

On a Generating Function and its Probability Distributions. A Contribution to the Theory of Transition Rates I

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A function of two complex variables with two real parameters a and b is described, which generates a sequence of probability distributions of two integer variables $m \geq 0$ and $n \geq 0$. Closed expressions for the special $b = 0$ and general case $b \neq 0$ and recurrence equations for calculating the probability distributions are derived. The probability distribution for $m = 0$ and a large enough is qualitatively bell-shaped, and that for $m \neq 0$ has multiple peak structures. In both cases, the b parameter influences solely the skewness of the curves. For small a values, the distributions fall rapidly from a value of nearly one, decreasing by a factor of 10^{10} or more as n increases from zero to $n = 10$. The influence of the b parameter on their properties can be pronounced. Finally, we note an important property of the distributions when two or several of them are convoluted with one another. The result is expressed in terms of an addition theorem in respect to the parameter a and describes a multidimensional distribution.

Key words: Generating Function; Function of Two Complex Variables; Probability Distributions; Multidimensional Probability Distributions; Transition Probabilities.

1. Introduction

It is not surprising that the computation of quantities in the analysis of physical systems leads to probability distributions, which have no counterparts in the classical theory of probability. This fact has made it possible to develop a very general theory, from which a whole sequence of functions of this latter kind can be derived. The mathematical formulation of this concept is best carried out by constructing a generating function of the complexity of the system being studied (e. g. including all internal degrees of freedom and their corresponding parameters). Moreover, the generating function approach offers the advantage that some physical properties can be expressed in a simple mathematical form, i. e., in terms of addition theorems. The procedure discussed in this article has its origin in a publication of the present author et al. [1], in which the general quantum theoretical formalism for the analysis is given. In particular, in this paper a function of two complex variables z and w in a bidisc $D^1 = (z = 0, 1) \otimes D^1(w = 0, 1)$ is derived [2], which generates a sequence of integer-valued probability distributions $I_1(m, n; a, b)$, where m and n can take all integer values ≥ 0 . The derivation of the generating function and its probability distributions

marked one of the first systematic attempts to work out an accurate theory of electronic transitions (radiative and nonradiative) in molecules and condensed matter. This subject has been developed in subsequent papers [3, 4] to an arbitrary N -dimensional manifold of vibrational modes, however the published mathematical details do not completely realize the potential of the method. The present paper serves to partially fill this gap.

After representing first the generating function in its full form, we examine in the next section the behaviour of this function in the special (zero temperature) case $w = 0$ and show how the probability distribution is obtained by an infinite series expansion of this function. We shall represent the probability distribution in terms of a homogeneous form in a and b and of a given degree n , where a and b are two real parameters appearing in the generating function and n is an integer ≥ 0 . Furthermore, we shall discuss some important properties of this distribution in terms of an addition theorem in respect to the parameter a and introduce multidimensional distributions.

Likewise, we show in the next section how the analysis can again be generalized to deal with the finite temperature case (setting $w \neq 0$) and derive a sequence

of further probability distributions. We conclude this section by listing the principal aims of the method described for the special case, where the second parameter appearing in the generating function, for example b , becomes zero.

2. The Generating Function Approach

2.1. Derivation of $I_1(0, n; a, b)$

As mentioned in the Introduction, in the present and the next sections we use the generating function formalism introduced in [1] to study a whole class of integer-valued probability distributions. To give a convenient representation of the generating function (GF), from which the distributions are obtained, we write the latter in (1) as a product of two functions, which have many of the same structural features (see below):

$$G_1(w, z; a, b) = (1 - b^2)^{1/2} \frac{\exp \left[\frac{-a(1-z)}{1-bz} \right]}{[(1-bz)(1+bz)]^{1/2}} \cdot \frac{\exp \left[\frac{(1+b)a \left(\frac{1-z}{1-bz} \right)^2 w}{1 - \left(\frac{z-b}{1-bz} \right) w} \right]}{\left[\left(1 - \frac{z-b}{1-bz} w \right) \left(1 - \frac{z+b}{1+bz} w \right) \right]^{1/2}}. \quad (1)$$

Here z and w are complex variables in the bidisc $D^1(0, 1) \otimes D^1(0, 1)$, and a and b are real parameters within the intervals $a \geq 0$ and $-1 < b < 1$. [Physically, the parameter a is associated with the Franck-Condon displacement (or Stokes shift) between the electronic states under consideration and the parameter b with the frequency change of the vibrational mode when going from one electronic state to another.] By going to the time-dependent representation of $G_1(t)$, for example, while calculating the spectral band shapes of electronic [5–11] and nonradiative [12] transitions, the complex variables are defined by $z = e^{i\omega^{(l)}t}$ and $w = e^{-\alpha/T - i\omega^{(e)}t}$, where $\omega^{(l)}$ and $\omega^{(e)}$ are vibrational frequencies of a molecule (crystal) in the ground and excited electronic states, respectively, and which accompany the electronic transition. The factor $e^{-\alpha/T}$ in the variable w is the Boltzmann weighting factor. The subscript 1 of the function G_1 denotes 1st order or the one-dimensional case and is associated with the power

of the denominator of G_1 . The function in (1) is regular in the bidisc and its infinite series representation is

$$G_1(w, z; a, b) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} I_1(m, n; a, b) w^m z^n, \quad (2)$$

where $I_1(m, n; a, b)$ is, as will be shown, for each integer $m \geq 0$ an integer-valued probability distribution of n and vice versa. Hence $I_1 \geq 0$ and

$$\sum_{n=0}^{\infty} I_1(m, n; a, b) = 1 \quad \text{for } m = 0, 1, 2, 3, \dots \quad (3)$$

In order to prove this, we first consider the special case $w = 0$. Physically, this case corresponds to the limit of zero temperature, where only the lowest (vibrational) level $m = 0$ of the initial electronic state is occupied. For this case, (1) together with (2) can be written as

$$G_1(0, z; a, b) = (1 - b^2)^{1/2} \frac{\exp \left[\frac{-a(1-z)}{1-bz} \right]}{[(1-bz)(1+bz)]^{1/2}} = \sum_{n=0}^{\infty} I_1(0, n; a, b) z^n. \quad (4)$$

The function in the exponent of (4) constitutes a homographic transformation which maps the unit circle $|z| = 1$ in a circle lying in the left z -half plane and passes tangential to the point $z = 0$. Therefore G_1 is regular over the unit circle $D^1(0, 1)$ and univalent if $a/1 + b \leq \pi$. This situation is summarized in Figure 1a. The shaded region lies entirely within a ring $\exp \left[-\frac{2a}{1+b} \right] \leq |G_1(0, z; a, b)| \leq 1$. For larger values of a , the function $G_1(0, z; a, b)$ becomes polyvalent (see Fig. 1b). In general the mapping has a fix point, which is 1 at $z = 1$, $G_1(0, 1; a, b) = 1$, and where $\max_{z \in D^1(0, 1)} |G_1(0, z; a, b)| = G_1(0, 1; a, b) = 1$. A significant conclusion may be drawn by regarding Fig. 1, if we take $G_1 = U + iV$ and $z = \exp(i\theta)$, where $0 \leq \theta \leq 2\pi$. The real quantity $U(\theta)$ is then found to be even, $U(\theta) = U(2\pi - \theta) = U(-\theta)$, whereas the imaginary part $V(\theta)$ is an odd function of θ , $V(\theta) = -V(2\pi - \theta) = -V(-\theta)$. This symmetry property of G_1 accurately reflects corresponding properties of G_1 , which will be evident if G_1 is represented by its power series of z . On the other hand, it is easy to check that the coefficients on the right-hand series of (4) for $n \geq 1$ are given by $I_1(0, n; a, b) = \frac{2}{\pi} \int_0^\pi U(\theta) \cos n\theta d\theta$, which

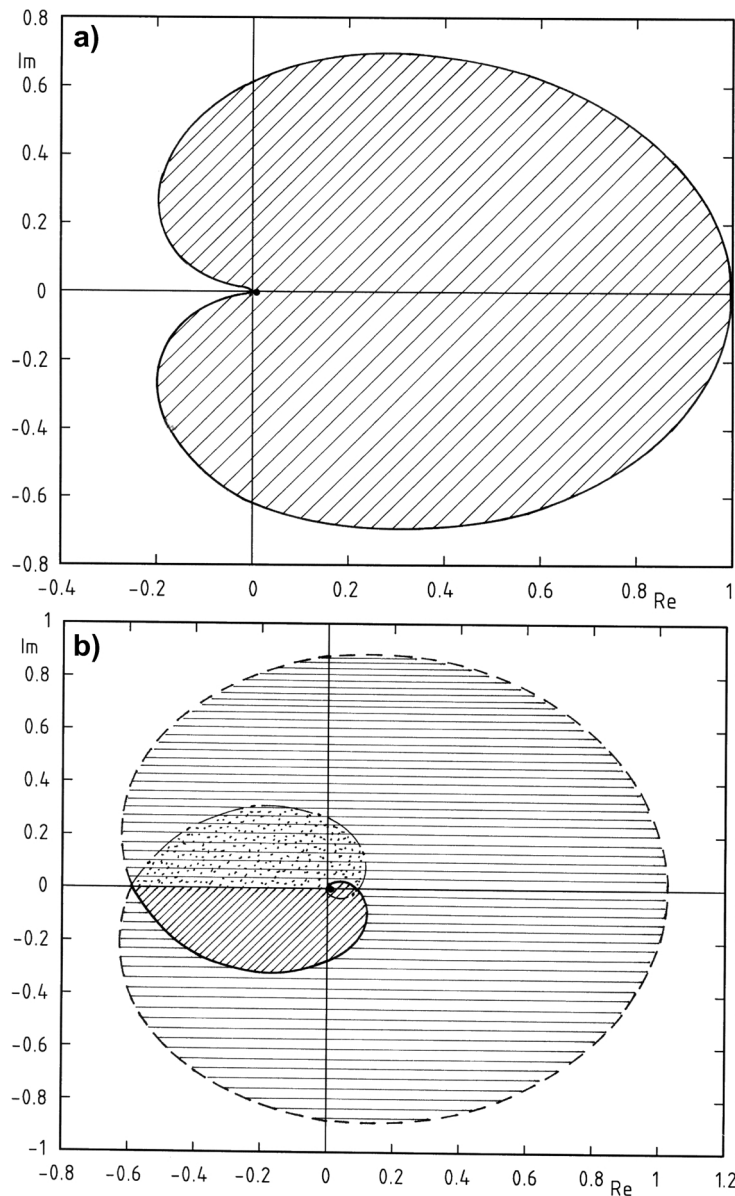


Fig. 1. (a) Analytic structure in the complex z -plane of $G_1(0, z; a, b)$ as given by (4) for $|z| \leq 1$, $a = 3.45$ and $b = 0.25$. (b) Same as (a), but now $a = 10$ and $b = 0.1$. The monovalent, divalent and trivalent areas of $G_1(0, z; a, b)$ are designated by different shadings. The closed region represented by the black dots in the center of the complex z -plane is avoided by $G_1(0, z; a, b)$.

are real and nonnegative numbers. To investigate this point more clearly, we expand the exponential term in (4) in a power series of z over the unit circle $D^1(0, 1)$:

$$\begin{aligned} \exp\left[\frac{-a(1-z)}{1-bz}\right] &= \exp(-a) \exp\left[\frac{-a(1-b)}{1-bz}z\right] \\ &= \exp(-a) \sum_{k=0}^{\infty} c_k z^k, \end{aligned} \quad (5)$$

where $c_0 = 1$ and

$$c_k = \sum_{i=1}^k k \frac{1}{i!} \binom{k-1}{i-1} a^i (1-b)^i b^{k-i}, \quad k \geq 1, \quad (6)$$

and representing the denominator of G_1 (or strictly, its regular branch of positive function value at $z = 0$) in terms of a binomial series. We now get the product of the two series. This gives, after rearranging and collecting terms of a^n ,

$$\begin{aligned}
I_1(0, n; a, b) &= (1 - b^2)^{1/2} \exp(-a) \\
&\cdot \left\{ (-1)^n b^n \sum_{i=0}^n (-1)^i \binom{-1/2}{n-i} \binom{-1/2}{i} + (-1)^{n-1} \frac{\bar{a}}{1!} b^{n-1} \sum_{i=1}^n (-1)^{i-1} \binom{-3/2}{n-i} \binom{-1/2}{n-1} \right. \\
&\quad + (-1)^{n-2} \frac{\bar{a}^2}{2!} b^{n-2} \sum_{i=2}^n (-1)^{i-2} \binom{-5/2}{n-i} \binom{-1/2}{i-2} + (-1)^{n-3} \frac{\bar{a}^3}{3!} b^{n-3} \sum_{i=3}^n (-1)^{i-3} \binom{-7/2}{n-i} \binom{-1/2}{i-3} \\
&\quad + \dots \\
&\quad \left. + (-1)^1 \frac{\bar{a}^{n-1}}{(n-1)!} b \sum_{i=n-1}^n (-1)^{i-n+1} \binom{-n+1/2}{n-i} \binom{-1/2}{i-n+1} + \frac{\bar{a}^n}{n!} \binom{-n-1/2}{0} \binom{-1/2}{0} \right\},
\end{aligned} \quad (7)$$

which satisfies the recurrence

$$\begin{aligned}
(n+1)I_1(0, n+1; a, b) &= (\bar{a} + nb)I_1(0, n; a, b) \\
&+ b(\bar{a} + nb)I_1(0, n-1; a, b) \\
&- (n-1)b^3I_1(0, n-2; a, b),
\end{aligned} \quad (8)$$

where $\bar{a} = a(1-b)$. Equation (8) represents a preferred method for calculating the values of $I_1(0, n; a, b)$, starting from the initial value $I_1(0, 0; a, b) = (1 - b^2)^{1/2} \exp(-a)$. The term in curly brackets in (7) is a square, so that $I_1(0, n; a, b)$ can be written as a square of a polynomial of

$$\begin{aligned}
I_1(0, n; a, b) &= (1 - b^2)^{1/2} \exp(-a) \frac{1}{n!} \\
&\cdot \left[\sum_{r=0}^{[n/2]} \frac{n!}{2^r (n-2r)! r!} b^r \bar{a}^{n/2-r} \right]^2.
\end{aligned} \quad (7a)$$

The right-hand series of (4) converges as $z \rightarrow 1$, hence by a simple substitution $z = 1$ it follows immediately that

$$\sum_{n=0}^{\infty} I_1(0, n; a, b) = 1. \quad (9)$$

The relation (9) of $I_1(0, n; a, b)$ can also be verified directly using (7).

2.2. The Addition Theorem

If $G_1(0, z; a_1, b)$ and $G_1(0, z; a_2, b)$ are generating functions described by (4), then the product

$$G_1(0, z; a_1, b) G_1(0, z; a_2, b) = G_2(0, z; a_1 + a_2, b)$$

is a generating function of the same kind, but of order (dimensionality) two. At the same time, as a con-

sequence of (4), we also have

$$\begin{aligned}
G_2(0, z; a_1 + a_2, b) &= \\
&= \left(\sum_{n_1=0}^{\infty} I_1(0, n_1; a_1, b) z^{n_1} \right) \left(\sum_{n_2=0}^{\infty} I_1(0, n_2; a_2, b) z^{n_2} \right) \\
&= \sum_{n=0}^{\infty} I_2(0, n; a_1 + a_2, b) z^n,
\end{aligned} \quad (10)$$

where the joined distribution of order two

$$\begin{aligned}
I_2(0, n; a_1 + a_2, b) &= \\
&= \sum_{n_1=0}^n I_1(0, n_1; a_1, b) I_1(0, n - n_1; a_2, b)
\end{aligned} \quad (11)$$

is obtained as a convolution of two probability distributions of dimensionality one. Equation (11) can also be proved directly from (7). Equation (11) expresses the so-called addition theorem in respect to the parameter a . The two-dimensional probability distribution on the left-hand side of (11) can simply be written as a convolution of one-dimensional probability distributions, the a -parameter of which is the sum $a = a_1 + a_2$. It must be emphasized that the one-dimensional distributions in (11) have the same b -parameter (for arguments). (This condition is given, for example, for components of a degenerate vibration.)

If we now define

$$\begin{aligned}
G_i(0, z; a, b) &= (1 - b^2)^{i/2} \frac{\exp \left[\frac{-a(1-z)}{1-bz} \right]}{[(1-bz)(1+bz)]^{i/2}} \\
&= \sum_{n=0}^{\infty} I_i(0, n; a, b) z^n,
\end{aligned} \quad (12)$$

where i is an arbitrary positive integer, the following addition theorem can be considered and calculated

similarly

$$\sum_{n_1=0}^n I_i(0, n_1; a_1, b) I_j(0, n - n_1; a_2, b) = I_{i+j}(0, n; a_1 + a_2, b). \quad (13)$$

Because of the convolution form of (13), it is obvious that the sum of $I_{i+j}(0, n; a, b)$ over n equals 1. As before, the distribution addition theorem (13) is obtained by summing the a parameters $a_1 + a_2 = a$ and by summing the orders $i + j$ to get the a parameter and the order of the convoluted distribution.

3. The Distributions $I_1(m, n; a, b)$

3.1. Derivation of $I_1(m, n; a, b)$

Having determined the probability distribution for $m = 0$, namely $I_1(0, n; a, b)$, we now proceed to the general case $m \neq 0$. For this purpose, the w -dependent factor of (1) may be expanded in power of w^m . This can be done by analogy to the expansion of $G_1(0, z; a, b)$, taking into account the following assignment:

$$z \rightarrow w, \quad a \rightarrow \frac{a(1-z)}{1-bz}, \quad b \rightarrow \left(\frac{z-b}{1-bz} \right). \quad (14)$$

Hence

$$1-b \rightarrow 1 - \left(\frac{z-b}{1-bz} \right) = (1+b) \left(\frac{1-z}{1-bz} \right), \quad (15)$$

and

$$\exp \left[\frac{a(1-b)}{1-bz} z \right] \rightarrow \exp \left[\frac{a(1+b) \left(\frac{1-z}{1-bz} \right)^2 w}{1 - \left(\frac{z-b}{1-bz} \right) w} \right] \quad (16)$$

or expanded

$$1 + \sum_{n=1}^{\infty} \left(\sum_{k=1}^n \frac{1}{k!} \binom{n-1}{k-1} a^k (1-b)^k b^{n-k} \right) z^n \rightarrow 1 + \sum_{m=1}^{\infty} A_m(z) w^m, \quad (17)$$

where

$$A_m(z) = \sum_{k=1}^m \frac{1}{k!} \binom{m-1}{k-1} a^k \cdot (1+b)^k \left(\frac{1-z}{1-bz} \right)^{2k} \left(\frac{z-b}{1-bz} \right)^{m-k}, \quad (18)$$

$m \geq 1$.

Note that by the assignment (14) the parameter a becomes complex in the z -plane, but with $\operatorname{Re} \frac{a(1-z)}{1-bz} \geq 0$, as it should be. Accordingly, $-1 \leq \operatorname{Re} \left(\frac{z-b}{1-bz} \right) \leq 1$ for $|z| \leq 1$, similar to $-1 < b < 1$.

Expanding the regular branch of

$$\left[\left(1 - \frac{z-b}{1-bz} w \right) \left(1 - \frac{z+b}{1+bz} w \right) \right]^{-1/2} = \sum_{n=0}^{\infty} B_n(z) w^n \quad (19)$$

in terms of binomial series, where

$$B_n(z) = (-1)^n \sum_{k=0}^n \binom{-1/2}{k} \binom{-1/2}{n-k} \cdot \left(\frac{z-b}{1-bz} \right)^k \left(\frac{z+b}{1+bz} \right)^{n-k}, \quad (20)$$

we now obtain the product

$$\begin{aligned} & \exp \left[\frac{(1+b)a \left(\frac{1-z}{1-bz} \right)^2 w}{1 - \left(\frac{z-b}{1-bz} \right) w} \right] \cdot \frac{1}{\left[\left(1 - \frac{z-b}{1-bz} w \right) \left(1 - \frac{z+b}{1+bz} w \right) \right]^{1/2}} \\ &= \left(1 + \sum_{n=1}^{\infty} A_n(z) w^n \right) \left(\sum_{n=0}^{\infty} B_n(z) w^n \right) \\ &= \sum_{m=0}^{\infty} C_1^{(m)}(z; a, b) w^m, \quad |w| < 1, \end{aligned} \quad (21)$$

where

$$C_1^{(m)}(z; a, b) = B_m(z) + \sum_{k=1}^m A_k(z) B_{m-k}(z), \quad (22)$$

or after substitution of (18) and (20) in (22) and after a somewhat lengthy derivation, we have

$$\begin{aligned}
C_1^{(m)}(z; a, b) &= (-1)^m \sum_{i=0}^m \binom{-1/2}{m-i} \binom{-1/2}{i} \left(\frac{z-b}{1-bz} \right)^{m-i} \left(\frac{z+b}{1+bz} \right)^i \\
&+ (-1)^{m-1} \frac{\hat{a}}{1!} \left(\frac{1-z}{1-bz} \right)^2 \sum_{i=1}^m \binom{-3/2}{m-i} \binom{-1/2}{i-1} \left(\frac{z-b}{1-bz} \right)^{m-i} \left(\frac{z+b}{1+bz} \right)^{i-1} \\
&+ (-1)^{m-2} \frac{\hat{a}^2}{2!} \left(\frac{1-z}{1-bz} \right)^4 \sum_{i=2}^m \binom{-5/2}{m-i} \binom{-1/2}{i-2} \left(\frac{z-b}{1-bz} \right)^{m-i} \left(\frac{z+b}{1+bz} \right)^{i-2} \\
&+ (-1)^{m-3} \frac{\hat{a}^3}{3!} \left(\frac{1-z}{1-bz} \right)^6 \sum_{i=3}^m \binom{-7/2}{m-i} \binom{-1/2}{i-3} \left(\frac{z-b}{1-bz} \right)^{m-i} \left(\frac{z+b}{1+bz} \right)^{i-3} \\
&+ \dots \dots \dots \\
&+ (-1)^1 \frac{\hat{a}^{m-1}}{(m-1)!} \left(\frac{1-z}{1-bz} \right)^{2m-2} \sum_{i=m-1}^m \binom{-m+1/2}{m-i} \binom{-1/2}{i-m+1} \left(\frac{z-b}{1-bz} \right)^{m-i} \left(\frac{z+b}{1+bz} \right)^{i-m+1} \\
&+ \binom{-m-1/2}{0} \binom{-1/2}{0} \frac{\hat{a}^m}{m!} \left(\frac{1-z}{1-bz} \right)^{2m}, \tag{23}
\end{aligned}$$

where $\hat{a} = a(1+b)$.

Substituting (4) and (21) in (1) and comparing terms of w^m in the two resulting series gives

$$\begin{aligned}
(1-b^2)^{1/2} \frac{\exp \left[\frac{-a(1-z)}{1-bz} \right]}{(1-b^2 z^2)^{1/2}} C_1^{(m)}(z; a, b) \\
= \sum_{n=0}^{\infty} I_1(m, n; a, b) z^n. \tag{24}
\end{aligned}$$

Using Leibnitz's formula for the n -th derivative of a product, we obtain

$$\begin{aligned}
I_1(m, n; a, b) &= \sum_{k=0}^n I_1(0, n-k; a, b) \\
&\cdot \left[\frac{1}{k!} \left(\frac{d}{dz} \right)^k C_1^{(m)}(0; a, b) \right], \tag{25}
\end{aligned}$$

where use has been made of (4). Note that (24) and (25) are valid for $m = 0$, since $C_1^{(0)}(z; a, b) = 1$. The left-hand side of (24) can be regarded for each integer $m \geq 0$ as a generating function of $I_1(m, n; a, b)$.

Summing both sides of (25) over n gives

$$\begin{aligned}
\sum_{n=0}^{\infty} I_1(m, n; a, b) \\
= \sum_{n=0}^{\infty} \left(\sum_{k=0}^n I_1(0, n-k; a, b) \frac{1}{k!} \left(\frac{d}{dz} \right)^k C_1^{(m)}(0; a, b) \right) \\
= \left(\sum_{n=0}^{\infty} I_1(0, n; a, b) \right) \left(\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n C_1^{(m)}(0; a, b) \right) \\
= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n C_1^{(m)}(0; a, b), \tag{26}
\end{aligned}$$

where we have used the fact that $I_1(0, n; a, b)$ satisfies (9). On the other hand, after simply substituting $z = 1$ in (23) and (24), the interpretation yields

$$\sum_{n=0}^{\infty} I_1(m, n; a, b) = C_1^{(m)}(1, a, b) = 1, \quad m \geq 0. \tag{27}$$

In view of the formulae (26) and (27), it is natural to expect simple relations among the developing coefficients of $C_1^{(m)}(z)$ appearing in the sum (26). To demon-

strate this, it suffices to note that the functions $C_1^{(m)}(z)$ appearing in (24) are not independent, but related by the following recurrence equation:

$$\begin{aligned} (m+1)C_1^{(m+1)}(z) &= \left[\hat{a} \left(\frac{1-z}{1-bz} \right)^2 + \left(2m + \frac{1}{2} \right) \left(\frac{z-b}{1-bz} \right) + \left(m + \frac{1}{2} \right) \left(\frac{z+b}{1+bz} \right) \right] C_1^{(m)}(z) \\ &- \left[\hat{a} \left(\frac{1-z}{1-bz} \right)^2 \left(\frac{z+b}{1+bz} \right) + \left(m - \frac{1}{2} \right) \left(\frac{z-b}{1-bz} \right)^2 + \left(2m - \frac{1}{2} \right) \left(\frac{z-b}{1-bz} \right) \left(\frac{z+b}{1+bz} \right) \right] C_1^{(m-1)}(z) \\ &+ (m-1) \left(\frac{z-b}{1-bz} \right)^2 \left(\frac{z+b}{1+bz} \right) C_1^{(m-2)}(z), \end{aligned} \quad (28)$$

or written, more compactly

$$\begin{aligned} (m+1)C_1^{(m+1)}(z) &= a_0^{(m)}(z; a, b)C_1^{(m)}(z) \\ &+ a_1^{(m)}(z; a, b)C_1^{(m-1)}(z) + a_2^{(m)}(z; b)C_1^{(m-2)}(z), \end{aligned} \quad (28a)$$

where we have now and throughout of the rest of this section assumed that $C_1^{(m)}(z) = C_1^{(m)}(z; a, b)$. Equation (28) is most often useful in the analysis of the functions $C_1^{(m)}(z)$ and in the determination of the distributions $I_1(m, n; a, b)$ (see below). Not only can the functions $C_1^{(m)}(z)$ and their derivatives be determined starting with the lowest one, specifically $C_1^{(0)}(z) = 1$,

but one can also obtain other quantities of interest from them. Essential formulae are the equations (A.4) to (A.6) of the Appendix, wherein the derivatives of $a_i^{(m)}(z)$ ($i = 0, 1, 2$) at $z = 0$ are also given.

Proof of consistency. We have to verify that the sum on the right-hand side of (26) is 1. Applying (28) for $m = 0$ and referring to (A.4) of Appendix, we have

$$\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n C_1^{(1)}(0) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n a_0^{(0)}(0) = 1.$$

Assuming that the same sum rule is valid for $C_1^{(m)}(z)$, by applying (28) repeatedly for $m+1$, we deduce, with use of (A.4) to (A.6) of the Appendix,

$$\begin{aligned} (m+1) \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n C_1^{(m+1)}(0) &= \sum_{i=0}^2 \left(\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n a_i^{(m)}(0) \right) \left(\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n C_1^{(m-i)}(0) \right) \\ &= \sum_{i=0}^2 \left(\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n a_i^{(m)}(0) \right) = (3m+1) - (3m-1) + (m-1) = m+1. \end{aligned}$$

Hence

$$\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n C_1^{(m+1)}(0) = 1 \quad (29)$$

is thus implicitly applicable for all values of m . This completes the proof of consistency. Equation (26) agrees demonstrably with (27).

Corollary. Comparing (7) with (23), we have the following relation:

$$\begin{aligned} I_1(0, n; a, b) &= (1-b^2)^{1/2} \exp(-a) C_1^{(n)}(0; a, -b) \\ &= I_1(n, 0; a, -b). \end{aligned} \quad (30)$$

It may be shown that the general symmetry property

$$I_1(m, n; a, b) = I_1(n, m; a, -b) \quad (31)$$

holds. This follows immediately from the symmetry property of $G_1(w, z; a, b) = G_1(z, w; a, -b)$.

3.2. The Addition Theorem for $I_1(m, n; a, b)$

For completeness we finally use (1) and (2) to derive the addition theorem for $I_1(m, n; a, b)$. In close analogy to the case $m = 0$, we have now

$$G_1(w, z; a_1, b) G_1(w, z; a_2, b) = G_2(w, z; a_1 + a_2, b) \quad (32)$$

and

$$\begin{aligned} &G_2(w, z; a_1 + a_2, b) \\ &= \left(\sum_{m_1=0}^{\infty} \sum_{n_1=0}^{\infty} I_1(m_1, n_1; a_1, b) w^{m_1} z^{n_1} \right) \end{aligned}$$

$$\cdot \left(\sum_{m_2=0}^{\infty} \sum_{n_2=0}^{\infty} I_1(m_2, n_2; a_2, b) w^{m_2} z^{n_2} \right) \quad (33)$$

$$= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} I_2(m, n; a_1 + a_2, b) w^m z^n,$$

where

$$I_2(m, n; a_1 + a_2, b) = \sum_{m_1+m_2=m} \sum_{n_1+n_2=n} I_1(m_1, n_1; a_1, b) I_1(m_2, n_2; a_2, b) \quad (34)$$

is again the convolution $I_1 \otimes I_1$. As before, the parameters a_1 and a_2 and the orders or dimensionalities of the distributions on the right-hand side are summed to give the a parameter and order of the convoluted distribution. The successive application of (34) gives

$$I_N = I_1 \otimes I_1 \otimes \dots \otimes I_1. \quad (35)$$

They have the norm

$$\sum_{n=0}^{\infty} I_N(m, n; \sum_{k=1}^N a_k, b) = \binom{N+m-1}{m}. \quad (36)$$

3.3. The Recurrence Formula

As already mentioned, the optimum strategy for finding quickly the values of $I_1(0, n; a, b)$ is given by applying the recurrence (8). The same pertains to the distribution $I_1(m, n; a, b)$. The corresponding recurrence may be derived by making use of (25) and (28). Indeed, starting from the relation (28a), we first determine the n -th derivative of $C_1^{(m+1)}(z)$ for $z = 0$:

$$(m+1) \left(\frac{d}{dz} \right)^n C_1^{(m+1)}(0)/n! = \sum_{i=0}^2 \left(\sum_{k=0}^n \left(\frac{d}{dz} \right)^k a_i^{(m)}(0) \left(\frac{d}{dz} \right)^{n-k} C_1^{(m-i)}(0)/k!(n-k)! \right) \quad (37)$$

and substitute this result in (25). After collecting terms

containing the same factor $\left(\frac{d}{dz} \right)^k a_i^{(m)}(0)/k!$, this yields

$$(m+1)I_1(m+1, n) = a_0^{(m)}(0)I_1(m, n) + \left(\frac{d}{dz} \right) a_0^{(m)}(0)I_1(m, n-1) + \frac{1}{2!} \left(\frac{d}{dz} \right)^2 a_0^{(m)}(0)I_1(m, n-2) + \dots + \frac{1}{n!} \left(\frac{d}{dz} \right)^n a_0^{(m)}(0)I_1(m, 0) + a_1^{(m)}(0)I_1(m-1, n) + \left(\frac{d}{dz} \right) a_1^{(m)}(0)I_1(m-1, n-1) + \frac{1}{2!} \left(\frac{d}{dz} \right)^2 a_1^{(m)}(0)I_1(m-1, n-2) + \dots + \frac{1}{n!} \left(\frac{d}{dz} \right)^n a_1^{(m)}(0)I_1(m-1, 0) + a_2^{(m)}(0)I_1(m-2, n) + \left(\frac{d}{dz} \right) a_2^{(m)}(0)I_1(m-2, n-1) + \frac{1}{2!} \left(\frac{d}{dz} \right)^2 a_2^{(m)}(0)I_1(m-2, n-2) + \dots + \frac{1}{n!} \left(\frac{d}{dz} \right)^n a_2^{(m)}(0)I_1(m-2, 0), \quad (38)$$

where we have assumed $I_1(m, n; a, b) = I_1(m, n)$. The coefficients $\left(\frac{d}{dz} \right)^k a_i^{(m)}(0)/k! (i = 0, 1, 2)$ are given explicitly in the Appendix. Equation (38) enables us to determine $I_1(m, n)$ completely for all values m and n , provided that the values of $I_1(0, n)$ are already available.

3.4. Case $b = 0$

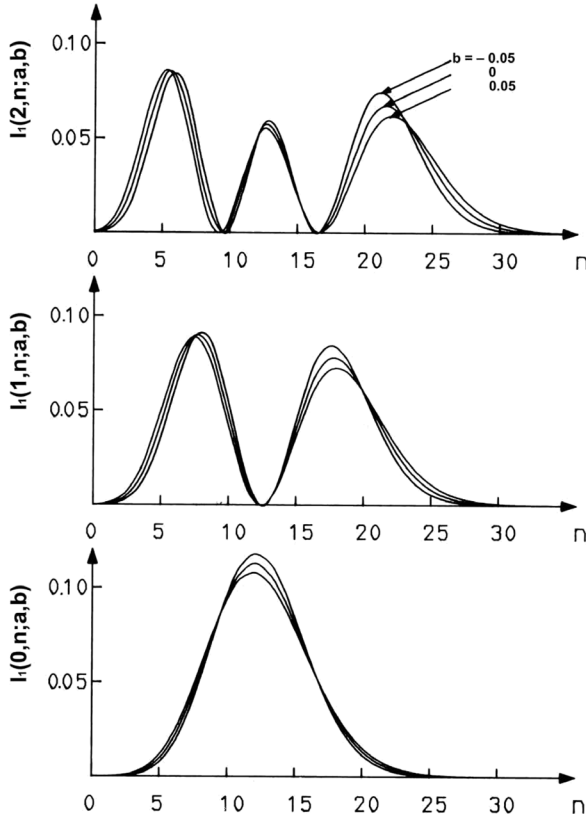
When $b = 0$, a special case of the formulae of the preceding section exists. In this case, the problem simplifies considerably, since

$$I_1(0, n; a, 0) = \exp(-a) \frac{a^n}{n!} \quad (39)$$

reduces to the Poisson distribution of probability theory with mean a . In comparison with the latter, $I_1(0, n; a, b)$ gives skew line shapes, with a skewness to lower n or to higher n values, depending on whether $b < 0$ or $b > 0$ (see Fig. 2). We can now use the exact

Table 1. The derivatives of $C_1^{(m)}(z; a, 0)$ for $m = 0, 1, 2, 3$ at $z = 0$.

m	$n = 0$	$n = 1$	$n = 2$	$\frac{1}{n!} \left(\frac{d}{dz} \right)^n C_1^{(m)}(0; a, 0)$ $n = 3$	$n = 4$	$n = 5$	$n = 6$
$C_1^{(0)}$	$(0) = 1$						
1	$a,$	$-2a + 1,$	a				
2	$\frac{a^2}{2!},$	$-2a^2 + 2a,$	$3a^2 - 4a + 1,$	$-2a^2 + 2a$	$\frac{a^2}{2!}$		
3	$\frac{a^3}{3!},$	$-a^3 + \frac{3}{2}a^2,$	$\frac{5}{2}a^3 - 6a^2 + 3a,$	$-\frac{10}{3}a^3 + 9a^2 - 6a + 1,$	$\frac{5}{2}a^3 - 6a^2 + 3a,$	$-a^3 + \frac{3}{2}a^2,$	$\frac{a^3}{3!}$

Fig. 2. The probability distributions $I_1(m, n; a, b)$ for the lowest m -levels ($m = 0, 1, 2$) and a value of $a = 12.5$. Shown is the weak b -dependence.

expression (23), but for $b = 0$:

$$C_1^{(m)}(z; a, 0) = z^m + \binom{m}{1} \frac{a}{1!} (1-z)^2 z^{m-1} + \binom{m}{2} \frac{a^2}{2!} (1-z)^4 z^{m-2} + \dots + \binom{m}{m} \frac{a^m}{m!} (1-z)^{2m}, \quad (40)$$

where use has been made of the fact that $\binom{-x}{k} = (-1)^k \binom{x+k-1}{k}$ for $x > 0$. Differentiating with respect

to z and substituting $z = 0$, we have

$$\begin{aligned} \frac{1}{n!} \left(\frac{d}{dz} \right)^n C_1^{(m)}(0; a, 0) = & (-1)^{n-m+1} \binom{2}{n-m+1} \binom{m}{1} \frac{a}{1!} \\ & + (-1)^{n-m+2} \binom{4}{n-m+2} \binom{m}{2} \frac{a^2}{2!} + \dots \quad (41) \\ & + (-1)^{n-1} \binom{2m-2}{n-1} \binom{m}{m-1} \frac{a^{m-1}}{(m-1)!} \\ & + (-1)^n \binom{2m}{n} \binom{m}{m} \frac{a^m}{m!} + \delta_{mn}, \end{aligned}$$

where δ_{mn} is the Kronecker delta.

Table 1 presents the derivatives $\frac{1}{n!} \left(\frac{d}{dz} \right)^n C_1^{(m)}(0; a, 0)$ for several of the values of m in terms of polynomials of a . It may be seen that they are now symmetrically distributed with respect to $n = m$ [where n denotes the n -th derivative of $C_1^{(m)}(z; a, 0)$] and the sum along each row equals 1, as (29) clearly shows. Moreover the number of the derivatives of $C_1^{(m)}(z; a, 0)$ for each m is finite. Substitution of (39) and (41) into (25) leads after rearrangement to

$$I_1(m, n; a, 0) = \exp(-a) \left(\frac{n!}{m!} a^{m-n} \right) [L_n^{m-n}(a)]^2, \quad (42)$$

where

$$L_n^\alpha(a) = \sum_{l=0}^n \frac{\Gamma(\alpha + n + 1)}{\Gamma(\alpha + l + 1)} \frac{(-a)^l}{l!(n-l)!}, \quad \alpha > -1 \quad (43)$$

is the Laguerre polynomial. In expression (42) it is assumed that $m \geq n$. If $n > m$, then simply exchange m and n .

3.5. Case $b \neq 0$

As with the result (42), an explicit representation of $I_1(m, n; a, b)$ is obtained from (38) for the general

case $b \neq 0$. The result is

$$I_1(m, n; a, b) = (1 - b^2)^{1/2} \exp(-a) \frac{m!n!}{2^{m+n}} \cdot \left[\sum_{i=0}^{\lfloor m/2 \rfloor} \sum_{r=0}^{\lfloor n/2 \rfloor} \frac{(-1)^i b^{i+r}}{(m-2i)!i!(n-2r)!r!} (n-2r)! \right. \\ \left. \cdot A^{m-n-2(i-r)} C^{n-2r} L_{n-2r}^{m-n-2(i-r)}(a) \right]^2, \quad (44)$$

where

$$\begin{aligned} A &= [2a(1+b)]^{1/2} = (2\hat{a})^{1/2}, \\ B &= -[2a(1-b)]^{1/2} = -(2\bar{a})^{1/2}, \\ C &= 2[(1-b)(1+b)]^{1/2}, \end{aligned} \quad (45)$$

and $L_{n-2r}^{m-n-2(i-r)}(a)$ are again Laguerre polynomials. As before, in the deriving expression (44) it is assumed that $m \geq n$ and $m-2i \geq n-2r$ (there is a case in which one can have $m-2i < n-2r$ for one or finitely limited values of i). In this case replace the corresponding factor (or factors)

$$\begin{aligned} (*) \quad & (n-2r)! A^{m-n-2(i-r)} C^{n-2r} L_{n-2r}^{m-n-2(i-r)}(a) \quad \text{by} \\ & (m-2i)! B^{n-m-2(i-r)} C^{m-2i} L_{m-2i}^{n-m-2(i-r)}(a). \end{aligned}$$

Analogously, if $m < n$,

$$I_1(m, n; a, b) = (1 - b^2)^{1/2} \exp(-a) \frac{m!n!}{2^{m+n}} \cdot \left[\sum_{i=0}^{\lfloor m/2 \rfloor} \sum_{r=0}^{\lfloor n/2 \rfloor} \frac{(-1)^i b^{i+r}}{(m-2i)!i!(n-2r)!r!} (m-2i)! \right. \\ \left. \cdot B^{n-m-2(r-i)} C^{m-2i} L_{m-2i}^{n-m-2(r-i)}(a) \right]^2, \quad (44a)$$

provided $n-2r \geq m-2i$ holds for all nonnegative integers i and r . Otherwise, perform an exchange of the appropriate factors appearing in (44a) according to (*), but in the reverse order. The term within the square bracket in (44) is a polynomial in a , the coefficients of which are polynomials of b . We have thus shown that each member of the sequence of $I_1(m, n; a, b)$ for different integers m is a square of a polynomial multiplied by a positive factor $(1 - b^2)^{1/2} \exp(-a) \left(\frac{m!n!}{2^{m+n}} \right)$. As mentioned earlier, the result (44) contains (42) as a special case when $b = 0$. The properties (27) and (44) are satisfactory features of definition of $I_1(m, n; a, b)$.

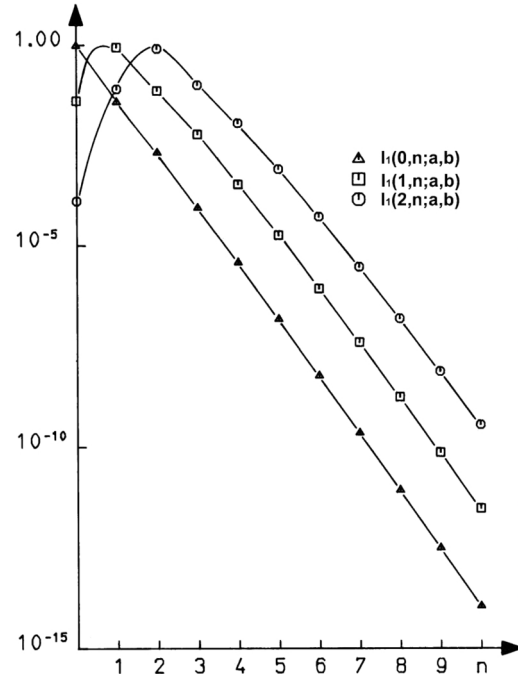


Fig. 3. Same as Fig. 2, but for $a = 0.045$ and $b = 0.025$.

3.6. Numerical Results

Finally, we illustrate in Figs. 2 and 3 the role of the parameters a and b on the distribution $I_1(m, n; a, b)$ for several of the (lowest) levels of m ($m = 0, 1, 2$). At values of $a > 1$ and $m \geq 0$, the distributions $I_1(m, n; a, b)$ have a multiple peak structure and the b dependence is very slight. The b parameter solely influences the skewness of the curves. The situation is quite different when a is small, i.e., $a \leq 1$. The distribution $I_1(m, n; a, b)$ now falls rapidly from a value of nearly one, decreasing by a factor of 10^{10} or more as n increases from zero to $n = 10$. What is remarkable, however, is that the distribution $I_1(m, n; a, b)$ increases by several orders of magnitude when the parameter b deviates from zero by only a value of 0.1 (frequency effect).

Appendix.

The Derivatives of $a_0^{(m)}(z)$, $a_1^{(m)}(z)$ and $a_2^{(m)}(z)$

Expanding the homographic functions appearing in (28) in power series of z , differentiating the expression of $a_0^{(m)}(z)$ in respect to z and substituting finally $z = 0$, we have for $m \geq 0$:

$$\frac{1}{n!} \left(\frac{d}{dz} \right)^n a_0^{(m)}(0) = \begin{cases} \hat{a} - mb, & n = 0, \\ \hat{a} [(n+1)b^n - 2nb^{n-1} + (n-1)b^{n-2}] + (1-b^2) [(2m+1/2)b^{n-1} + (m+1/2)(-1)^{n-1}b^{n-1}], & n \geq 1. \end{cases} \quad (\text{A.1})$$

Similarly for $m \geq 1$:

$$\frac{1}{n!} \left(\frac{d}{dz} \right)^n a_1^{(m)}(0) = \begin{cases} -\hat{a}b + mb^2, & n = 0, \\ -\hat{a} \left(nb^{n-1} - 2b^{n-2} \left\{ \frac{n/2}{(n-1)/2} + b^{n-3} \left\{ \frac{(n-2)/2}{(n-1)/2} + b^{n+1} \left\{ \frac{(n+2)/2}{(n+1)/2} - 2b^n \left\{ \frac{n/2}{(n+1)/2} \right\} \right\} \right\} \right. \\ \left. - (2m-1/2) \begin{cases} b^{n-2} - b^{n+2}, & n - \text{even} \\ 0, & n - \text{odd} \end{cases} - (m-1/2)[(n-1)b^{n-2} - 2nb^n + (n+1)b^{n+2}] \right), & n \geq 1 \end{cases} \quad (\text{A.2})$$

and

$$\frac{1}{n!} \left(\frac{d}{dz} \right)^n a_2^{(m)}(0) = \begin{cases} (m-1)b^3, & n = 0, \\ (m-1) \left(b^{n-3} \left\{ \frac{(n-2)/2}{(n-1)/2} - b^{n-1} \left\{ \frac{n/2}{(n-1)/2} - b^{n+1} \left\{ \frac{n/2}{(n+1)/2} \right\} \right\} \right. \right. \\ \left. \left. + b^{n+3} \left\{ \frac{(n+2)/2, n - \text{even}}{(n+1)/2, n - \text{odd}} \right\} \right) \right). \end{cases} \quad (\text{A.3})$$

We can now use these results to evaluate the sum

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n a_0^{(m)}(0) &= -mb + \hat{a} \sum_{n=0}^{\infty} [(n+1)b^n - 2nb^{n-1}] + \hat{a} \sum_{n=1}^{\infty} (n-1)b^{n-2} \\ &\quad + (1-b^2) \left[\left(2m + \frac{1}{2} \right) \sum_{n=0}^{\infty} b^n + \left(m + \frac{1}{2} \right) \sum_{n=0}^{\infty} (-1)^n b^n \right] \\ &= -mb + \left[\left(2m + \frac{1}{2} \right) (1+b) + \left(m + \frac{1}{2} \right) (1-b) \right] \\ &= -mb + [(3m+1) + mb] \\ &= 3m+1. \end{aligned} \quad (\text{A.4})$$

Analogously:

$$\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n a_1^{(m)}(0) = -(3m-1) \quad (\text{A.5})$$

and

$$\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dz} \right)^n a_2^{(m)}(0) = m-1. \quad (\text{A.6})$$

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