omega_{pi}^2}{\omega^2 - \omega_{Bi}^2}, \quad \varepsilon_2 = -\sum_i \frac{\omega_{pi}^2 \omega}{\omega_{Bi}(\omega^2 - \omega_{Bi}^2)},$$

$$\varepsilon_3 = 1 + \frac{\omega_{pe}^2}{\omega^2} 2z_{0e}^2 (1 + i\sqrt{\pi} z_{0e} W(z_{0e})).$$

Here $z_{0e} = \omega / \sqrt{2}k_\parallel v_{Te}$ and $W(\zeta)$ is the plasma dispersion function.

Power carried by the ray Q is defined as $Q = Q_0 e^{-\Gamma}$ where Q_0 is initial power and

$$\Gamma = \int_o^T \text{Im}\, \vec{k}\, \frac{\partial \vec{r}}{\partial t}\, dt \cdot \qquad (10)$$

The following parameters of the plasma and excited FW were used in the numerical calculations: deuterium plasma with the addition of hydrogen ($n_h / n_d(0) = 5 \ldots 16$ %), $n_e = 3.1 \cdot 10^{13} cm^{-3}$ is the density of the deuterium in the core, $T_{i,e} = 1 \ldots 3$ keV are the ion deuterium and hydrogen) and electron temperatures, $B(0) = 1.8$ T is magnetic field in the center of column, $l = 8$ is toroidal wave number, $\omega = 1.822 \cdot 10^8$ rad/s is FW frequency (Fig. 2).
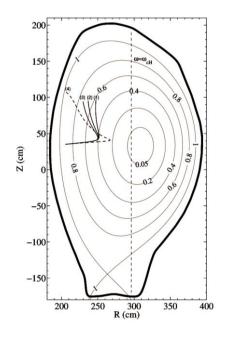

Fig. 2. Ray trajectories in JET-like tokamak for cases: $n_h / n_d(0) = 16\%$ $T_{i,e}(0) = 1$ keV (1); $n_h / n_d(0) = 16\%$, $T_{i,e}(0) = 2$ keV (2); $n_h / n_d(0) = 16\%$, $T_{i,e}(0) = 3$ keV (3); ($n_h / n_d(0) = 5\%$, $T_{i,e}(0) = 3$ keV (4)

A detailed analysis of that RF plasma heating scenario in JET-like tokamak is not the subject of thispaper. Moreover, the full investigation of this scenario requires as well the use of the 1-D wave model to solve boundary problem for the system of Maxwell-Vlasov equations, that also leads to massive computations of the plasma dispersion function. However, it is easy to see that the application of the technique presented in this paper for the plasma dispersion function evaluation allows approximately twice to accelerate calculations on the base both models.

CONCLUSIONS

1. On the base of nonsingular form for Cauchy integrals and the Euler-Maclaurin formula a new method for computing the complex error function for real values of argument is given.

2. Comparison of this method with the most successful one of Gautschi -Poppe-Wijers has shown that doubled efficiency for real argument values in the most "expensive" in terms of computational time region R.

3. This method can be used as well for computation of any Cauchy integrals defined on the real axis, provided that the density of the corresponding integral vanishes at infinity.

4. The efficiency of using this method was shown in application for investigation of ICRF plasma heating in JET-type tokamaks, where it has been implemented to ray tracing code. As far as this code usually featured for the study of the shortwave IBW in tokamak JET, it leads to a large number of trajectories and a large number of calculations of the plasma dispersion function during calculation of each trajectory. For acceleration of such calculations this method was applied to.

REFERENCES

1. G. Poppe & C. Wijers. More Efficient Computation of the Complex Error Function // *ACM Transactions on Mathematical Software*. 1990, v. 16 (1), p. 38-46.
2. V. Fadeev, N. Terent'ev. *Tables of values of the function* $w(z) = \exp(-z^2)[1 + 2i / \sqrt{\pi} \int_0^z \exp(t^2)dt]$ *for complex argument*. Moscow: "Gosud. Izdat. Teh.-Teor. Lit.", 1954.
3. B.D. Fried, S.D. Conte. *The Plasma Dispersion Function. The Hilbert Transform of Gaussian*. New York: "Academic Press", 1961.
4. W. Gautschi. Efficient computation of the complex error function // *SIAM Journal on Numerical Analysis*. 1969, v. 7, p. 187-198.
5. J.A.C. Weideman. Computation of the Complex Error Function // *SIAM Journal on Numerical Analysis*. 1994, v. 31(5), p. 1497-1518.
6. M. Zaghoul, A. Ali. Algorithm 916 Computing the Fadeeva and Voight Functions // *ACM Transactions on Mathematical Software*. 2011, v. 38(2), p. 1-22.
7. S. Abrarov, B. Quine. Efficient algorithmic implementation of the Voigt/complex error function based on exponential series approximation // *Appl. Math. Comp*. 2011, v. 218(5), p. 1894-1902.
8. M. Abramowitz, I. Stegun. *Handbook of Mathematical Functions*. New York: "National Bureau of Standards", 1964.
9. F. Castejón, S. Pavlov. Relativistic plasma dielectric tensor evaluation based on the exact plasma dispersion function concept // *Physics of Plasmas*. 2006, v. 13.
10. E.R. Tracy, A.J. Brizard, A.S. Richardson, A.N. Kaufman. *Ray Tracing and Beyond*. Cambridge: "University Press", 2014.
11. http://www.ccfe.ac.uk/JET.aspx
12. A.V. Longinov, K.N. Stepano. Radio-frequency heating in the ion cyclotron frequency range, p. 93-238. The book: *High-Frequency Plasma Heating*, Editor A.G. Litvak. AIP: "New York", 1992.
13. https://fusion.gat.com/theory/Efit.

БЫСТРОЕ ВЫЧИСЛЕНИЕ КОМПЛЕКСНОЙ ФУНКЦИИ ОШИБОК РЕАЛЬНОГО АРГУМЕНТА

С.В. Малко, С.С. Павлов, К.К. Третьяк

Предлагается новый эффективный метод вычисления комплексной функции ошибок реального аргумента на основе несингулярной интегральной формы Коши и формулы Эйлера-Маклорена. Показано, что для действительных значений аргумента, которые являются наиболее "дорогими" по времени вычислений, новый алгоритм примерно в два раза быстрее, чем алгоритм 680 с той же точностью. Алгоритм был успешно использован в коде лучевых траекторий, который применялся для исследования ИЦР-нагрева плазмы в токамаке типа JET.

ШВИДКЕ ОБЧИСЛЕННЯ КОМПЛЕКСНОЇ ФУНКЦІЇ ПОМИЛОК РЕАЛЬНОГО АРГУМЕНТУ

С.В. Малко, С.С. Павлов, К.К. Трет'як

Пропонується новий ефективний метод обчислення комплексної функції помилок реального аргументу на основі несінгулярної інтегральної форми Коші та формули Ейлера-Маклорена. Показано, що для дійсних значень аргументу, які є найбільш "дорогими" за часом обчислень, новий алгоритм приблизно в два рази швидший, ніж алгоритм 680 з тією ж точністю. Алгоритм був успішно використаний в коді променевих траєкторій, який застосовувався для дослідження ІЦР-нагріву плазми в токамаці типу JET.