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Notes

On the Computation of the Generalized Integral in Glow Curve Theory

An improvement in the method for computing the value of the integral $\int_{T_0}^{T} \exp(-E/kT')\, dT'$ was given previously [1]; where T_0 is the temperature (in °K) at which the crystal is excited, T the variable temperature (°K), k the Boltzmann constant, and E the activation energy (eV). A more general theory taking into account a possible dependence of the frequency factor s on temperature, $s = s''T^a$, where s'' is a constant [2, 3], includes the integral $\int_{T_0}^{T} T'^a \exp(-E/kT')\, dT'$. The value of a was reported [4, 5] to be usually between -2 and 2, and in most cases it is an integer or half-integer. The purpose of the present note is to improve the computation of this generalized integral in a way similar to that which was done for the specific case of $a = 0$ [1]. It is obvious that for another specific case, $a = -2$, the function is integrable and therefore its evaluation is trivial.

Let us define

$$F(T, E, a) = \int_0^T T'^a \exp(-E/kT')\, dT', \tag{1}$$

then the integral we are interested in will be

$$\int_{T_0}^{T} T'^a \exp(-E/kT')\, dT' = F(T, E, a) - F(T_0, E, a). \tag{2}$$

By integrating by parts we have from Eq. (1)

$$F(T, E, a) = \frac{kT^{a+2}}{E} \exp\left(\frac{-E}{kT}\right) \times \left\{1 - \frac{1}{\Gamma(a+2)} \sum_{n=2} \left(\frac{kT}{E}\right)^{n-1} (-1)^{n-1}\, \Gamma(a+n+1)\right\}. \tag{3}$$

If we take N terms in this series the absolute value of the possible error $|R_N|$ would not exceed the $(N+1)$th term. The integral is represented to a good approximation by the series in the case where E/kT is larger than unity. In most cases dealt with in glow curve theory, $E/kT \gtrsim 20$; only in extreme cases does it get as low as 10. The absolute value of the terms decreases with n up to a certain $n = N$, after which the absolute values of the terms start to increase. The turning point would be N for which $|a_N/a_{N-1}| \approx 1$, which in the general case would give

$$N \approx E/kT - a. \tag{4}$$

As explained previously [1] for the case of $a = 0$, it is of advantage to take $N - 1$ terms in the series (Eq. (3)), and to add one half of the Nth term. The possible error would thus be equal to $a_N/2$.

In a way similar to that which was done for $a = 0$, we now develop a method for estimating the possible error incurred in the evaluation of the integral by the series. This possible error, R_N, would be given as a function of a and E/kT, without actually computing the terms of the series. In accordance with Eq. (3) we have

$$|R_N| \cong \left|\frac{a_N}{2}\right| = \left(\frac{kT}{E}\right)^{N-1} \frac{\Gamma(a+N+1)}{2\Gamma(a+2)}. \tag{5}$$

If we choose N to be the largest integer smaller than $E/kT - a$, we have

$$N = E/kT - a - \alpha, \tag{6}$$

where α is a positive number between 0 and 1. Thus we have

$$|R_N| \cong \left(\frac{kT}{E}\right)^{N-1} \frac{\Gamma(E/kT + 1 - \alpha)}{2\Gamma(a+2)}. \tag{7}$$

Using the generalized Stirling formula (see, for example, [6])

$$\Gamma(x+1) \cong x^{x+1/2} e^{-x} \sqrt{2\pi}, \tag{8}$$

and making use of the fact that $E/kT - \alpha$ is always 10 or more, we have to a good approximation that

$$|R_N| \cong \left(\frac{kT}{E}\right)^{N-1} \left(\frac{E}{kT}\right)^{N+a+1/2} \left(1 - \frac{\alpha}{E/kT}\right)^{E/kT-\alpha+1/2} \times \exp\left(\frac{-E}{kT}\right) \frac{e^{\alpha}\sqrt{2\pi}}{2\Gamma(a+2)}. \tag{9}$$

Again, since E/kT is rather large, we have that

$$\left(1 - \frac{\alpha}{E/kT}\right)^{E/kT} \approx e^{-\alpha}. \tag{10}$$

Thus our final result is

$$|R_N| = \sqrt{\pi/2}\left(\frac{E}{kT}\right)^{a+3/2} \frac{\exp(-E/kT)}{\Gamma(a+2)}. \tag{11}$$

The relative error can be found according to Eq. (3) by dividing the value given in Eq. (11) by the expression

$$1 - \frac{1}{\Gamma(a+2)} \sum_{n=2}^{N} \left(\frac{kT}{E}\right)^{n-1} (-1)^n \Gamma(a+n+1)$$

This expression is usually smaller than unity by only 10–20 %; thus the value of R_N itself is a good approximation for the relative error. It is immediately seen that Eq. (11) reduces to Eq. (13) of [1] for $a = 0$.

The evaluation of $\Gamma(a + 2)$ for Eq. (11) is trivial for integral values of a. For half-integers or other nonintegrals its value can be found using tables (for example, see [7]) and the equation $\Gamma(m + 1) = m\Gamma(m)$.

It is to be noted that although the Γ-function appears twice in Eq. (3), one does not have to find its values for calculating each term in the series; it is much easier, especially while working with the computer, to use the fact that $\Gamma(a + n + 1)/\Gamma(a + 2)$ is the same as $(a + n)(a + n - 1) \cdots (a + 2)$. Finally, the conventional assumption that $F(T, E, a) \gg F(T_0, E, a)$ can be checked in a way similar to that explained in [1] for $a = 0$. When one does not want to bother about the validity of this assumption there is no problem in calculating $F(T_0, E, a)$ and using Eq. (2).

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