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Note

Evaluation of the Integral $\int_0^\infty t^n \exp(-t^2 - x/t) dt$

1. Introduction

In many problems [1, 2] that involve the motion of particles having Maxwellian distribution there appears the function $T_n(x)$, defined by the integral

$$T_n(x) = \int_0^\infty t^n e^{-t^2 - x/t}\, dt, \tag{1.1}$$

where x is real and positive and the parameter n belongs to the set of natural numbers. The properties of $T_n(x)$ are well established [3, 4] and tabulated values are available [5] for the functions T_1, T_2, T_3 in the range $0 \leqslant x \leqslant 1$ to 4 significant figures.

More recently numerical values of $T_n(x)$ have been required with higher precision by Cole and Pack [6] and for relatively high values of the parameter n (up to 20) by Boffi, De Socio, Gaffuri and Pescatore [7]. In principle, with the use of high speed computers, the T_n functions may be evaluated numerically for any $x \geqslant 0$ and any value of n. However care must be taken to ensure that the required precision be maintained in the calculations. For example, there are some numerical differences between certain results in [7] and those of Loyalka [8], even though as pointed out by Cole [9], the relevant algebraic expressions in both papers are equivalent and ought to yield identical results. It is possible that these discrepancies are associated with the evaluation of the T_n functions. The aim of the present note is to establish criteria for the accurate computation of $T_n(x)$ and to generalize the formulae to include negative values of n.

2. Properties of $T_n(x)$

Let x belong to the domain L_n defined by

$$L_n = \begin{cases} [0, \infty) & \text{if} \quad n > -1, \\ (0, \infty) & \text{if} \quad n \leqslant -1. \end{cases} \tag{2.1}$$

The integral function (1.1) exists in L_n and satisfies the following properties;

$$g_n(x) = -g'_{n+1}(x), \tag{2.2}$$

$$x g_{n-1}(x) + (n+1)\, g_n(x) - 2 g_{n+2}(x) = 0, \tag{2.3}$$

$$2T_1(x) = \sum_{k=0}^{\infty} (a_k \ln x + b_k)\, x^k, \tag{2.4}$$

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where

$$a_k = -\frac{2a_{k-2}}{k(k-1)(k-2)}, \qquad b_k = \frac{-2b_{k-2} - (3k^2 - 6k + 2)\,a_k}{k(k-1)(k-2)}, \qquad k \geqslant 3, \tag{2.5}$$

with $a_0 = a_1 = 0$, $b_0 = -a_2 = 1$, $b_1 = -\pi^{1/2}$, $b_2 = 3(1-\gamma)/2$, γ being the Euler constant. The asymptotic series [4, 5] are valid throughout L_n subject to the condition $\epsilon \gg 1$, where ϵ is defined by

$$\epsilon = \frac{2x^2}{|n|^3}. \tag{2.6}$$

Following [5] we write

$$T_n(x) \sim \left(\frac{\pi}{3}\right)^{1/2} \left(\frac{z}{3}\right)^{n/2} e^{-z} \sum_{p=0}^{\infty} c_{n,p} z^{-p}, \tag{2.7}$$

where $z = 3(x/2)^{2/3}$ and

$$\begin{aligned} c_{n,0} &= 1,\; c_{n,1} = (3n^2 + 3n - 1)/12, \\ 12(p+2)\,c_{n,p+2} &= -(12p^2 + 36p - 3n^2 - 3n + 25)\,c_{n,p+1} \\ &\quad + \tfrac{1}{2}(n-2p)(2p+3-n)(2p+3-2n)\,c_{n,p}, \quad p = 0, 1, \ldots . \end{aligned} \tag{2.8}$$

In the limit as $x \to 0$

$$T_n(0) = \frac{1}{2}\,\Gamma\left(\frac{n+1}{2}\right), \qquad n > -1, \tag{2.9}$$

$$\frac{T_{-(m+1)}(x)}{T_{-m}(x)} \sim \frac{m-1}{x}, \qquad m > 1. \tag{2.10}$$

For small and moderate values of x a typical calculation proceeds as follows. First $T_1(x)$ is computed by means of the series (2.4). Next, by differentiation and integrating and using (2.2) and (2.9) corresponding series may be found for $T_0(x)$ and $T_2(x)$. Finally, these values may be inserted into the recurrence relation (2.3) to generate $T_n(x)$, $n = 2, -1, \pm 3, \pm 4, \ldots, \pm N$ say. Although the task of computing the various expressions is straightforward, numerical difficulties may arise. For a given target precision for $T_1(x)$ there will be a critical calue for x, x_L, above which the series (2.4) fails, in practical terms, to converge fast enough. On switching to the asymptotic expression (2.7), valid for $\epsilon \gg 1$, a corresponding critical value of x, x_U, exists, below which the representation cannot achieve the required accuracy. If $x_U > x_L$, a third method must be used to evaluate $T_1(x)$ to the required precision, for example, Padè approximants or direct numerical integration. But even if T_0, T_1 and T_2 can be found with the required precision, the use of the recurrence (2.3) may generate numerical errors which grow and eventually swamp the function $T_n(x)$. It is well known [10, 11] that stability in recurrence relations may depend on (a) the particular solution of the difference equation being computed; (b) the values of x or other parameters (in this case, n) in the difference equation, and (c) the direction in which the recursion is followed.

3. Choice of Recursive Direction

We associate with recurrence relation (2.3) fundamental solutions $y_{1,n}$, $y_{2,n}$, $y_{3,n}$. Numerical errors introduced either initially or subsequently by rounding are propagated by all three solutions as the recursion proceeds. We wish to contain the relative error of $T_n(x)$ for fixed x and different n. The conclusion of Oliver [11] is thus appropriate, namely that recursion is effective in the direction for which the required solution dominates. It is necessary then to identify which solution corresponds to the required T_n function. The cases n positive and n negative are dealt with separately.

Case (a) *n positive*

Asymptotic forms, for fixed x and sufficiently large n, of the fundamental solutions $y_{i,n}$ of (2.3) may be obtained by making appropriate balances between the three terms. On neglecting the first member of (2.3), the resulting balance may be written

$$\frac{g_{n+2}(x)}{g_n(x)} \sim \frac{n+1}{2}. \tag{3.1}$$

Equation (3.1) yields two uncoupled solutions, which can be expressed

$$\frac{y_{1,n}}{y_{1,n-1}} \sim \left(\frac{n}{2}\right)^{1/2}, \tag{3.2}$$

$$\frac{y_{2,n}}{y_{2,n-1}} \sim -\left(\frac{n}{2}\right)^{1/2}. \tag{3.3}$$

The term neglected in (2.3), namely xg_{n-1} has order of magnitude $\epsilon^{1/2}$ relative to the retained terms. A third solution of (2.3) can be found by neglecting the third member, yielding

$$\frac{y_{3,n}}{y_{3,n-1}} \sim -\frac{x}{n}. \tag{3.4}$$

Here the neglected term has order of magnitude $O(\epsilon)$. It is useful to note also that

$$\left| \frac{y_{3,n}}{y_{3,n-1}} \Big/ \frac{y_{1,n}}{y_{1,n-1}} \right| = O(\epsilon^{1/2}). \tag{3.5}$$

Thus, when $\epsilon \ll 1$, that is, when $2x^2 \ll n^3$, the three fundamental solutions are given by (3.2)–(3.4). We see from equation (3.5) that the solution pair $y_{1,n}$, $y_{2,n}$ dominates for forward recursion whilst $y_{3,n}$ dominates for backward recursion.

A third balance is possible between the terms of (2.3), by neglecting the second member. We then obtain

$$\frac{g_n(x)}{g_{n-3}(x)} \sim \frac{x}{2}. \tag{3.6}$$

All three solutions of type (3.6) have effectively uncoupled. The fundamental solutions satisfy

$$\left|\frac{z_{i,n}}{z_{i,n-1}}\right| \sim \left(\frac{x}{2}\right)^{1/3}, \qquad i = 1, 2, 3. \tag{3.7}$$

This time the neglected member has order of magnitude $O(\epsilon^{-1/3})$, which means that solutions (3.6) are valid when $2x^2 \gg n^3$. Thus forward recursion is *stable* for both $\epsilon \gg 1$ $(z_{i,n})$ and $\epsilon \ll 1$ $(y_{1,n})$. Backwards recursion is *stable* for $\epsilon \gg 1$ $(z_{i,n})$ but *unstable* for $\epsilon \ll 1 (y_{1,n})$. For the purpose of identifying the T_n functions the cases $\epsilon \ll 1$ and $\epsilon \gg 1$ are considered separately.

(i) $\epsilon \ll 1$. From (2.9) and the result $\Gamma(z + a)/\Gamma(z + b) \sim z^{a-b}$ as $z \to \infty$ [5] we find

$$\frac{T_n(0)}{T_{n-1}(0)} \sim \left(\frac{n}{2}\right)^{1/2}. \tag{3.8}$$

When $x = 0$ behaviour similar to (3.8) for $T_n(x)$ may be inferred from the inequality

$$T_n(x) \geqslant e^{-x}(T_n(0) - 1/(n + 1)). \tag{3.9}$$

Since $T_n(x)$ is identified with (3.2), forward recursion is *stable*. However backward recursion is *not*, due to the dominance of solution (3.4) in ratio (3.5).

(ii) $\epsilon \gg 1$. From (2.7) we have

$$\frac{T_n(x)}{T_{n-1}(x)} \sim \left(\frac{x}{2}\right)^{1/3}, \tag{3.10}$$

which corresponds to (3.7). Thus the recursion relation is stable forwards *and* backwards.

Case (b) *n negative*

It proves convenient to re-express (2.3), setting $n = -m$, in the form

$$-2g_{-(m-2)}(x) - (m - 1)\, g_{-m}(x) + x g_{-(m+1)}(x) = 0. \tag{3.11}$$

Corresponding to the balances which lead to equations (3.2)–(3.5) we find solutions, for sufficiently large m, of type

$$\left|\frac{y_{i,-m}}{y_{i,-(m-1)}}\right| \sim \left(\frac{2}{m}\right)^{1/2}, \qquad i = 1, 2, \quad \epsilon \ll 1, \tag{3.12}$$

$$\frac{y_{3,-m}}{y_{3,-(m-1)}} \sim \frac{m-1}{x}, \qquad \epsilon \ll 1, \tag{3.13}$$

with

$$\left|\frac{y_{1,-m}}{y_{1,-(m-1)}}\right| \Big/ \left|\frac{y_{3,-m}}{y_{3,-(m-1)}}\right| = O(\epsilon^{1/2}). \tag{3.14}$$

Equation (3.14) shows that for m increasing $y_{3,-m}$ dominates $y_{1,-m}$ whereas for positive n, (3.5) shows the reverse. We therefore expect $y_{3,-m}$ to dominate for forward (m increasing) recursion and $y_{1,-m}$ to dominate for backwards recursion.

The third possible balance, corresponding to (3.6) gives the three uncoupled solutions

$$\frac{g_{-m}}{g_{-(m-3)}} \sim \frac{2}{x}, \tag{3.15}$$

valid, and stable in both directions, for $\epsilon \gg 1$. The behaviour of $y_{3,-m}$ (3.13), corresponds to the $T_{-m}(x)$ behaviour in (2.10). Thus, the $T_{-m}(x)$ are *stable* forward and *unstable* backwards. For $\epsilon \gg 1$ however the $T_{-m}(x)$ are stable in both directions.

To sum up; if the starting values T_0, T_1 and T_2 are known for a given $x = 0$, then recursion may proceed safely for T_n whether n is positive or negative. Recursion *towards* T_0 is only stable within the regime $\epsilon \gg 1$.

4. Evaluation of $T_0(x)$, $T_1(x)$, $T_2(x)$

For any $x > 0$, the $T_n(x)$ are stable when computed by forward recurrence because the relative error does not grow with increasing $|n|$. The relative accuracy of T_n therefore depends upon the relative accuracy of T_0, T_1 and T_2. The coefficients of the series expansion (2.4) may be obtained recursively from (2.5) and (2.6) without fear of numerical instability. The number of terms required to achieve a given relative accuracy increases with x. For example, when x equals five, twentyfour terms in the series (2.4) are needed for nine significant figures (SF) using double precision arithmetic. Single precision calculations were found to lead to 9SF accuracy only for $x < 3$. For higher values of x the situation is worse.

The asymptotic series (2.7) on the other hand is available for high enough x. For $x = 20$ ten terms in the asymptotic series for T_i, $i = 0,\ldots, 20$, sufficed for 9SF accuracy. For larger values of x fewer terms were needed. In the interval $7 \leqslant x \leqslant 10$ numerical integration was necessary to calculate the integral (1.1). The substitution

$t = (1 - u)^{-1} - \frac{1}{2}$ transforms the range of integration from $[0, \infty)$ into $[-1, 1]$; the numerical procedure employed was based on the optimum addition of points to the Gauss quadrature formula [12, 13]. This procedure was used also to verify the results from the convergent and asymptotic series.

NUMERICAL RESULTS

In Table I we illustrate the stability of forward of forward recursion. In column 1 the starting value T_0 is given (for $x = 30$) with precision ranging from 9 to 1 SF. Starting values for T_1 and T_2 are similarly supplied. Recurrence relation (2.3) is used to generate T_{50}, whose value is shown in the second column, and T_{-50}, shown in column three. It is clear that the accuracy of $T_{\pm 50}$ is maintained relative to the accuracy of T_0. This behaviour was repeated in test runs where x ranged from 0.001 to 100.

TABLE I

Stability of Forward Recursion, $x = 30$

$T_0 \times 10^8$	$T_{50} \times 10^{21}$	$T_{-50} \times 10^{12}$
1.212 640 12	4.397 683 68	3.504 994 33
1.212 640	4.397 683 56	3.504 994 2
1.212 6	4.397 62	3.504 95
1.21	4.394	3.502
1	4.1	3.3

In Table II we illustrate some stable and unstable features of backward recursion. It proves instructive to consider a relatively high value, $x = 30$, for which there exist regions $\epsilon \ll 1$ and $\epsilon \gg 1$ depending upon n. As $|n|$ ranges from 1 to 10 ϵ ranges from approximately two thousand to two, so we expect the backwards recursion to be essentially stable. This is seen in column two of the Table where the bold face figure represents the machine accuracy (16 for calculations in which $n > 0$ and 14 for $n < 0$, using two different machines). For $|n| = 20$, $\epsilon \approx \frac{1}{4}$ and we expect mild backwards instability between $|n| = 20$ and 10, shown in column three. For higher starting values of $|n|$ the instability sharpens until at $|n| = 50$ the instability devastates T_0 (column 6). An interesting feature to note is that, as predicted, the relative accuracy is essentially held between $|n| = 10$ and $n = 0$.

In Table III we present values of T_0, T_1 and T_2 for x in the range 10^{-3} to 10^2 to 9SF. Entries for $x \leqslant 5$ were computed from the convergent series expression (2.4), the number of terms in the series for $T_1(x)$ being shown in column 5. Entries for $x \geqslant 20$ were computed from the asymptotic expansion (2.7) and for the remaining interval $7 \leqslant x \leqslant 10$ numerical quadrature was employed. All entries agree to 9SF with quadrature calculations of Siewert and Grandjean [14]. Comparison was also made

TABLE II
Stability of Backward Recursion, $x = 30$

	$\lvert T^a_{nb} - T^b_{nf} \rvert / T_{nf} = 0(10^r)$				
n	r	r	r	r	r
−50					**−14**
−40				**−14**	−7
−30			**−14**	−8	0
−20		**−14**	−11	−3	+5
−10	**−14**	−12	−8	0	+8
0	−14	−11	−7	+1	+8
0	−16	−14	−11	−4	+4
10	**−16**	−14	−11	−4	+4
20		**−16**	−13	−5	+2
30			**−16**	−10	−3
40				**−16**	−10
50					**−16**

[a] T_{nb} computed by backwards recurrence from bold face figure.
[b] T_{nf} computed by forwards recurrence from T_2 onwards.

TABLE III
Values of $T_0(x)$, $T_1(x)$ and $T_2(x)$ to 9SF

x	$T_0(x)$	$T_1(x)$	$T_2(x)$	abc
0.001	8.791 841 09(−01)	4.991 175 44(−01)	4.426 139 05(−01)	4[a]
0.01	8.387 458 48(−01)	4.913 999 91(−01)	4.381 568 45(−01)	6[a]
0.10	6.343 215 82(−01)	4.263 396 79(−01)	3.969 925 50(−01)	8[a]
0.50	2.987 173 53(−01)	2.531 761 74(−01)	2.653 830 44(−01)	10[a]
1.00	1.500 459 65(−01)	1.465 633 81(−01)	1.684 873 48(−01)	14[a]
1.25	1.111 466 24(−01)	1.142 154 71(−01)	1.360 920 00(−01)	14[a]
1.50	8.390 956 72(−20)	9.002 630 74(−02)	1.107 033 00(−01)	14[a]
1.75	6.429 963 93(−02)	7.162 928 43(−02)	9.059 828 06(−02)	16[a]
2.00	4.987 649 66(−02)	5.744 661 43(−02)	7.453 878 20(−02)	16[a]
2.50	3.089 888 50(−02)	3.768 758 33(−02)	5.114 826 80(−02)	18[a]
3.00	1.973 853 52(−02)	2.526 371 96(−02)	3.564 180 87(−02)	18[a]
4.00	8.619 308 83(−03)	1.193 080 33(−02)	1.795 659 00(−02)	20[a]
5.00	4.022 478 82(−03)	5.927 054 23(−03)	9.405 873 71(−03)	24[a]
7.00	1.004 586 83(−03)	1.630 738 21(−03)	2.814 956 54(−03)	127[b]
8.00	5.280 881 90(−04)	8.915 091 47(−04)	1.593 208 90(−03)	127[b]
9.00	2.849 775 27(−04)	4.981 821 05(−04)	9.184 689 10(−04)	127[b]
10.00	1.572 691 73(−04)	2.837 185 19(−04)	5.380 869 64(−04)	127[b]
20.00	9.122 975 92(−07)	2.034 457 89(−06)	4.689 067 84(−06)	10[c]
30.00	1.212 640 12(−08)	3.071 140 15(−08)	7.980 178 53(−08)	7[c]
40.00	2.562 828 77(−10)	7.111 651 72(−10)	2.016 154 49(−09)	7[c]
50.00	7.398 758 77(−12)	2.205 050 08(−11)	6.695 044 40(−11)	6[c]
100.00	2.119 813 72(−18)	7.904 590 64(−18)	2.982 882 70(−17)	5[c]

[a] No. of terms used in convergent series.
[b] No. of function evaluations in quadrature formula.
[c] No. of terms used in asymptotic series.

between values of $T_n(x)$ for $|n| \geqslant 2$ by the asymptotic formula and by the recurrence formula. For fixed x, as $|n|$ increased, so decreasing ϵ, more terms in the asymptotic series were needed for satisfactory agreement, which suggests that the recurrence relation ought to be used to generate $T_n(x)$, $|n| > 2$, whatever the method used to generate the starting values T_0, T_1 and T_2.

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