THE CALCULATION OF arg $\Gamma(ia+1)$

By JAMES G. BECKERLEY

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ABSTRACT. A convenient, rapidly-converging finite sum formula is derived for the numerical evaluation of arg $\Gamma(ia+1)$. This formula is then employed to construct a four-place table of arg $\Gamma(ia+1)$ for $a = .1, .2, .3, \ldots, 2.0$. The asymptotic formula is shown to be satisfactory for computing the function when $a > 2.0$

$\Gamma(z)$ for complex values of z has been tabulated to a limited extent[1,2,3]. Nevertheless, in the use of these tables the physicist must spend considerable time in understanding an author's notation (see reference 2) or considerable effort in securing interpolated values (see reference 1). Besides, the periodicals in which some of the tables appear are not always available (*e.g.*, reference 3). So it is convenient to have a simple closed formula with which any desired $\Gamma(z)$ may be calculated, a formula whose element may be obtained from commonly available tables.

The purpose of this paper is to present such formulas for the function $\Gamma(ia+1) = (ia)$. This function occurs frequently in problems involving positive energy hydrogen functions.[4]

It is unnecessary to discuss the calculation of the absolute value[5] of this function, as the exact formula for the absolute value is quite convenient for numerical calculation. $|\Gamma(ia+1)| = \sqrt{(\pi a)/(\sinh \pi a)}$. However, the exact formula[6] for the argument (or angle) is an infinite sum whose terms diminish so slowly as to make addition impractical.

$$\arg \Gamma(ia+1) = -Ca + \sum_{n=1}^{\infty} \left(\frac{a}{n} - \operatorname{arctg} \frac{a}{n} \right)$$

where C = Euler's constant $= .5772156665\ldots$

The obvious solution to this difficulty is to break the series off at the Nth term, substitute the power series for arctg (a/n), sum the resulting series analytically, leaving only a finite sum to be evaluated. This is done in the following procedure.

$$\arg \Gamma(ia+1) = -Ca + \sum_{n=1}^{N} \left(\frac{a}{n} - \operatorname{arctg} \frac{a}{n} \right) + \sum_{n=N+1}^{\infty} \left[\frac{1}{3}\left(\frac{a}{n}\right)^3 - \frac{1}{5}\left(\frac{a}{n}\right)^5 \ldots \right]$$

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$$= -\sum_{n=1}^{N} \operatorname{arctg}\frac{a}{n} + \left(S_1^N - C\right)a + \left\{ \sum_{n=1}^{\infty}\left[\frac{1}{3}\left(\frac{a}{n}\right)^3 - \frac{1}{5}\left(\frac{a}{n}\right)^5 \ldots\right] - \sum_{n=1}^{N}\left[\frac{1}{3}\left(\frac{a}{n}\right)^3 - \frac{1}{5}\left(\frac{a}{n}\right)^5 \ldots\right]\right\}.$$

Thus,

$$(1) \quad \arg\Gamma(ia+1) = -\sum_{n=1}^{N} \operatorname{arctg}\frac{a}{n} + \left(S_1^N - C\right)a - \sum_{n=1}^{\infty}\frac{(-1)^n a^{2n+1}}{2n+1}\Delta S_{2n+1}^N$$

where $S_\mu^\nu = \sum_{n=1}^{n=\nu}\left(\frac{1}{n}\right)^\mu$; $\Delta S_\mu^\nu = S_\mu^\infty - S_\mu^\nu$.

The series S_μ^ν are the well-known numerical series whose values can be obtained analytically and which have been tabulated[7] for a reasonable range of values of μ. Now one convenient feature of formula (1) is that *the* ΔS_{2n+1}^N *diminishes very rapidly with increasing* n. This is shown in Table I, where ΔS_{2n+1}^N is tabulated for $n=1, 2, \ldots, 5$ and $N=1, 2, \ldots, 5$. It is apparent that the convergence becomes even better with increasing N. (Also included in Table I are values of S_1^N for $N=1, 2, \ldots, 5$.)

TABLE I. Values of $\Delta S_{2n+1}^N = \sum_{\mu=1}^{\infty}\left(\frac{1}{\mu}\right)^{2n+1} - \sum_{\mu=1}^{N}\left(\frac{1}{\mu}\right)^{2n+1}$

n	ΔS_{2n+1}^1	ΔS_{2n+1}^2	ΔS_{2n+1}^3	ΔS_{2n+1}^4	ΔS_{2n+1}^5	N	S_1^N
		$\times 10^{-4}$	$\times 10^{-4}$	$\times 10^{-6}$	$\times 10^{-6}$		
1	.202057	770.569	400.199	24394.9	16394.9	1	1.0000
2	.036928	56.777	15.6253	585.97	265.97	2	1.5000
3	.008349	5.3678	.7953	18.495	5.695	3	1.8333
4	.002008	.55268	.0446	.648	.136	4	2.0833
5	.000494	.05908	.0263	.025	.005	5	2.2833

An even more convenient feature of formula (1) is the *alternating* character of the infinite series. This makes it possible to rewrite (1) as a finite series with a remainder term :

$$(2) \quad \arg\Gamma(ia+1) = -\sum_{n=1}^{N} \operatorname{arctg}\frac{a}{n} + (S_1^N - C)a - \sum_{n=1}^{P}\frac{(-1)^n \Delta S_{2n+1}^N}{2n+1}a^{2n+1} + R_P$$

$$|R_P| < \frac{\Delta S^N_{2P+3}}{(2P+3)} \times a^{2P+3}$$

where the infinite series of (1) has been terminated with the Pth term.

To illustrate the usefulness of formula (2), let us choose values of N and P such that $|R_P| < 10^{-5}$ for $0 \leq a \leq 2$. Inspection of Table I shows that we can choose either N=4, P=4 or N=5, P=3.

If we take the latter values for N and P, then the resulting finite series will be suitable for calculating a four-place table of arg $\Gamma(ia+1)$ in the range $0 \leq a \leq 2$. Substituting the values for the coefficients from Table I, we obtain the desired formula :

$$\text{(3)} \quad \arg\Gamma(ia+1) = -\sum_{n=1}^{5} \operatorname{arctg}\frac{a}{n} + \sum_{n=1}^{4} \alpha_{2n-1}a^{2n-1} - R$$

$$\alpha_1 = +1.706118\,; \qquad \alpha_5 = -5.32 \times 10^{-5}$$

$$|R| < 15 \times 10^{-9}a^9$$

$$\alpha_3 = +.005465\,; \qquad \alpha_7 = +8.14 \times 10^{-7}$$

The rapidly diminishing coefficients indicate the extreme usefulness of the general formula (2) in numerical calculations of arg $\Gamma(ia+1)$. So far as the five-term arctangent sum is concerned, this is not an inconvenience, since many accurate tables of this function exist.

To complete the present paper, Table II is presented. In this are listed the values of arg $\Gamma(ia+1)$ for $a = .1, .2, \ldots, 2.0$. The values have been calculated from formula (3) above. It is hoped that this table will be of use to physicists who are engaged in numerical calculations involving the "Coulomb phase factors" which occur in the continuous spectrum wave functions of hydrogenic atoms ; and it is further hoped that the table might be of use to mathematicians working in those branches of analysis which involve gamma functions of purely imaginary argument. *

As the table is restricted to values of $|a| \leq 2$ (negative values simply yield complex conjugates, which multiply the arguments by -1), it is necessary to consider the method of calculating arg $\Gamma(ia+1)$ when $|a| > 2$. For these higher values of a, the asymptotic formula[9]

$$\text{(4)} \qquad \arg\Gamma(ia+1) \simeq (\pi/4) + a(\ln a - 1) - (1/12a)$$

is applicable with diminishing error for increasing values of a. This is illustrated in Table II, where for $1.5 \leq a \leq 2.0$ the values obtained from the asymptotic formula (4) have been placed in a column parallel to the values obtained from (3).

* Strictly speaking, $\Gamma(ia+1)$ is not a "gamma function of purely imaginary argument" but is related to such a function by the simple identity : $\Gamma(ia) = [\Gamma(ia+1)]/(ia)$. $\Gamma(ia+1)$ is, however, a factorial function of purely imaginary argument : $\Gamma(ia+1) = (ia)!$.

Comparison of the exact and asymptotic values shows that, at least as far as the physicist is concerned, formula (4) is quite adequate even for values of $a \geq 1.5$. However, for more accurate numerical work it is necessary to extend calculation to higher values of a before using the asymptotic formula.

TABLE II. Four-place Table of arg $\Gamma(ia+1)$ for $a = 0.0, 0.1, 0.2, \ldots, 2.0$ including Comparison with Asymptotic Formula [Equation (4)]

a	arg $\Gamma(ia+1)$	a	arg $\Gamma(ia+1)$	Asymptotic arg $\Gamma(ia+1)$
0.0	.0000	1.1	−.2883	...
.1	−.0572	1.2	−.2673	...
.2	−.1122	1.3	−.2392	...
.3	−.1634	1.4	−.2043	...
.4	−.2072	1.5	−.1620	−.1620
.5	−.2441			
.6	−.2727	1.6	−.1155	−.1147
.7	−.2928	1.7	−.0622	−.0616
.8	−.3042	1.8	−.0034	−.0039
.9	−.3071	1.9	+.0606	+.0611
1.0	−.3016	2.0	+.1297	+.1300

In conclusion, it is seen that the formulas derived minimize the labour necessary in numerical calculation of arg $\Gamma(ia+1)$ — or arg (ia) ! — and that the construction of a complete table of this function for an extended range of the variable is quite possible. That such a generally useful function, the factorial function, has never been completely tabulated for imaginary values of its argument, is rather a curious fact. It illustrates well the axiom that a computer's field is unbounded.

JUDSON COLLEGE,
UNIVERSITY OF RANGOON.

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