GENERALIZATION AND APPLICATION OF LAPLACE TRANSFORMATION FORMULAS FOR DIFFUSION

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Abstract—The present work generalizes the relation between image functions as $e^{-qx}q^{-m}(q+h)^{-n}$ and their original ones f(t). The resultant equation is valid for any integer pairs (m,n) and it will analyze some diffusion problems easily and systematically. In addition, some characteristics of error functions are mentioned.

NOMENCLATURE

A, V,area and volume; D, diffusivity; arbitrary constant but 0 < e' < 1 or $e' \approx 1/2$; variables $x/(4Dt)^{1/2}$ and $h(Dt)^{1/2}$: F, H,h, h',K/D and V/A; j, k, m, n, r, s, integers; Κ, constant; distance; Laplace transformation operator; inverse Laplace transformation operator; p, q,parameters for $\mathcal{L}[f(t)]$ $= \int_0^\infty f(t) e^{-pt} dt \text{ and } q = (p/D)^{1/2};$ f(t)original function; $g(\xi)$, auxiliary function; i'' erfc(ξ), integrated error function $\int_{\xi}^{\infty} i^{n-1} \operatorname{erfc}(\xi) d\xi \text{ with } i^{0} \operatorname{erfc}(\xi)$ $\int_{\xi} = \operatorname{erfc}(\xi) = (2/\sqrt{\pi}) \int_{\xi}^{\infty} \exp(-\xi^{2}) d\xi;$ $H_n(\xi)$, Hermite's polynomials, $(-)^n \exp(\xi^2)(d/d\xi)^n \exp(-\xi^2)$ $\Gamma(\xi)$, gamma function; unit function: $1(\xi)$ [m/2],Gauss symbol; (m+n-j)extended binomial coefficient; α, β, reals, $\alpha + \beta = h$; 0, initial: I, II, phases I, II;

INTRODUCTION

Laplace transformed.

It is well known that the Laplace transformation method has been frequently used to study many diffusion problems for mass and heat transfer. In an analysis of some partial differential equations for the diffusion with the transformation, the related subsidiary equations are usually written in terms of characteristic image functions such as $\exp(-qx)q^{-m}(q+h)^{-n}$.

The image function uniquely corresponds to its original one with the preparation of a set (m, n). Consequently, if the relation between two functions could be unified and calculated for any integer pair (m, n), the solution of many diffusion problems could be greatly simplified.

Carslaw and Jaeger [1], Crank [2], and Erdelyi et al. [3] have tabulated many individual Laplace transformation formulas for lower pairs of (m,n) values. These have often been very useful. However, it is necessary for any higher (m,n) values to deduce a suitable relation corresponding to one of the pair or to derive one of the formulas from the fundamental definition of the inversion theorem. This may be very time consuming.

The purpose of the present work is to obtain a generalized relation which is applicable to an arbitrary integer pair (m, n) where, of course, negative m and/or n may be present. Comparisons between the present result and the previous discrete relations are presented instead of a proof of the new equation (which is possible by the inductive method), together with some illustrative examples of diffusion problems.

DERIVATION

Let an original function be given by f(t) with respect to time. The f(t) is, in fact, dependent on space variables, diffusivity and so on, as shown later, but these are neglected for simplicity.

A definition for the transformation is given by the following equation in the usual way:

$$\int_0^\infty f(t) e^{-pt} dt = \mathcal{L}\{f(t)\} = \frac{e^{-qx}}{q^m (q+h)^n}$$
 (1)

where

$$q = (p/D)^{1/2}. (2)$$

Furthermore the notation \mathcal{L}^{-1} , the Laplace inversion operator, will be used for convenience,

$$f(t) = \mathcal{L}^{-1} \left[\frac{e^{-qx}}{q^m (q+h)^n} \right]. \tag{3}$$

In order to obtain the original function f(t) from its image or vice versa, various methods are available. Here it is advantageous to introduce an operator

 $(h-d/dx)^n$ into equation (3) and to solve the resultant ordinary differential equation (4), because characteristic relationships between diffusion phenomena and error functions may be used,

$$\left(h - \frac{\mathrm{d}}{\mathrm{d}x}\right)^{n} f(t) = \mathcal{L}^{-1} \left[\left(h - \frac{\mathrm{d}}{\mathrm{d}x}\right)^{n} \frac{\mathrm{e}^{-qx}}{q^{m}(q+h)^{n}} \right]$$
$$= \mathcal{L}^{-1} \left[\frac{\mathrm{e}^{-qx}}{q^{m}} \right]. \quad (4)$$

This equation can be solved and gives the following solution under the conditions of $m \ge 2$ and $n \ge 1$:

$$\mathcal{L}^{-1} \left[\frac{e^{-qx}}{q^m (q+h)^n} \right]_{n>0}^{m \ge 2} = (-)^m D \frac{(2H)^{m-2}}{h^{m+n-2}}$$

$$\times \exp(-F^2) \left\{ \sum_{j=0}^{m-2} {m+n-j-3 \choose n-1} (-)^j (2H)^{j-m+2} \right\}$$

$$\times \exp(F^2) i^j \operatorname{erfc}(F) - \sum_{j=0}^{n-1} {m+n-j-3 \choose m-2} (2H)^{j-m+2}$$

$$\times \exp[(F+H)^2] i^j \operatorname{erfc}(F+H) \right\}$$
(5)

because the following relation is valid

$$\mathcal{L}^{-1}\left(\frac{e^{-qx}}{q^{2+k}}\right) = D[(4Dt)^{1/2}]^k i^k \operatorname{erfc}(F)$$
 (6)

where k = 0, 1, 2, ...

On the other hand, for m < 2, if m is forced to assign inconvenient values in equation (5), the rule of an empty sum means that the sum will be zero. Therefore the series in the original function does not depend on the variable $x/[(4Dt)^{1/2}]$ but on the combined term $x/(4Dt)^{1/2} + h(Dt)^{1/2}$.

With a change in the order of k in $(h-d/dx)^k$ or extending k in equation (5) to negative values, the same procedure as at $m \ge 2$ gives the following equation:

$$\mathcal{L}^{-1} \left[\frac{e^{-qx}}{q^m (q+h)^n} \right]_{n>0}^{m<2} = (-)^{m+1} D \frac{(2H)^{m-2}}{h^{m+n-2}}$$

$$\times \exp(-F^2) \sum_{j=m+n-2}^{n-1} {m+n-j-3 \choose m-2} (2H)^{j-m+2}$$

$$\times \exp[(F+H)^2] i^j \operatorname{erfc}(F+H) \quad (7)$$

where the coefficient $\binom{m+n-j-3}{m-2}$ is an extended binomial coefficient, as explained in the Appendix.

The coefficient which includes any negative elements can be classified into three types at most, and each of these may be evaluated with the aid of a gamma function and its functional formulas. In some cases the limit value calculation has to be carried out using the following two formulas:

$$\frac{\Gamma(-\zeta+k)}{\Gamma(-\zeta)} = (-)^k \frac{\Gamma(\zeta+1)}{\Gamma(\zeta-k+1)},\tag{8}$$

$$\frac{\Gamma(\xi)}{\Gamma(\xi-k)} = (-)^k \frac{\Gamma(-\xi+k+1)}{\Gamma(-\xi+1)}.$$
 (9)

Equation (9) may be used for the reverse procedure to equation (8) and vice versa.

Now, comparing equation (5) with equation (7), it is clear that the extension of m from positive to negative does not change the basic form of the relation, but lets the first term in the remainder series start from a different index.

Therefore, it is also considered that there is no essential difference for the extension of n to negative values. Thus, it may be concluded that only the initial term in the first series of equation (5) should be changed. If $m \ge 2$, then

$$\mathcal{L}^{-1} \left[\frac{e^{-qx}}{q^m (q+h)^n} \right]_{\substack{m \ge 2 \\ n \le 0}}^{m \ge 2} = (-)^m D \frac{(2H)^{m-2}}{h^{m+n-2}}$$

$$\times \exp(-F^2) \sum_{\substack{j=m+n-2}}^{m-2} \binom{m+n-j-3}{n-1} (-)^j (2H)^{j-m+2}$$

$$\times \exp(F^2) i^j \operatorname{erfc}(F) \quad (10)$$

where the exponential forms are not eliminated on purpose because of formalization. In the remaining case, $n \le 0$ and m < 2, repeated differentiations of the image function and the original one with x give

$$\mathcal{L}^{-1} \left[\frac{e^{-qx}}{q^m (q+h)^n} \right]_{\substack{m < 2 \\ n \le 0}}^{m < 2} = (-)^m D \frac{(2H)^{m-2}}{h^{m+n-2}}$$

$$\times \exp(-F^2) \sum_{\substack{j=m+n-2}}^{m-2} {m+n-j-3 \choose n-1} (-)^j (2H)^{j-m+2}$$

$$\times \exp(F^2) i^j \operatorname{erfc}(F). \quad (11)$$

The integer j in part of equations (7) and (10) and all j in equation (11) take negative integers. Under such conditions, the function i^j erfc() seems to have not been used widely. But the function with negative j may be especially recommended in differential or integral analyses for the group of error functions since repeated integrations are just differentiations with negative orders (and vice versa).

Now, let us introduce Hermite polynomials defined as

$$H_m(\xi) = (-)^m \exp(\xi^2) \left(\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^m \exp(-\xi^2)$$
$$= \sum_{j=0}^{\lfloor m/2 \rfloor} \frac{(-)^j m! (2\xi)^{m-2j}}{j! (m-2j)!}. \quad (12)$$

Then we can express i^{j} erfc (x) with negative j as follows $(i \rightarrow -m)$:

$$\exp(\xi^2) i^{-m} \operatorname{erfc}(\xi) = \left(\frac{2}{\sqrt{\pi}}\right) H_{m-1}(\xi), \quad (m \ge 1). \quad (13)$$

Therefore equation (11) has the following form:

$$\mathcal{L}^{-1} \left[\frac{e^{-qx}}{q^m (q+h)^n} \right]_{\substack{m \le 2 \\ n \le 0}}^{m \le 2} = (-)^m D \frac{(2H)^{m-2}}{h^{m+n-2}}$$

$$\times \exp(-F^2) \frac{2}{\sqrt{\pi}} \sum_{j=m+n-2}^{m-2} \binom{m+n-j-3}{n-1}$$

$$\times (-)^j (2H)^{j-m+2} H_{-(j+1)}(F). \quad (14)$$

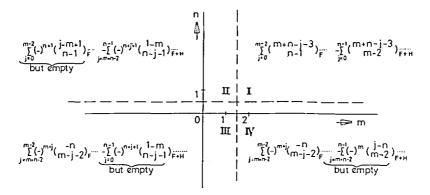


Fig. 1. Particular forms in parts of binomial coefficients and the first suffix in equation (15). Quadrants I-IV are sectioned by two dashed axes.

Equations (7) and (10) may be rewritten in terms of Hermite functions at required points where j < 0. As mentioned above, expressions between the image and original functions are slightly altered according to whether m and n are greater than 2-e' or less than 1-e', respectively. The numeral e' is real 0 < e' < 1, and for simplicity, let it equal a half integer 1/2 here. The differences in the equations are taken away with the aid of a unit function a

$$\mathcal{L}^{-1} \left[\frac{e^{-qx}}{q^m (q+h)^n} \right] = (-)^m D \frac{(2H)^{m-2}}{h^{m+n-2}}$$

$$\times \exp(-F^2) \sum_{j=(m+n-2)(1-1(n-1/2))}^{m-2} \binom{m+n-j-3}{n-1}$$

$$\times (-)^j (2H)^{j-m+2} \exp(F^2) i^j \operatorname{erfc}(F)$$

$$- \sum_{j=(m+n-2)v(2-v)}^{n-1} \binom{m+n-j-3}{m-2} (2H)^{j-m+2}$$

$$\times \exp\left[(F+H)^2 \right] i^j \operatorname{erfc}(F+H) \tag{15}$$

where

$$v = 1(m-3/2) + 1(n-1/2)$$
.

Modified forms for the extended binomial coefficient and the first index in the series are shown in Fig. 1.

APPLICATION AND DISCUSSION

Comparison with the previous equations

The generalized equation (15) can be proved by the induction method. But here, instead of this, we will illustrate how all previous equations are covered by equation (15).

The case n > 0 is shown in Table 1. The previous

equations [1-3] and the present one seem to be slightly different at first glance, but this is because the integrated error functions; were not used in the earlier works. Therefore, these are actually quite trivial. The present results have rather complicated forms but they are clearly systematic and have wide applicability: any change in n may be easily followed.

Table 2 shows results for the case of n=0 and for various m. The present results are also shown in both intermediate and rearranged forms. In this case only, however, it is not always necessary to carry out the analysis via the combination of Hermite functions, because a direct calculation from equation (5) is possible both for positive m (strictly speaking $m \ge 2$) and for other m with the aid of a relation between the integrated error functions with negative orders and a single Hermite function. The equations in Table 2 reveal an interesting feature of Hermite equations which have a combined variable—they can be transformed to single variable functions with simple manipulations.

An original image-relation with negative n has not been found in previous tabulations. Hence, let us examine the case for n < 0, which is also explained by the present equation. If h is considered to be merely one of the parameters in the expression $(q+h)^n|_{n<0}$, this can be binomially expanded for q.

Considering that both the whole original functions for $\exp(-qx)q^{-m}$ have analogous forms, and that the Laplace transformation has a linear nature, we can write equation (16):

$$\frac{e^{-qx}}{q^{m}(q+h)^{n}}\bigg|_{n<0} = \sum_{j=0}^{-n} {\binom{-n}{j}} q^{-n-j-m} h^{j} e^{-qx} = \mathcal{L}[f(t)].$$
(16)

For example, let us consider an original f(t) whose m and n are arbitrarily 4 and -3, respectively. This solution can be constructed from some standard

[†] The unit function $1(\xi)$ has values of 1, 1/2 or 0 for $\xi > 0$, $\xi = 0$, $\xi < 0$, respectively. The arguments in the forms of (2m+1)/2 [or (2n+1)/2] eliminate the case where functional values are of one half.

[‡] Integrated error functions have been discussed by D. R. Hartree, Mem. Manchr. Lit. Phil. Soc. 80, 85-102 (1936).

Table 1. Comparison between the present and the previous equations for $\exp(-qx)/q^n/(q+h)^n = \mathcal{L}[f(t)]$ at n > 0 where $F = x/(4Dt)^{1/2}$ and $H = h(Dt)^{1/2}$

m,n		present	previous [1,2,3]
= 4	n	$4D\frac{\sqrt{Dt}^{n+2}}{H^{n}}e^{-F^{2}}\left(\sum_{j=0}^{2}{\binom{n-j+1}{n-1}}\right)\frac{(-)^{j}e^{F^{2}}i^{j}erfc(F)}{(2H)^{2-j}}-\sum_{j=0}^{n-1}{\binom{n-j+1}{2}}\frac{e^{(F+H)^{2}}i^{j}erfc(F+H)}{(2H)^{2-j}}\right)$	
	1	$4D\frac{\sqrt{Dt^{3}}}{H}\left\{\frac{erfc(F)}{(2H)^{2}} - \frac{ierfc(F)}{2H} + \frac{i^{2}erfc(F)}{1} - \frac{e^{-F^{2}}e^{(F+H)^{2}}erfc(F+H)}{(2H)^{2}}\right\}$	$-\frac{D}{h^3}e^{(2FH+H^2)}erfc(F+H)-\frac{D}{h^3}\left\{erfc(F)-(2H)ierfc(F)+(2H)^2i^2erfc(F)\right\}$
ε	2	$4D \frac{(Dt)^{2}}{H^{2}} \left[\left(\frac{3erfc(F)}{(2H)^{2}} - \frac{2ierfc(F)}{2H} + \frac{1 \cdot i^{2}erfc(F)}{2H} \right) - e^{-F^{2}} e^{(F+H)^{2}} \left(\frac{3erfc(F+H)}{(2H)^{2}} + \frac{1ierfc(F+H)}{2H} \right) \right]$	
	n	$-2D \frac{\sqrt{Dt} \stackrel{n+1}{H}^{n+1}}{H^{n}} e^{-F^{2}} \left\{ \sum_{j=0}^{t} \binom{n-j}{n-j} \right\} \frac{(-)^{j} e^{F^{2}} \stackrel{j}{i} erfc(F)}{(2H)^{1-j}} - \sum_{j=0}^{n-i} \binom{n-j}{j} \right\} \frac{e^{(F+H)^{2}} \stackrel{j}{i} erfc(F+H)}{(2H)^{1-j}} $ $-2D \frac{Dt}{H} \left\{ \frac{erfc(F)}{2H} - \frac{ierfc(F)}{1} - \frac{e^{-F^{2}} e^{(F+H)^{2}} erfc(F+H)}{2H} \right\}$	
m = 3	1	$-2D \frac{Dt}{H} \left\{ \frac{erfc(F)}{2H} - \frac{ierfc(F)}{1} - \frac{e^{-F^2}e^{(F+H)^2}erfc(F+H)}{2H} \right\}$	$\frac{2}{h}\sqrt{\frac{D^3t}{\pi}}e^{-F^2} - \frac{1+2FH}{h^2} \operatorname{erfc}(F) + \frac{D}{h^2}e^{(2FH+H^2)}\operatorname{erfc}(F+H)$
	2	$-2D\frac{\sqrt{Dt}^{3}}{H^{2}}\left[\left(\frac{2erfc(F)}{2H} - \frac{1 \cdot ierfc(F)}{1}\right) - e^{-F^{2}}e^{(F+H)^{2}}\left(\frac{2erfc(F+H)}{2H} + \frac{1 \cdot ierfc(F+H)}{1}\right)\right]$	
	n	$D \frac{\sqrt{Dt}^{n}}{H^{n}} e^{-F^{2}} \left\{ \sum_{j=0}^{0} {n-j-1 \choose n-1} (-2H)^{j} e^{F^{2}} i^{j} erfc(F) \sum_{j=0}^{n-1} {n-j-1 \choose 0} (2H)^{j} e^{(F+H)^{2}} i^{j} erfc(F+H) \right\}$	
m = 2	1	$D\frac{\sqrt{Dt}}{H}\left\{ erfc(F) - e^{-F^2}e^{(F+H)^2} erfc(F+H) \right\}$	$\frac{D}{h}$ erfc(F) - $\frac{D}{h}$ e ^(2FH+H²) erfc(F+H)
	2	$D \frac{Dt}{H^2} \left[erfc(F) - e^{-F^2} e^{(F+H)^2} \left\{ erfc(F+H) + (2H) ierfc(F+H) \right\} \right]$	$\frac{D}{h^2}$ erfc(F) - $\frac{2}{h}\sqrt{\frac{Dt}{\pi}}$ e^{-F^2} - $\frac{1}{h^2}$ (1-2FH-2H ²) $e^{(2FH+H^2)}$ erfc(F+H)
	3	$D\frac{\sqrt{Dt^{3}}}{H^{3}} \left[erfc(F) - e^{-F^{2}}e^{(F+H)^{2}} \left\{ erfc(F+H) + (2H) ierfc(F+H) + (2H)^{2} i^{2} erfc(F+H) \right\} \right]$	
E	n	$(\frac{D}{2})\frac{\sqrt{D1}}{H^n}^{n-1}e^{-F^2\sum_{j=n-1}^{n-1}}(\frac{0}{n-j-1})(-)^{(n+j+1)}(2H)^{(j+1)}e^{(F+H)^2}i^{j}erfc(F+H)$	
	1	De ^{-F²} e ^{(F+H)²} erfc(F+H)	De ^(2FH+H²) erfc(F+H)
	2	2D√Dt e ^{-F²} e ^{(F+H)²} ierfc(F+H)	$2\sqrt{\frac{D^2t}{\pi c}}e^{-F^2} - (2D^2ht + 2D\sqrt{Dt}F)e^{(2FH+H^2)}er(c(F+H)$
	3	4D·Dt e-f2e (F+H)2 i2erfc(F+H)	

Table 1 (continued)

0 = @	U	$(\frac{D}{4})\frac{\sqrt{Dt}^{n-2}}{H^n}e^{-F^2\sum\limits_{j+n-2}^{n-1}(\frac{1}{n-j-1})(-)^{(n+j)}}(2H)^{(j+2)}e^{(F+H)^2}i^{j}erfc(F+H)$	
	1	$(\frac{D}{4}) \frac{1}{H\sqrt{Dt}} e^{-F^2} \left\{ (2H) \frac{2}{\sqrt{\pi}} H_0^2 (F+H) - (2H)^2 e^{(F+H)^2} erfc(F+H) \right\}$	$\sqrt{\frac{D}{\pi t}} e^{-F^2} - Dh e^{(2FH+H^2)} erfc(F+H)$
	2	$(\frac{D}{4})\frac{1}{H^2}e^{-F^2}e^{(F+H)^2}\{(2H)^2erfc(F+H)-(2H)^3ierfc(F+H)\}$	$-2h\sqrt{\frac{D^3t}{\pi}}e^{-F^2}+D(1+2FH+2H^2)e^{(2FH+H^2)}erfc(F+H)$
	3	$(\frac{D}{4})\sqrt{\frac{Dt}{H^3}}e^{-F^2}e^{(F+H)^2}\left((2H)^3ierfc(F+H)-(2H)^4i^2erfc(F+H)\right)$	
	n	$(\frac{D}{8})^{\sqrt{\frac{Dt}{H^n}}} e^{-F^2 \sum_{j=n-3}^{n-1} (\frac{2}{n-j-1}) (-)^{(n+j+1)} (2H)^{(j+3)} e^{(F+H)^2 i^{j}} e^{rfc(F+H)}$	
8	1	$(\frac{D}{8})\frac{1}{HDt}e^{-F^2}\left[\frac{2}{\sqrt{\pi}}\left\{(2H)\mathcal{H}_1(F+H)-2(2H)^2\mathcal{H}_0(F+H)\right\}+(2H)^3e^{(F+H)^2}ertc(F+H)\right]$	1/√π t (F-H) e ^{-F²} + Dh² e ^(2FH+H²) erfc(F+H)
	2	$(\frac{D}{8})\frac{1}{H^2\sqrt{Dt}}e^{-F^2}[(2H)^2\frac{2}{\sqrt{\pi}}\mathcal{H}_0(F+H)-e^{(F+H)^2}\{2(2H)^3\text{ertc}(F+H)-(2H)^4\text{icrfc}(F+H)\}]$	
m = -2	n	$(\frac{D}{16})\frac{\sqrt{Dt}^{n-4}}{H^n}e^{-F^2\sum_{j=n-4}^{n-1}(\frac{3}{n-j-1})(-)^{(n+j)}}(2H)^{(j+4)}e^{(F+H)^2}i^{j}erfc(F+H)$	
	1	$(\frac{D}{16})\frac{1}{H\sqrt{Dt^3}}e^{-F^2}\left[\frac{2}{\sqrt{\pi}}\left\{(2H)\mathcal{X}_2(F+H)-3(2H)^2\mathcal{X}_1(F+H)+3(2H)^3\mathcal{X}_0(F+H)\right\}-(2H)^4e^{(F+H)^2}e^{-f}c(F+H)\right]$	$\frac{1}{\sqrt{\pi D} \sqrt{t^3}} (F^2 - \frac{1}{2} - \frac{2FH}{2} + H^2) e^{F^2} - Dh^3 e^{(2FH+H^2)} erfc(F+H)$
	2	$(\frac{D}{16})\frac{1}{H^2Dt}e^{-F^2}\left[\frac{2}{\sqrt{\pi}}\left((2H)^2\mathcal{H}_1(F+H)-3(2H)^3\mathcal{H}_0(F+H)\right) + e^{(F+H)^2}\left(3(2H)^4crfc(F+H)-(2H)^5ierfc(F+H)\right)\right]$	

Table 2. Comparison between the present and the previous equations for $\exp(-qx)/q^m/(q+h)^n = \mathcal{L}[f(t)]$ at n=0

			
	present	, rearanged	previous [1,2,3]
m	$(-)^{m}D\sqrt{4Dt}^{m-2}e^{-F^{2}\left\{\prod\limits_{j=0}^{m-2}(Tn-j-3)\frac{(-)^{j}e^{F^{2}}i^{j}erfc(F)}{(2H)^{m-j-2}}-\frac{-1}{j-m^{2}}\frac{1-m}{(-j-1)}\frac{(-)^{j}e^{(F+H)^{2}}i^{j}erfc(F+H)}{(2H)^{m-j-2}}\right\}}$		D√4Dt ^{m-2} i ^{m-2} erfc(F)
4	$D(4Dt) e^{-F^2} \left(\binom{-1}{-1} e^{F^2} i^2 ertc(F) - 0 \right)$	= D(4Dt)i ² erfc(F)	$D^2t\left\{(1-2F^2)erfc(F)-\frac{2}{\sqrt{\pi}}Fe^{-F^2}\right\}$
3	$D\sqrt{4Dt} e^{-F^2} \left\{ \binom{-1}{-1} e^{F^2} i erfc(F) - 0 \right\}$	= D√4Dtierfc(F)	$D\sqrt{4Dt}\left\{\frac{1}{\sqrt{\pi}}e^{-F^2}-Ferfc(F)\right\}$
2	$De^{-F^2}\left\{ \left(\frac{-1}{-1} \right) e^{F^2} erfc(F) - 0 \right\}$	= Dertc(F)	Derfc(F)
1	$-\frac{D}{\sqrt{4Dt}}e^{-F^{2}}\left[0-\frac{2}{\sqrt{\pi}}\left(\binom{0}{0}\right)\mathcal{H}_{0}(F+H)\right]$	$= \frac{2}{\sqrt{\pi}} \frac{D}{\sqrt{4Dt}} e^{-F^2} \mathcal{H}_0(F)$	$\sqrt{\frac{D}{\pi t}} e^{-F^2}$
0	$\frac{D}{4Dt} e^{-F^{2}} \left[0 + \frac{2}{\sqrt{\pi}} \left\{ \binom{1}{1} \mathcal{N}_{i} (F+H) - \binom{1}{0} (2H) \mathcal{N}_{o} (F+H) \right\} \right]$	$= \frac{2}{\sqrt{\pi}} \frac{D}{\sqrt{4Dt}} {}_{2} e^{-F^{2}} \mathcal{L}_{1}(F)$	1 √75t Fe-F?
	$-\frac{D}{\sqrt{4Dt^3}}e^{-F^2}\left[0-\frac{2}{\sqrt{c}}\left\{\binom{2}{2}\right\}\mathcal{K}_2(F+H)-\binom{2}{1}(2H)\mathcal{K}_1(F+H)+\binom{2}{0}(2H)^2\mathcal{K}_0(F+H)\right]$		$\frac{1}{2\sqrt{\pi Ot^3}} (2F^2-1)e^{-F^2}$
-2	$\frac{D}{(4Dt)^2}e^{-F^2}[0+\frac{2}{\sqrt{\pi}}(\frac{1}{3})J\zeta_3(F+H)-(\frac{3}{2})(2H)J\zeta_2(F+H)+(\frac{3}{4})(2H)^2J\zeta_4(F+H)-(\frac{3}{6})(2H)^3J\zeta_6(F+H)$	$= \frac{2}{\sqrt{\pi}} \frac{D}{\sqrt{4Dt}} e^{-F^2} \mathcal{X}_3(F)$	$\frac{1}{2\sqrt{\pi}Dt^2}(2F^3-3F)e^{-F^2}$

relations for n = 0 and m = -1, -2, -3 and -4,

$$f(t) = \frac{D}{(4Dt)^{1/2}} \exp(-F^2) \left(\frac{2}{\sqrt{\pi}}\right) + 3hD \exp(-F^2)$$

$$\times \left[\exp(F^2)\operatorname{erfc}(F)\right] + 3h^2D(4Dt)^{1/2} \exp(-F^2)$$

$$\times \left[\exp(F^2)\operatorname{i}\operatorname{erfc}(F)\right] + h^3D(4Dt)\exp(-F^2)$$

$$\times \left[\exp(F^2)\operatorname{i}^2\operatorname{erfc}(F)\right]. \tag{17}$$

Meanwhile from a direct substitution of (m,n) = (4, -3) into equation (16), we can get the next equation,

$$f(t) = (-)^{4}D \frac{[(4Dt)^{1/2}]^{4-2}}{h^{-3}} \exp(-F^{2})$$

$$\times \left[\sum_{j=4-3-2}^{4-2} {4-3-j-3 \choose -4} (-)^{j} (2H)^{j-4+2} \right]$$

$$\times \exp(F^{2}) i^{j} \operatorname{erfc}(F) + \operatorname{empty}$$

$$= Dh^{3} (4Dt) \exp(-F^{2})$$

$$\times \left[-{1 \choose -4} (2H)^{-3} \exp(F^{2}) i^{-1} \operatorname{erfc}(F) \right]$$

$$+ {-2 \choose -4} (2H)^{-2} \exp(F^{2}) \operatorname{erfc}(F)$$

$$-{3 \choose -4} (2H)^{-1} \exp(F^{2}) i \operatorname{erfc}(F)$$

$$+{4 \choose -4} \exp(F^{2}) i^{2} \operatorname{erfc}(F)$$

$$+{4 \choose -4} \exp(F^{2}) i^{2} \operatorname{erfc}(F)$$

$$(18)$$

Here, the binomial coefficients with the limit value calculation are used as

$$-\begin{pmatrix} -1 \\ -4 \end{pmatrix} = 1, \quad \begin{pmatrix} -2 \\ -4 \end{pmatrix} = 3,$$
$$-\begin{pmatrix} -3 \\ -4 \end{pmatrix} = 3, \quad \begin{pmatrix} -4 \\ -4 \end{pmatrix} = 1.$$
 (19)

It is quite clear that equation (18) is just the same as equation (17). A combination of n and negative m does not make any difference in the final form between direct and indirect calculations.

One more example is with both negative m and n, values of -5 and -2, respectively. From equation (17) we have

$$\mathcal{L}[f(t)] = q^7 e^{-qx} - 2hq^6 e^{-qx} + h^2q^5 e^{-qx}$$
. (20)

This equation is constructed by a sum of m = -7, -6,-5 at n = 0. Therefore the original function for the above equation is shown by

$$f(t) = \frac{D i^{-9} \operatorname{erfc}(F)}{[(4Dt)^{1/2}]^9} + \frac{2hD i^{-8} \operatorname{erfc}(F)}{[(4Dt)^{1/2}]^8} + \frac{h^2D i^{-7} \operatorname{erfc}(F)}{[(4Dt)^{1/2}]^7}.$$
 (21)

On the other hand, we can get directly the next original

equation from equation (15),

$$f(t) = \frac{Dh^{2}}{[(4Dt)^{1/2}]^{7}} \exp(-F^{2})$$

$$\times \left\{ \begin{bmatrix} 2 \\ 2 \end{bmatrix} \frac{\exp(F^{2}) i^{-9} \operatorname{erfc}(F)}{(2H)^{2}} + \begin{pmatrix} 2 \\ 1 \end{pmatrix} \frac{\exp(F^{2}) i^{-8} \operatorname{erfc}(F)}{(2H)^{1}} + \begin{pmatrix} 2 \\ 0 \end{pmatrix} \frac{\exp(F^{2}) i^{-7} \operatorname{erfc}(F)}{(2H)^{0}} \right\} + \operatorname{empty}. \tag{22}$$

In the application of equation (15), the existence of the second series for another combined variable may be uncertain, but this is cleared by the empty sum rule. Although this empty is stressed by a term 'empty' in the latter equation, this is naturally zero. This example also shows the identity between the direct and indirect calculations.

Application to diffusion problems

Let us apply the derived equation (15) to boundary value problems for diffusion which have been discussed in rather complicated forms. Here the only procedure which should be carried out is the fractionization of subsidiary equations in terms of the fundamental image function.

Example (1). Suppose the initial solute concentration, C_{10} , in a well-stirred phase I of volume V. A solute is transferred from phase I to another phase, labelled II, where the initial solute concentration is zero and the diffusivity is D. It is supposed that the rate is controlled by diffusion in phase II, that there is no mechanical energy transfer between the phases, and that the flux at the interface is in proportion to the concentration difference between phases I and II, where the proportional coefficient is a constant K.

A set of boundary conditions can be written as

$$V\frac{dC_{I}}{dt} + AK(C_{I} - C_{II}) = 0$$

$$D\frac{\partial C_{II}}{\partial x} + K(C_{I} - C_{II}) = 0$$

$$\begin{cases} x = 0, t > 0. \end{cases}$$
(23)

With the usual Laplace transformation method, a subsidiary equation concerning phase II is given by

$$\bar{C}_{II} = \frac{hC_{I0}}{D} \frac{e^{-qx}}{(q^2 + hq + hh')q}$$
 (25)

where

$$\mathcal{L}(C_{II}) = \bar{C}_{II}, \quad q = (p/D)^{1/2},$$

 $h = K/D \quad \text{and} \quad h' = V/A.$

The denominator is rewritten into a simple quadratic form,

$$q^2 + hq + hh' = \left(q + \frac{h}{2}\right)^2 + \left(hh' - \frac{h^2}{4}\right).$$
 (26)

In order to make the form $\exp(-qx)q^{-m}(q+h)^{-n}$, the reciprocal of equation (26) is expanded into an infinite series,

$$\bar{C}_{II} = \frac{hC_{IO}}{D} \frac{e^{-qx}}{q \left[\left(q + \frac{h}{2} \right)^2 + \left(hh' - \frac{h^2}{4} \right) \right]}$$

$$= \frac{hC_{IO}}{D} \sum_{k=0}^{\infty} \frac{\left(\frac{h^2}{4} - hh' \right)^k e^{-qx}}{q \left(q + \frac{h}{2} \right)^{2k+2}}$$
(27)

or letting k start from 1,

$$\bar{C}_{II} = \frac{hC_{10}}{D} \sum_{k=0}^{\infty} \left(\frac{h^2}{4} - hh' \right)^{k-1} \frac{e^{-qx}}{q \left(q + \frac{h}{2} \right)^{2k}}.$$
 (28)

Since the images in the above equation are assigned for m, n and h to 1, 2k and h/2, respectively, the inverse relation is possible. Namely the concentration profile C_{II} can be expressed as

$$C_{II} = hC_{I0} \exp(-F^2) \sum_{k=1}^{\infty} \left(\frac{h^2}{4} - hh'\right)^{k-1} \left[(4Dt)^{1/2} \right]^{2k-1} \times \exp\left[\left(F + \frac{H}{2}\right)^2 \right] i^{2k-1} \operatorname{erfc}\left(F + \frac{H}{2}\right).$$
 (29)

or a slightly altered equation becomes a solution of the problem,

$$C_{II} = 2C_{I0} \frac{\exp(-F^2)}{(h - 4h')(Dt)^{1/2}} \sum_{k=1}^{\infty} (h^2 Dt - 4Dthh')^k \times \exp\left[\left(F + \frac{H}{2}\right)^2\right] i^{2k-1} \operatorname{erfc}\left(F + \frac{H}{2}\right). \quad (30)$$

This problem has been already solved elsewhere [1]. The previous analysis used a factorization of the quadratic form $q^2 + hq + hh'$ as

$$q^2 + hq + hh' = (q + \alpha)(q + \beta) \tag{31}$$

and partial fractionizations of $(q + \alpha)$ and $(q + \beta)$. This procedure gives the solution as

$$C_{II} = C_{I0} \frac{h}{\beta - \alpha} \left\{ \exp(\alpha x + \alpha^2 Dt) \operatorname{erfc} \left[F + \alpha (Dt)^{1/2} \right] - \exp(\beta x + \beta^2 Dt) \operatorname{erfc} \left[F + \beta (Dt)^{1/2} \right] \right\}.$$
(32)

Therefore the present and previous solutions must be identical in spite of the apparent differences between them.

Before giving the proof for this identity, let us compare the two equations. The earlier solution has a simple form but takes complex variables if the discriminant of equation (26) has a negative value. In that case error functions of complex variables are involved. This makes the analysis cumbersome in spite of the simple form. Meanwhile, the present result has more complication only in the characteristics of the systematic forms and the avoidance of complex variables. Both of these will facilitate the analysis.

Next, the identity for real α and β will be given.

Proof. Let us introduce an auxiliary function $g(\xi)\dagger$, where ξ is an arbitrary real variable,

$$g(\xi) = \exp\{ [\xi(Dt)^{1/2} + F]^2 \} \operatorname{erfc} [\xi(Dt)^{1/2} + F].$$
 (33)

Expanding as a Taylor series at $\xi = h/2$, we can get

$$g(\xi) = \sum_{k=0}^{\infty} \left[-(4Dt)^{1/2} \right]^k \exp\left\{ \left[\left(\frac{h}{2} \right) (Dt)^{1/2} + F \right]^2 \right\}$$

$$\times i^k \operatorname{erfc} \left[\left(\frac{h}{2} \right) (Dt)^{1/2} + F \right] \left[\xi - \left(\frac{h}{2} \right) \right]^k. \quad (34)$$

Because ξ is arbitrary, to make $g(\alpha)$ and $g(\beta)$, subtraction gives

$$g(\alpha) - g(\beta) = \sum_{k=0}^{\infty} \left[-(4Dt)^{1/2} \right]^k \exp\left\{ \left[\left(\frac{H}{2} \right) + F \right]^2 \right\}$$
$$i^k \operatorname{erfc} \left[\left(\frac{H}{2} \right) + F \right] \left\{ \left[\alpha - \left(\frac{h}{2} \right) \right]^k - \left[\beta - \left(\frac{h}{2} \right) \right]^k \right\}. \tag{35}$$

Furthermore, suppose that with $\alpha + \beta = h$, the last term in equation (35) is rearranged to give

$$\left\{ \left[\alpha - \left(\frac{h}{2} \right) \right]^k - \left[\beta - \left(\frac{h}{2} \right) \right]^k \right\} = \left(\frac{\alpha - \beta}{2} \right)^k - \left(\frac{\beta - \alpha}{2} \right)^k \tag{36}$$

where only odd k's determine the nonzero values $2[(\alpha-\beta)/2]^k$. Therefore renumbering for k, we have the following equation for $g(\alpha)-g(\beta)$:

$$g(\alpha) - g(\beta) = -2 \sum_{k=1}^{\infty} \left[(4Dt)^{1/2} \right]^{2k-1} \left(\frac{\alpha - \beta}{2} \right)^{2k-1} \times \exp\left[\left(\frac{H}{2} + F \right)^{2} \right] i^{2k-1} \operatorname{erfc}\left[\left(\frac{H}{2} \right) + F \right]. \quad (37)$$

Substituting equation (37) into equation (31) and rearranging for exponentials we arrive at

$$C_{\rm II} = C_{10} \frac{h}{(\alpha - \beta)^2 (Dt)^{1/2}} \exp(-F^2) \sum_{k=1}^{\infty} \left[(\alpha - \beta)(Dt)^{1/2} \right]^{2k}$$

$$\times \exp\left[F + \left(\frac{H}{2}\right)^2\right] i^{2k-1} \operatorname{erfc}\left[F + \left(\frac{H}{2}\right)\right].$$
 (38)

Now, remembering equations (26) and (27),

$$\alpha + \beta = h$$
, $\alpha \beta = hh'$,

and making use of the perfect-square form,

$$(\alpha - \beta)^2 = h^2 - 4hh'.$$

[†] This function or generally $\exp(x^2)i^n$ erfc(x) is more recommendable than i^n erfc(x) in analyses. When n is larger, i^n erfc(x) will take smaller values with poor precision. It may be dangerous to conclude at a glance that i^n erfc(x) with larger n is negligible because it often appears together with some multiplicating factor which includes the parameter n and which may have a significant value. From such points of view as the precision and the formalism, the auxiliary function g(x) will play an important role in various analyses. Some relationships of g(x) with i^n erfc(x) will be reported later.

Substitution of these into equation (38) gives equation (30). Thus the identity has been proved.

Example (2). Let us consider next a problem with a restricted region of x ($0 \le x \le 1$), where the initial concentration C_0 is constant. Suppose that a solute moves out through one of the boundaries, x = 1, to the other phase. The flux at x = 1 is in proportion to the concentration and there is no flux at x = 0.

A subsidiary equation in the restricted area is given by equation (39)

$$\frac{d^2\bar{C}}{dx^2} - q^2\bar{C} = -\frac{C_0}{D}, \quad (0 < x < l). \tag{39}$$

The boundary conditions are

$$\frac{\mathrm{d}\bar{C}}{\mathrm{d}x} = 0, \quad \text{at } x = 0,$$

$$\frac{d\bar{C}}{dx} + h\bar{C} = 0, \quad \text{at } x = l. \tag{41}$$

A solution for \bar{C} of equation (39) is

$$\bar{C} = \frac{C_0}{p} - \frac{hC_0}{D} \frac{\cosh(qx)}{q^2 [q \sinh(ql) + h \cosh(ql)]}.$$
 (42)

An inversion of C_0/p is straightforwardly C_0 , but the second term in the equation has a rather complicated form. This term can be simplified by changing hyperbolic functions into exponential functions, and reforming the equation into terms of the type $\exp(-qx)q^{-m}(q+h)^{-n}$. This gives

$$\frac{\cosh(qx)}{q \sinh(ql) + h \cosh(ql)} = \frac{e^{-q(l-x)} + e^{-q(l+x)}}{(q+h) - (q-h) e^{-2ql}},$$
 (43)

and taking a reciprocal of a denominator in equation (42) gives

$$\frac{1}{(q+h)-(q-h)e^{-2qI}} = \sum_{i=0}^{\infty} \frac{(q+h-2h)^{i} e^{-2qIJ}}{(q+h)^{j+1}}.$$
 (44)

Applying a binomial expansion to $(q+h-2h)^{j}$ gives

$$(q+h-2h)^{j} = \sum_{k=0}^{j} {j \choose k} (q+h)^{j-k} (-2h)^{j}.$$
 (45)

From equations (42)-(45), we get the image relation

$$\bar{C} = \frac{C_0}{p} - \frac{C_0 h}{D} \sum_{j=0}^{\infty} \sum_{k=0}^{j} {j \choose k} (-2h)^k \\
\times \left(\frac{e^{-q[(2j+1)l-x]}}{q^2 (q+h)^{k+1}} - \frac{e^{-q[(2j+1)l+x]}}{q^2 (q+h)^{k+1}} \right).$$
(46)

The inversion of the image function can also be written out as

$$C = C_0 - C_0 \sum_{j=0}^{\infty} \sum_{k=0}^{j} {j \choose k} (-2)^k$$

$$\times \left\{ \operatorname{erfc}(\xi_-) + \operatorname{erfc}(\xi_+) - \exp(-\xi_-^2) \sum_{r=0}^{k} (2H)^r \right\}$$

$$\times \exp\left[(\xi_- + H)^2 \right] i^r \operatorname{erfc}(\xi_- + H)$$

$$-\exp(-\xi_{+}^{2}) \sum_{r=0}^{k} (2H)^{r} \exp[(\xi_{+} + H)^{2}] i^{r}$$

$$\times \operatorname{erfc}(\xi_{+} + H) \bigg\} \bigg|_{\xi_{-\text{or}+} = \frac{(2j+1)l-x}{(4Dl)^{1/2}} \operatorname{or} \frac{(2j+1)l+x}{(4Dl)^{1/2}}}$$
(47)

Taking out a term for j = 0 corresponds to a known profile [1],

(39)
$$C = C_0 - C_0 \left\{ \operatorname{erfc} \left[\frac{l - x}{(4Dt)^{1/2}} \right] + \operatorname{erfc} \left[\frac{l + x}{(4Dt)^{1/2}} \right] - \exp\left[h(l - x) + h^2 Dt \right] \operatorname{erfc} \left[h(Dt)^{1/2} + \frac{l - x}{(4Dt)^{1/2}} \right] \right]$$

$$(40) \quad - \exp\left[h(l + x) + h^2 Dt \right] \operatorname{erfc} \left[h(Dt) + \frac{l + x}{4(Dt)^{1/2}} \right] + \dots \right\}.$$
(41)

CONCLUSION

When diffusion problems are analyzed by the Laplace transformation method, we meet frequently typical image functions in the form of

$$\exp(-qx)q^{-m}(q+h)^{-n}.$$

It has been usual for relations between these images and their original functions are tabulated or treated for every m and n. The present equation can cover the previous relations. In addition to this, two diffusion problems which are rather complicated are systematically illustrated with the generalized relation. As the examples show, the method which uses the decomposition of the subsidiary equations into polynomials of the type $\sum C_{mn} \exp(-qx)q^m(q+h)^n$ is not restricted to a single form but it may be possible to combine increased m and decreased n or vice versa. However this does not deny the uniqueness of the solution but apparent differences may be eliminated by some formulas for integrated error functions.

In order to evaluate numerically the analytical results computers will be required. Therefore, it will be necessary to estimate the effect of the relationships between arguments and integral orders in error functions on computing time, as well as the choice for polynomials.

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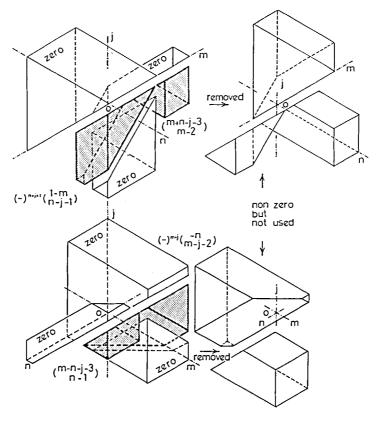


Fig. 2. Binomial coefficients $\binom{m+n-j-3}{m-2}$ and $\binom{m+n-j-3}{n-1}$. Shaded blocks are used in this treatment.

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APPENDIX

EXTENDED BINOMIAL COEFFICIENT FOR NEGATIVE ARGUMENTS TOGETHER WITH POSITIVE ONES

The standard binomial coefficient is defined as

$$\binom{r}{s} = \frac{r!}{s!(r-s)!}$$

where r, s and r-s are not negative integers. But here, let us extend r and s to be any integers which may be constructed with two or more integer variables in order to make a wider coefficient. We call this simply 'the coefficient', or the 'extended binomial coefficient'.

In order to calculate the coefficient, let us rewrite the factorial functions with the aid of gamma functions,

$$\binom{r}{s} = \frac{\Gamma(r+1)}{\Gamma(s+1)\Gamma(r-s+1)}.$$

Now, for coefficients with three gamma functions, it may be possible to classify them according to whether their arguments are positive, negative or zero,

(i)
$$r+1 \ge 1$$
, $s+1 \ge 1$, $r-s+1 \ge 1$
(ii) $r+1 \ge 1$, $s+1 \ge 1$, $r-s+1 < 1$

(iii)
$$r+1 \ge 1$$
, $s+1 < 1$, $r-s+1 \ge 1$
(iv) $r+1 \ge 1$, $s+1 < 1$, $r-s+1 < 1$
(v) $r+1 < 1$, $s+1 \ge 1$, $r-s+1 \ge 1$
(vi) $r+1 < 1$, $s+1 \ge 1$, $r-s+1 < 1$
(vii) $r+1 < 1$, $s+1 < 1$, $r-s+1 \ge 1$
(viii) $r+1 < 1$, $s+1 < 1$, $r-s+1 < 1$.

In the above classifications, (iv) and (v) are not possible because of the contradiction among the conditions. In addition, the coefficients in the cases (ii), (iii) and (viii) are zero, since a value in the denominator is infinite from the definition of the gamma function with non-positive integer arguments. The case (i) follows the usual manner. In the remaining cases, (vi) and (vii), two infinities, one in the numerator and the other in the denominator make the coefficients indefinite. But they may turn out to be definite with the limit value calculation by the aid of functional equations.

Therefore the coefficient can possess an original form and two other forms. The additional forms can be rewritten in a cyclic way with the two reversible equations (8) and (9).

Next, the variation of the two actual coefficients which appeared in the main description with the integer parameter set (j, m, n) is shown in Fig. 2, provided that the three parameters are all less than 5. In order to reduce the intricacy somewhat, the blocks which are formed with non-zero coefficients but not used because of the empty-sum rule, are removed from the cubes. The remainder contains three zero-valued blocks. In the numerical calculations, these may also be excluded. Concerning the final non-zeros, the coefficients with negative terms are rewritten as usual with the previous reversible formulas and the results are noted.

GENERALISATION ET APPLICATION DES FORMULES DE TRANSFORMATION DE LAPLACE POUR LA DIFFUSION

Résumé—On généralise la relation entre la fonction image du type $e^{-qx}q^{-m}(q+h)^{-n}$ et son original f(t). L'équation résultante est donnée pour tout couple (m,n) et quelques problèmes de diffusion sont analysés facilement et systématiquement. On donne de plus quelques natures caractéristiques reliées à la fonction d'erreur.

VERALLGEMEINERUNG UND ANWENDUNG VON LAPLACE-TRANSFORMATIONSGLEICHUNGEN AUF DIE DIFFUSION

Zusammenfassung—Die vorliegende Arbeit verallgemeinert die Beziehung zwischen Bildfunktionen, wie z. B. vom Typ $e^{-qx}q^{-m}(g+h)^{-n}$ und ihren Originalfunktionen f(t). Die sich ergebende Gleichung gilt für jedes ganzzahlige Paar (m,n) und eignet sich zur leichten und systematischen Lösung einiger Diffusionsprobleme. Zusätzlich wird auf einige charakteristische Umstände bezüglich Fehlerfunktionen hingewiesen.

ОБОБЩЕНИЕ И ПРИМЕНЕНИЕ ПРЕОБРАЗОВАНИЙ ЛАПЛАСА ДЛЯ ОПИСАНИЯ ДИФФУЗИИ

Аннотамия—Дано обобщенное соотношение, связывающее образы функции типа $e^{-qx}q^{-m}(q+h)^{-n}$ с их оригиналами f(t). Получены результаты для любой пары целых чисел (m,n), что позволяет легко и систематически анализировать некоторые задачи диффузии. Кроме того, рассмотрены некоторые свойства функций ошибок.