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Computation of the Exponential Trap Population Integral of Glow Curve Theory*

1. Introduction

In the analysis of thermally stimulated currents (TSC) it is frequently necessary to compute an integral

$$\varphi(x) \equiv \int_x^\infty e^{-u}u^{-2}\,du = \frac{e^{-x}}{x} + E_i(-x). \tag{1}$$

This arises, for example, in the evaluation of the light output of a thermoluminescence (glow curve) experiment in the case of fast retrapping, or of the TSC of a thin specimen in which the small interelectrode spacing allows collection of the full released charge.

The expression evaluated is usually given in the form [1]

$$I = n_0 s e^{-E/kT} e^{-s/\beta \int_0^T e^{-E/kT}\,dT}, \tag{2}$$

where the lower limit of the integral is taken as zero if the starting temperature corresponds to a stable population of trapped carriers. The integral appearing in the exponent is usually integrated by parts to obtain an asymptotic series, either directly, or by identification with the exponential integral to which it is related. One [2], two [3], or four [4] terms of the asymptotic series are usually used. Recently Chen [5] has proposed optimal use of the asymptotic series by continuing it to the next smallest term and then adding one half of the smallest term. (These approximations are herein designated as A1, A2, A4, and AO, respectively.) Dussel and Bube [6] had already recognized the extremely slow convergence of the asymptotic series and had resorted to numerical integration for values of the argument, x, less than 15. The incorporation of one half of the last term in the AO approximation makes a substantial improvement over the simple summation.

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Simple change of variable in (2) leads to the form given in (1),

$$
\begin{aligned}
I &= n_0 s e^{-x} e^{-sE/\beta k} \int_{\infty}^{x} e^{-u} d(u^{-1}) \\
&= n_0 s e^{-x} e^{-\lambda} \int_{x}^{\infty} e^{-u} u^{-2}\, du \qquad (3) \\
&= n_0 s \exp(-x - \lambda\varphi)
\end{aligned}
$$

where

I = stimulated particle current;
n_0 = initial trapped particles;
s = effective attempt-to-escape frequency;
E = trap depth;
$x \equiv E/kT$;
$\lambda \equiv sE/\beta k$.

2. Accuracy Requirement

Two points must be considered in deciding what accuracy is required:

(1) The value of λ in various applications ranges of the order of 10^8 to 10^{15}, with 10^{12} typical. This is the number by which absolute error must be multiplied to determine errors in the calculated TSC. For this reason an absolute error of 10^{-13} in φ may lead to *order-of-magnitude* error in I.

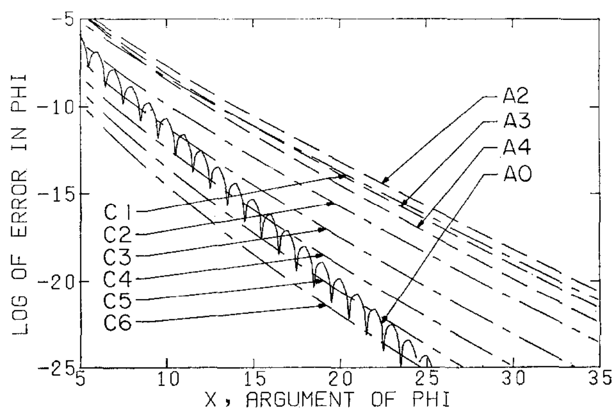

Fig. 1. Absolute errors in approximations to $\varphi(x)$. Long dashes, short dashes, and solid lines represent continued fraction, fixed-length asymptotic, and variable-length asymptotic approximations, respectively.

(2) The error of the most accurate asymptotic method (AO approximation) is *oscillatory*, having zeros located between integer values of the argument. Owing to the rapid fluctuation of error with argument values, the use of AO can lead to distortion of the shape of TSC curves used, for example, for the testing of half-width and other shape-dependent analytic methods.

A family of approximations to φ, based on the successive convergents of the continued fraction development of the Prym function originally due to Laplace [7], has been investigated for this application.

The relative error of the first six convergents (labeled C1, C2,..., C6) is depicted, together with the errors of A2, A3, A4, and AO in Fig. 1.

3. Approximations Employed and their Accuracy

The continued fraction employed is

$$\varphi(x) = e^{-x}x^{-1}\left(\frac{1}{x+2} - \frac{2}{x+4} - \frac{6}{x+6} - \cdots - \frac{n(n+1)}{x+2(n+1)} - \cdots\right). \tag{4}$$

The first three convergents of (4) are

$$\text{C1:} \qquad \varphi \approx \frac{e^{-x}}{x(x+2)}, \tag{5a}$$

$$\text{C2:} \qquad \varphi \approx \frac{e^{-x}(x+4)}{x(x^2+6x+6)}, \tag{5b}$$

$$\text{C3:} \qquad \varphi \approx \frac{e^{-x}(x^2+10x+18)}{x^3+12x^2+36x+24}. \tag{5c}$$

Comparing C1 with the two-term asymptotic expansion most used in deriving analytical results

$$\text{A2:} \qquad \varphi \approx \frac{e^{-x}}{x^2}\left(1 - \frac{2}{x}\right), \tag{6}$$

we see that the expansions are of comparable complexity. Figure 1 reveals a lesser error of C1 throughout its range, becoming appreciably superior for small values of the argument.

Where numerical evaluations, rather than analytic results, are sought, the C series of approximants is markedly advantageous. C3 would seem to be sufficiently accurate for most applications, even with large values of λ. Where higher accuracy is desired, C6 yields better performance than even AO (except at AO's isolated points of zero error), without the potential pitfalls of a rapidly changing error.

For convenience in comparing proposed approximations, selected values of φ and the errors of various approximations, all computed from C16, are presented in Table I.

TABLE I

Errors in Various Approximations

x	$\varphi(x)$ Calculated from C16	$\varphi_{\text{approx}} - \varphi_{C16}$						
		A2	A4	AO	C1	C2	C3	C6
5	1.9929380854(−4)	3.8(−5)	2.5(−5)	1.2(−6)	6.8(−6)	4.7(−7)	4.8(−8)	1.8(−10)
10	3.8302404656(−7)	2.0(−8)	3.5(−9)	2.0(−11)	4.7(−9)	1.3(−10)	6.1(−12)	2.9(−15)
15	1.2072091120(−9)	2.9(−11)	2.3(−12)	5.0(−16)	7.6(−12)	1.2(−13)	3.1(−15)	3.4(−19)
20	4.7024282154(−12)	6.5(−14)	3.0(−15)	1.5(−20)	1.8(−14)	1.8(−16)	3.0(−18)	1.1(−22)
25	2.0627779065(−14)	1.9(−16)	5.5(−18)	4.8(−25)	5.3(−17)	7.6(−19)	4.3(−21)	5.8(−26)
30	9.7655645591(−17)	6.1(−19)	1.3(−20)	1.7(−29)	1.8(−19)	8.9(−22)	8.0(−24)	4.8(−29)

4. Remark on Programming

A note regarding the computation is in order. While the rational forms (5a) and (5b) are most appropriate for analytic derivations, more accurate numerical work using the third or higher convergent is best programmed in the continued fraction form (4). This situation prevails in most modern machines having division speeds comparable to those for multiplication.

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