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Note

On Computing the Integral of Glow Curve Theory*

The integral in question arises in theories of thermoluminescence and thermally induced currents. It is $F(T, E) = \int_0^T \exp(-E/ks)ds$, where T denotes temperature, E energy, and k is Boltzmann's constant. In [1], Chen discusses the evaluation of $F(T, E)$ by means of the asymptotic expansion

$$F(T, E) \approx T \exp\left(-\frac{E}{kT}\right) \sum_{n=1}^{N} \left(\frac{E}{kT}\right)^{-n} (-1)^{n-1}\, n! \tag{1}$$

and recommends that N be chosen as the largest integer less than or equal to E/kT. In what follows, this will be called Chen's method; and for notational convenience we will define $E/kT \equiv x$.

Researchers in the Lockheed Palo Alto Material Sciences Laboratory studying thermally induced currents in microelectronic structures were interested in a potential range of $2 < x < 150$. Since the asymptotic expansion approach is not valid for small x (note that for $x = N = 2$, Eq. (1) reduces to zero), and N becomes large for large x when Chen's method is used, the author was asked to reexamine the evaluation of $F(T, E)$. The purpose of this paper is twofold: to present a reasonable alternative to Chen's method when the asymptotic expansion is used; and to present a new method of approximating $F(T, E)$ which is computationally very fast and whose error is uniformly bounded by $\pm(2 \times 10^{-8})$ for all $x \geqslant 1$.

Returning to the integration by parts which produced Eq. (1), we find

$$\begin{aligned} I(x, N) &\equiv F(T, E) - Te^{-x} S_N(x) \\ &= (-1)^N \frac{(N+1)!\, e^{x}}{x^N} E_{N+2}(x) \end{aligned} \tag{2}$$

where $S_N(x)$ is the summation appearing in Eq. (1) and

$$E_{N+2}(x) = \int_1^\infty \frac{e^{-xy}}{y^{N+2}}\, dy. \tag{3}$$

The integral of interest appears in Glow Curve Theory as a multiplicative factor of the form

$$\exp\left(-\frac{1}{b\tau} F(T, E)\right), \tag{4}$$

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where b is an experimentally controlled heating rate and τ has units of time. It follows then that the real concern is to bound the relative error in approximating Eq. (4), i.e., we wish to have

$$\left| \frac{\exp(-(1/b\tau)\, F(T, E)) - \exp(-(Te^{-x}/b\tau)\, S_N(x))}{\exp(-(1/b\tau)\, F(T, E))} \right| < \rho, \tag{5}$$

where ρ is under the experimenters control. Assuming an even number of terms of the asymptotic expansion are used, Eqs. (2) and (5) lead to the requirement that

$$I(x, N) < b\tau \ln (1 + \rho). \tag{6}$$

It is known (see [2, Chap. 5] that $E_{N+2}(x)$ satisfies the inequalities $1/(x + N + 2) < e^x E_{N+2}(x) \leqslant 1/(x + N + 1)$; therefore from Eqs. (2) and (6) it becomes reasonable to seek for an (even) integer N such that

$$\frac{(N+1)!}{x^N(x + N + 2)} < I(x, N) \leqslant \frac{(N+1)!}{x^N(x + N + 1)} < b\tau \ln(1 + \rho) \tag{7}$$

is satisfied. Note that the Nth term of the asymptotic expansion, except for sign, is $N!/x^N$. It is therefore a simple one-step operation to check the third inequality in (7). The proposed modification to Chen's method is now simply stated: Stop the computation of the asymptotic expansion terms at the first even integer, if any, for which that inequality is satisfied. This method, which we will call the Modified Asymptotic Expansion (MAE) method, was programmed to run on a minicalculator (HP 9820) in such a way that it retreats to Chen's method when ρ is sufficiently small. Results will be discussed later in the paper.

We now return to the original integral $F(T, E)$. It was fortuitously discovered that

$$F(T, E) = \int_0^T \exp\left(-\frac{E}{ks}\right) ds \equiv T\left(e^{-x} - x \int_x^\infty \frac{e^{-y}}{y}\, dy\right). \tag{8}$$

(The substitution $s = E/ky$ yields $F(T, E) = E/k \int_x^\infty e^{-y} y^{-2}\, dy$. Integrating by parts, $\int u\, dv$, with $u = -(y/2)e^{-y}$, $dv = -(2/y^{-3})\, dy$ yields after some algebraic manipulation, Eq. (8)—recall that $x = E/kT$.) The integral in (8) has been extensively studied in the open literature where it is identified as $E_1(x)$ or $-E_i(-x)$ [2, 3]. Specifically in [2, 3] there is presented a Tschebyscheff rational approximation of $E_1(x)$ of the form $xe^x E_1(x) = R(x) + \epsilon(x)$, where $R(x)$ is the quotient of two fourth-degree polynomials, and $\epsilon(x)$, the error associated with the approximation, oscillates between $\pm(2 \cdot 10^{-8})$ for all $x \geqslant 1$. Five of the nine zeros of the error curve are inside the interval (2, 150). Writing $R(x) = A(x)/B(x)$ and substituting into Eq. (8), we obtain the particularly simple, easily computed approximation

$$F(T, E) \approx Te^{-x}(1 - A(x)/B(x)). \tag{9}$$

The coefficients of $A(x)$ and $B(x)$, taken from [2], are listed in Table I.

TABLE I

Coefficients of $A(x)$ and $B(x)$

$A(x) = \sum_{n=0}^{4} a_n x^n$	$B(x) = \sum_{n=0}^{4} b_n x^n$
$a_0 = 0.2677737343$	$b_0 = 3.9584969228$
$a_1 = 8.6347608925$	$b_1 = 21.0996530827$
$a_2 = 18.0590169730$	$b_2 = 25.6329561486$
$a_3 = 8.5733287401$	$b_3 = 9.5733223454$
$a_4 = 1$	$b_4 = 1$

The relative error associated with using Eq. (9) is not investigated here since there is a convergent series representation for $E_1(x)$ (see, e.g., [2]). This series was programmed to run on a minicalculator (the HP 9820) and a direct comparison was made between Eqs. (8) and (9) for x in the interval $2 \leqslant x \leqslant 6$, an interval which contains two of the extrema of the error function $\epsilon(x)$. Sufficiently many terms of the series were used to evaluate Eq. (8) correctly to 10 decimal digits, the output capability of the calculator. The results of this comparison can be summarized as follows: In a neighborhood of the extrema, the first five decimal digits agree; away from the extrema, up to eight decimal digits are in agreement. The absolute error associated with Eq. (9) is a constant times $|\epsilon(x)|(e^{-x}/x)$ which decreases as x increases, so we would expect even better agreement near the other extreme values of $\epsilon(x)$.

The three methods of computing $F(T, E)$ were compared in a manner which we will now discuss. By restricting attention to only integer values of x, both the Chen and MAE methods could be programmed to calculate in a very efficient manner; that is, both become a simple evaluation of $\sum(-1)^n\, n!\, x^{-n}$ for $n = 1$ to x in Chen's method and to $\leqslant x$ for the MAE method (the multiplicative factor Te^{-x}, common to all the methods, was suppressed). Since the method of Eq. (9) is known to be the most accurate for small x, it was selected as the reference and comparisons were made of the basis of the number of decimal-digits-of-agreement (DDA). The interval $5 \leqslant x \leqslant 30$ was selected. The MAE method, with $b\tau = 1$ and $\rho = 10^{-5}$ in Eq. (7), retreated to the Chen method for $5 \leqslant x \leqslant 13$, and in this interval the DDA increased from 1 to 3. The DDA for the Chen method continued to increase to 6 at $x = 21$, and remained constant thereafter. The DDA for the MAE method remained at 4 for $14 \leqslant x \leqslant 25$ but used fewer terms as x increased; for example, only six terms were used for $17 \leqslant x \leqslant 25$. For $25 \leqslant x \leqslant 30$, the DDA decreased to 3. The method of Eq. (9) required 5 sec of computing time for the 26 cases, Chen's method needed 72 sec, and the MAE required 34 sec.

A referee has kindly pointed out that there are even more accurate approximations to $E_1(x)$ (and $E_n(x)$) available in the open literature [4, 5]; however, the fourth-order method discussed above has been proven to provide sufficient accuracy for the Lockheed Microelectronics experimental work.

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