

PROGRAMS FOR THE LANDAU AND THE VAVILOV DISTRIBUTIONS AND THE CORRESPONDING RANDOM NUMBERS

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PROGRAM SUMMARY

Title of program: LANDAU

Catalogue number: AAUI

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: CDC 6600; *Installation:* CERN, Geneva

Operating system: CDC Scope

Programming language used: FORTRAN IV

High speed storage required: 1114 words

No. of bits in a word: 60

Overlay structure: None

No. of magnetic tapes required: None

Other peripherals used: Card reader, line printer

No. of cards in combined program and test deck: 300

Card punching code: BCD

Keywords: Nuclear, Landau distribution, energy loss, thin absorber, random number generation.

PROGRAM SUMMARY

Title of program: VAVILOV

Catalogue number: AAUI

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: CDC 6600; *Installation:* CERN, Geneva

Operating system: CDC Scope

Programming language used: FORTRAN IV

High speed storage required: 3246 words

No. of bits in a word: 60

Overlay structure: None

No. of magnetic tapes required: None

Other peripherals used: Card reader, pine printer

No. of cards in combined program and test deck: 636

Card punching code: BCD

Keywords: Nuclear, Vavilov distribution, energy loss, thin absorber, random number generation.

Nature of the physical problem

The Landau [1] and the Vavilov [2] distributions are used to describe the energy loss of charged particles traversing a thin layer of matter. For Monte Carlo simulations it is of particular interest to have a random number generator for these distributions.

Method of solution

Fourier series are used to approximate the probability density functions, the cumulative distribution functions and the inverses of the conditional distribution functions.

Restrictions on the complexity of the problem

Theoretical considerations, together with numerical tests, show that in the case of the densities and the distribution functions three to five significant digits are obtained. In the case of the inverses of the conditional distribution functions three significant figures are obtained almost everywhere, except near the end points of the interval, where a relative error of up to 5–6% may occur.

Typical running time

Running times in msec on CDC 6600 for the Landau distribution.

| | |
|--------------|------|
| DISLAN(X, 0) | 2.75 |
| DISLAN(X, 1) | 2.42 |
| DINLAN(X) | 1.99 |

References

- [1] L. Landau, J. Phys. 8 (1944) 201–205.
 [2] P.V. Vavilov, Zh. Exper. Teor. Fiz. 32 (1957) 920–923
 [English transl. JETP 5 (1957) 749–751].

Running times in msec on CDC 6600 for the Vavilov distribution.

| | $\kappa=0.01,$ $\beta^2=0.5$ | $\kappa=4.0,$ $\beta^2=0.5$ | $\kappa=10.0,$ $\beta^2=0.5$ |
|------------------------|---------------------------------|--------------------------------|---------------------------------|
| COEDIS(RKA, BE2, 0, J) | 78.0 | 12.0 | 12.0 |
| COEDIS(RKA, BE2, 1, J) | 81.0 | 12.0 | 13.0 |
| COEDIN(RKA, BE2, J) | 9957.0 | 7911.0 | 7838.0 |
| DISVAV(X, 0) | 0.21 | 0.024 | 0.023 |
| DISVAV(X, 1) | 0.21 | 0.022 | 0.022 |
| DINVAV(X) | 1.56 | 1.54 | 1.55 |

LONG WRITE-UP

1. Introduction

The Landau distribution and its generalization, the Vavilov distribution, are often used to describe the energy loss of charged particles traversing a thin layer of matter. The Laplace transform of the probability density function of the Landau distribution was found by Landau [1] to describe the energy loss of fast particles which have traversed a layer of matter of a given thickness, the corresponding probability density of Λ is given by

$$f_0(\lambda) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{s\ln s + \lambda s} ds, \quad (1.1)$$

where c is an arbitrary real positive constant. This function was tabulated by Börsch-Supan [2] in 1961 for $-4 \leq \lambda \leq 100$.

A generalization of the Landau distribution was given by Vavilov [3] in 1956. This distribution takes into account the maximum allowed energy transfer in a single collision of a particle with an atomic electron. Again, if Λ is the random variable introduced by Landau, the corresponding probability density function of the Vavilov distribution is given by

$$f(\lambda) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \phi(s) e^{\lambda s} ds, \quad (1.2)$$

where

$$\phi(s) = C \exp[\psi(s)], \quad (1.3)$$

$$C = \exp[\kappa(1 + \beta^2\gamma)], \quad (1.4)$$

$$\psi(s) = s \ln \kappa + (s + \beta^2\kappa)$$

$$\times \left(\int_0^1 \frac{1 - \exp(-st/\kappa)}{t} dt - \gamma \right) - \kappa e^{-s/\kappa}, \quad (1.5)$$

$$\gamma = 0.5772 \dots \text{ (Euler's constant)}, \quad (1.6)$$

and c is an arbitrary real constant. The parameters κ and β^2 with

$$\kappa > 0, \quad 0 \leq \beta^2 \leq 1, \quad (1.7)$$

have the following meaning. κ is proportional to the ratio of the mean energy loss over the path length of the particles to the largest energy transfer possible in a single collision with an atomic electron. The parameter β^2 is given by

$$\beta^2 = v^2/c^2, \quad (1.8)$$

where v is the velocity of the particle and c the speed of light.

It can be proved that $f(\lambda)$ converges to $f_0(\lambda)$ as $\kappa \rightarrow 0$. In [3] it is shown that for $\kappa \leq 0.01$ the Vavilov distribution may be replaced by the Landau distribution. Seltzer and Berger [4] have tabulated the function $f(\lambda)$ for $\kappa = 0.01, 0.04, 0.07, 0.1, 0.4, 0.7, 1.0, 4.0, 7.0, 10.0$ and $\beta^2 = 0.0 (0.1) 1.0$. In addition they have demonstrated that for $\kappa \geq 10.0$ the Vavilov distribution may be replaced by a gaussian distribution with mean value

$$\mu = \gamma - 1 - \beta^2 - \ln \kappa \quad (1.9)$$

and variance

$$\sigma^2 = (2 - \beta^2)/2\kappa. \quad (1.10)$$

We shall therefore consider only the cases where

$$0.01 \leq \kappa \leq 10.0, \quad 0 \leq \beta^2 \leq 1. \quad (1.11)$$

The computer programs described in this paper provide physicists with a means to calculate in a fast way the probability density functions $f_0(\lambda)$ and $f(\lambda)$, the cumulative distribution functions

$$F_0(\lambda) = \int_{-\infty}^{\lambda} f_0(\xi) d\xi, \quad (1.12)$$

$$F(\lambda) = \int_{-\infty}^{\lambda} f(\xi) d\xi, \quad (1.13)$$

and the inverse functions of F_0 and F which are used for the generation of random numbers according to the Landau and the Vavilov distributions.

In all of these programs the main emphasis was put on speed of calculation; consequently the precision of the calculated function values, though sufficient for practical purposes, is not very great. The numerical methods which are applied can, in principle, also be used to obtain a higher precision by just changing some parameters as can be seen later.

2. Method of computation

The functions $f_0(\lambda)$ and $f(\lambda)$ are continuous, and have only one maximum, in the neighbourhood of zero, as can be seen from [4]. In addition they tend exponentially to zero as $|\lambda| \rightarrow \infty$, except that $f_0(\lambda)$ behaves as $O(\lambda^{-2})$ as $\lambda \rightarrow +\infty$ (see ref. [2]). We can therefore use the following method, described in [5], to compute the function values of $f_0(\lambda)$, $f(\lambda)$, $F_0(\lambda)$, and $F(\lambda)$, at least in a certain finite interval. We give the formulae only for $f(\lambda)$ and $F(\lambda)$, since those for the Landau distribution are of the same form.

Let ϵ_- and ϵ_+ be two given small positive numbers and let T_- and T_+ be two quantities such that

$$\int_{-\infty}^{T_-} f(\lambda) d\lambda \leq \epsilon_-, \quad (2.1)$$

$$\int_{T_+}^{\infty} f(\lambda) d\lambda \leq \epsilon_+. \quad (2.2)$$

We then define the following two functions

$$g(\lambda) = \frac{\omega}{\pi} \left[\frac{1}{2} + \sum_{k=1}^{\infty} \left(A_k \cos k\omega\lambda + B_k \sin k\omega\lambda \right) \right], \quad (2.3)$$

$$G(\lambda) = \frac{1}{\pi} \left[A + \frac{1}{2} \omega\lambda + \sum_{k=1}^{\infty} \left(\frac{A_k}{k} \sin k\omega\lambda - \frac{B_k}{k} \cos k\omega\lambda \right) \right], \quad (2.4)$$

with

$$\omega = 2\pi/T, \quad T = T_+ - T_-, \quad (2.5)$$

$$A = -\frac{1}{2} \omega T_- - \sum_{k=1}^{\infty} \left(\frac{A_k}{k} \sin k\omega T_- - \frac{B_k}{k} \cos k\omega T_- \right), \quad (2.6)$$

$$A_k = \operatorname{Re} \phi(ik\omega), \quad B_k = -\operatorname{Im} \phi(ik\omega) \quad (2.7, 8)$$

for $k = 0, \pm 1, \pm 2, \dots$. It is then shown in [5] that, for $T_- \leq \lambda \leq T_+$, we have

$$g(\lambda) = f(\lambda) + \sum_{k=1}^{\infty} \left[f(\lambda + kT) + f(\lambda - kT) \right], \quad (2.9)$$

$$0 \leq g(\lambda) - f(\lambda) \leq f(T_-) + f(T_+) + \frac{\epsilon_- + \epsilon_+}{T}, \quad (2.10)$$

$$-\epsilon_- \leq G(\lambda) - F(\lambda) \leq \epsilon_+. \quad (2.11)$$

These formulae show us that we can take $g(\lambda)$ as an approximation to $f(\lambda)$ and $G(\lambda)$ to $F(\lambda)$. Since $f(\lambda)$ tends to zero for $|\lambda| \rightarrow \infty$, we only have to make $|T_-|$ and T_+ large enough to obtain reasonable error bounds in (2.10) and (2.11). Naturally, in the neighbourhood of the end points of the interval (T_-, T_+) the function $g(\lambda)$ is a very bad approximation to $f(\lambda)$. However, in general, the values of $f(\lambda)$ will be so small there that, from the point of view of using $f(\lambda)$ to compute probabilities over different intervals, it is irrelevant whether we have an error of one hundred per cent or even more. What counts from a practical point of view is the fact that (2.11) is valid for all λ with $T_- \leq \lambda \leq T_+$.

Taking into account that we know $\phi(s)$, given by (1.3), and

$$\phi_0(s) = e^{s \ln s}, \quad (2.12)$$

which is the Laplace transform of $f_0(\lambda)$, the only quantities we still have to determine, given ϵ_- and ϵ_+ , are T_- , T_+ and N , where N is the number of terms used in the Fourier series. The choice of these parameters is discussed in the next two sections.

3. Determination of T_- and T_+

In Section 2 we already mentioned that $f(\lambda)$ tends exponentially to zero as $|\lambda| \rightarrow \infty$ and $f_0(\lambda)$ does the same for $\lambda \rightarrow -\infty$. Therefore, there exist $c_+ > 0$, $c_- < 0$, $M_+ > 0$ and $M_- > 0$ such that

$$\exp(-c_+ \lambda) f(\lambda) \leq M_- \text{ for all } \lambda \leq 0, \quad (3.1)$$

$$\exp(-c_- \lambda) f(\lambda) \leq M_+ \text{ for all } \lambda \geq 0. \quad (3.2)$$

Using this fact, we know from [5], theorem 1, that for every $T_- \leq T_-^{(0)}$ and $T_+ \geq T_+^{(0)}$ the inequalities (2.1) and (2.2) are satisfied, where

$$T_-^{(0)} = \sup_{\alpha \in (0, c_+)} \left(\frac{1}{\alpha} \ln \frac{\epsilon_-}{\phi(\alpha)} \right), \quad (3.3)$$

$$T_+^{(0)} = \inf_{\alpha \in (c_-, 0)} \left(\frac{1}{\alpha} \ln \frac{\epsilon_+}{\phi(\alpha)} \right). \quad (3.4)$$

These formulae allow us to determine T_+ for $f(\lambda)$ and T_- for $f(\lambda)$ and $f_0(\lambda)$. The determination of T_+ for $f_0(\lambda)$ requires a different method.

Taking into account that in (1.2) the real constant c may be chosen arbitrarily, it is seen that for the Vavilov distribution we can take $c_- = -\infty$ and $c_+ = +\infty$ in (3.3) and (3.4), respectively. We may therefore seek to obtain the extrema of (3.3) and (3.4) by equating the derivative of

$$U_{\pm}(\alpha) = \frac{1}{\alpha} \ln \frac{\epsilon_{\pm}}{\phi(\alpha)} \quad (3.5)$$

to zero. Substituting (1.3) in (3.5), we obtain the roots α_{\pm} of $U'_{\pm}(\alpha) = 0$ and take $T_{\pm}^{(0)} = U_{\pm}(\alpha_{\pm})$. Setting $x_{\pm} = \alpha_{\pm}/\kappa$, it then follows after a lengthy but straight forward calculation that

$$T_{\pm}^{(0)} = T_{\pm} = \frac{1}{x_{\pm}} \left[\frac{1}{\kappa} \ln \epsilon_{\pm} - 1 - \beta^2 \gamma - x_{\pm} \ln \kappa + \exp(-x_{\pm}) - (x_{\pm} + \beta^2) [\ln |x_{\pm}| + E_1(x_{\pm})] \right], \quad (3.6)$$

where x_+ is the negative root and x_- is the positive root of the equation

$$(1 - \beta^2) e^{-x} - \beta^2 [\ln |x| + E_1(x)] = 1 - \beta^2(1 - \gamma) - \frac{1}{\kappa} \ln \epsilon_{\pm} - x. \quad (3.7)$$

The function $E_1(x)$ is the exponential integral defined according to [6], No. 5.1.39 and 5.1.1, by

$$E_1(x) = -\gamma - \ln |x| + \int_0^x \frac{1 - e^{-t}}{t} dt = \int_x^{\infty} \frac{e^{-t}}{t} dt, \quad (3.8)$$

where for $x < 0$ we have to take the principal value of the integral on the right-hand side of (3.8).

Numerical calculations show that the expression

$$x_0 = 1 - \beta^2(1 - \gamma) - \frac{1}{\kappa} \ln \epsilon_- \quad (3.9)$$

is an approximation to the root x_- of (3.7), which is sufficient for practical purposes. In other words, by substituting (3.9) into (3.6) we obtain a T_- value which is only slightly smaller than $T_-^{(0)}$. The root x_+ has to be determined numerically.

As has already been mentioned, for the Landau distribution $T_- (= T_-^{(0)})$ can also be determined by (3.3). Using (2.12) in (3.3) we easily find:

$$T_- = T_-^{(0)} = -1 - \ln \ln \frac{1}{\epsilon_-}. \quad (3.10)$$

To determine T_+ for the Landau distribution we mention that Börsch-Supan [2] has given an asymptotic expansion of $f_0(\lambda)$ for large, positive λ . This expansion has been used in [5] to show that for $T_+ \geq 200$:

$$\int_{T_+}^{\infty} f_0(\lambda) d\lambda \leq \frac{1.043}{T_+} + \frac{1}{T_+^3} + \frac{8}{T_+^4}. \quad (3.11)$$

We observe that the last two terms on the right-hand side of (3.11) are very small. We therefore drop these terms and obtain

$$T_+ = 1.043/\epsilon_+, \quad (3.12)$$

by taking the equality sign in (3.11) and replacing the left-hand side by ϵ_+ . The quantities T_{\pm} are thus given as functions of ϵ_{\pm} by (3.6) for the Vavilov distribution and by (3.10) and (3.12) in the case of the Landau distribution. The choice of ϵ_{\pm} will be discussed later.

4. Determination of N

From (2.7) and (2.8) we can see that, the larger ω , the faster the Fourier coefficients A_k and B_k tend to zero. For a fixed precision the number N of terms required in the Fourier expansion will therefore decrease with increasing ω . On the other hand, using (2.5) and (3.6) it can be shown that ω increases with increasing κ for fixed β^2 in the case of the Vavilov distribution. Therefore we try to find an expression for N as a function of κ , β^2 and some parameter ϵ which determines the precision. In the case of the Landau distribution we determine N simply by trials on the computer, since the Landau distribution is independent of any parameter.

From (2.3), (2.7) and (2.8) we have for the absolute value R_N of the remainder of the series in (2.3):

$$\begin{aligned} R_N &= \frac{\omega}{\pi} \left| \sum_{k=N+1}^{\infty} (A_k \cos k\omega\lambda + B_k \sin k\omega\lambda) \right| \\ &= \frac{\omega}{2\pi} \left| \sum_{k=N+1}^{\infty} [\phi(ik\omega) e^{ik\omega\lambda} + \phi(-ik\omega) e^{-ik\omega\lambda}] \right| \\ &\leq \frac{\omega}{\pi} \sum_{k=N+1}^{\infty} |\phi(ik\omega)|. \end{aligned} \quad (4.1)$$

According to [6], No. 5.2.1 and 5.2.2, the sine and the cosine integrals are given by

$$\text{Si}(x) = \int_0^x \frac{\sin t}{t} dt, \quad (4.2)$$

$$\text{Ci}(x) = \gamma + \ln x + \int_0^x \frac{\cos t - 1}{t} dt \quad (4.3)$$

for $x > 0$. Therefore, for $x > 0$,

$$\int_0^x \frac{1-e^{-it}}{t} dt - \gamma = \ln x - \text{Ci}(x) + \text{Si}(x). \quad (4.4)$$

Using (1.3), (1.5) and (4.4), we obtain after some calculation

$$\frac{\omega}{\pi} |\phi(ik\omega)| = \frac{\omega}{\pi} C(k\omega/\kappa)^{\beta^2\kappa}$$

$$\times \exp \left[-\kappa \cos \frac{k\omega}{\kappa} - \beta^2 \kappa \text{Ci} \left(\frac{k\omega}{\kappa} \right) - k\omega \text{Si} \left(\frac{k\omega}{\kappa} \right) \right]. \quad (4.5)$$

Since $\text{Si}(x) \rightarrow \frac{1}{2}\pi$, $\text{Ci}(x) \rightarrow 0$ for $x \rightarrow \infty$ and $|\cos x| \leq 1$, we obtain:

$$\begin{aligned} \frac{\omega}{\pi} |\phi(ik\omega)| &\leq \frac{\omega}{\pi} C e^{\kappa(k\omega/\kappa)^{\beta^2\kappa}} e^{-\pi\omega k/2 + u_k} \\ &= u_k + v_k, \end{aligned} \quad (4.6)$$

where v_k converges faster to zero than u_k as $k \rightarrow \infty$.

Using (1.4) and (4.6) in (4.1) yields

$$\begin{aligned} R_N &\leq \frac{1}{2}\pi\omega D \sum_{k=N+1}^{\infty} k^{\beta^2\kappa} e^{-\pi\omega k/2} \\ &+ \sum_{k=N+1}^{\infty} v_k = U_N + V_N, \end{aligned} \quad (4.7)$$

with

$$D = (2/\pi^2)(\omega/\kappa)^{\beta^2\kappa} e^{\kappa(2+\beta^2\gamma)}. \quad (4.8)$$

Here again, V_N converges faster to zero than U_N as $N \rightarrow \infty$. We therefore use only U_N for the determination of an expression for N . It then follows easily after a change of variable and integration by parts that

$$\begin{aligned} U_N &\leq \frac{1}{2}\pi\omega D \int_N^{\infty} x^{\beta^2\kappa} e^{-\pi\omega x/2} dx \\ &= \frac{1}{2}\pi\omega D N^{\beta^2\kappa} e^{-\pi\omega N/2} \int_0^{\infty} (1+y/N)^{\beta^2\kappa} e^{-\pi\omega y/2} dy \\ &\leq D N^{\beta^2\kappa} e^{-\pi\omega N/2} + Z_N = W_N + Z_N, \end{aligned} \quad (4.9)$$

where again, Z_N converges faster to zero than W_N for $N \rightarrow \infty$. With W_N we have found our final expression to determine N . We set

$$D N^{\beta^2\kappa} e^{-\pi\omega N/2} = \epsilon, \quad (4.10)$$

where ϵ is a suitably smaller number, and we determine the root N of (4.10) numerically. For $\beta^2 = 0$ (4.10) can be solved analytically, giving

$$N = (2/\pi\omega) \ln(D/\epsilon) \quad \text{for } \beta^2 = 0. \quad (4.11)$$

The choice of a suitable ϵ will be discussed later.

5. The inverse of the distribution functions

One of our goals is the generation of random numbers according to the Landau and the Vavilov distributions. Let us assume that we have an analytic expression for the inverse function $P(x)$ of the distribution function $F(\lambda)$. Then, if w is a random number from a uniform distribution over $(0, 1)$,

$$y = P(w) \quad (5.1)$$

is a Vavilov-distributed random number. We therefore try to find at least an approximation to $P(x)$.

Let $Q(x)$ be the inverse function of $G(\lambda)$ where $G(\lambda)$ is given by (2.4). Then $Q(x)$ is an approximation to $P(x)$. We now give an analytic expression for $Q(x)$. From the definition of $G(\lambda)$ we know that

$$Q(0) = T_-, \quad Q(1) = T_+. \quad (5.2)$$

We define the following odd function

$$\begin{aligned} R(x) &= -f_- - Tx + Q(x), & 0 \leq x \leq 1, \\ T_- - Tx - Q(-x), & -1 \leq x \leq 0. \end{aligned} \quad (5.3)$$

$R(x)$ can be expanded in a Fourier sine series

$$R(x) = \sum_{k=1}^{\infty} D_k \sin k\pi x, \quad (5.4)$$

with

$$D_k = 2 \int_0^1 R(x) \sin k\pi x \, dx, \quad k = 1, 2, \dots \quad (5.5)$$

Therefore, with (5.3) and (5.4) we obtain

$$Q(x) = T_- + Tx + \sum_{k=1}^{\infty} D_k \sin k\pi x. \quad (5.6)$$

Integrating (5.5) by parts gives

$$D_k = \frac{2}{k\pi} \int_0^1 Q'(x) \cos k\pi x \, dx. \quad (5.7)$$

Then the transformation $x = G(\lambda)$ finally yields

$$D_k = \frac{2}{k\pi} \int_{T_-}^{T_+} \cos[k\pi G(\lambda)] \, d\lambda, \quad k = 1, 2, \dots \quad (5.8)$$

To summarize, the inverse of $G(\lambda)$ is given by (5.6), where the coefficients D_k are given by (5.8). The integrals in (5.8) must be calculated numerically, for instance by the trapezoidal rule, or Simpson's rule. A practical criterion for the choice of the number M of coefficients D_k in (5.6) will be discussed later.

Remark: It is evident that we can also find a sine series representation for the inverse of the conditional distribution function

$$F_S(\lambda|T') = P(\Lambda \leq \lambda | \Lambda \leq T'), \quad (5.9)$$

where T' is a fixed value with $T_- < T' \leq T_+$. If $G_S(\lambda|T')$ is the conditional distribution function corresponding to the distribution function $G(\lambda)$, then $G_S(\lambda|T')$ is an approximation to $F_S(\lambda|T')$; moreover, if

$$S = G(T'), \quad (5.10)$$

we have

$$G_S(\lambda|T') = G(\lambda)/S. \quad (5.11)$$

Let $Q_S(x)$ be the inverse of $G_S(\lambda|T')$; it is then easily seen that

$$Q_S(x) = T_- + (T' - T_-)x + \sum_{k=1}^{\infty} C_k \sin k\pi x, \quad (5.12)$$

where

$$C_k = \frac{2}{k\pi} \int_{T_-}^{T'} \cos[(k\pi/S)G(\lambda)] \, d\lambda, \quad k = 1, 2, \dots \quad (5.13)$$

For practical reasons we shall use later $Q_S(x)$ instead of $Q(x)$, for $S = 0.99$ and $S = 0.995$, depending on the value of κ .

6. Precision and the free parameters

In the actual programs the free parameters T_{\pm} , N , M , S and so on have been chosen in the following way. For the density and the distribution function of the Landau distribution we have taken

$$T_- = -5, \quad T_+ = 233.5, \quad N = 200. \quad (6.1)$$

This choice guarantees a precision of at least three correct decimal places for both functions. In many cases the precision is even higher as has been found by numerical tests.

In the case of the Vavilov distribution T_- , T_+ and N are always calculated according to the corresponding formulae derived in Sections 3 and 4. As has already been mentioned there, the values of T_{\pm} and N are dependent on the choice of ϵ_{\pm} and ϵ , respectively. In the program we have chosen

$$\epsilon_- = \epsilon_+ = \epsilon = 0.0005, \quad (6.2)$$

giving at least the same precision as in the case of the Landau distribution. In both of these cases the precision of the distribution function is higher than that of the density, for the reason given in Section 2. The choice of the parameter in (6.1) and (6.2) was made partly by theoretical considerations and partly by numerical tests.

We finally have to discuss the inverse function. Numerical tests showed that the series (5.6) converges fairly slowly. However, the series (5.12) converges much faster when taking, for instance,

$$S = 0.99 \quad \text{for} \quad 0.01 \leq \kappa \leq 0.04, \quad (6.3)$$

$$S = 0.995 \quad \text{for} \quad 0.04 \leq \kappa \leq 10.0,$$

in the case of the Vavilov distribution, and $S = 0.99$ in the case of the Landau distribution. In practical terms it means that we replace the original distribution by a new distribution (the conditional distribution) which has a shorter tail on the right-hand side. We have cut off a part of the tail which contains 1% and 0.5%, respectively, of the probability content of the original distribution, which can be tolerated in practice; in fact, for small κ , the long tail on the right-hand side is physically meaningless. Taking S as indicated in (6.3) and (6.4), and taking $M = 260$ for the Landau distribution and $M = 200$ for the Vavilov distribution, $Q_S(x)$ is almost everywhere accurate to three decimal places or more with an error up to 5–6% occurring only in the immediate neighbourhood of the end points of $(0, 1)$.

7. The routines

7.1. Landau distribution

(1) *DISLAN*(X, I). This is a function subprogram which computes for $I = 0$ the value of the density function, and for $I = 1$ the value of the distribution

function, at the point X . It uses eqs. (2.3) and (2.6), where the Fourier coefficients are given in DATA statements. The method for the summation of the Fourier series is the one recommended by Clenshaw [7], applied by Håvie [8] in the subprogram TRISUM for the summation of trigonometric series. (It is used in all other routines in this paper where Fourier series occur.) *DISLAN* is independent of any other subroutine. It is defined for all real X . Especially we have

$$\begin{aligned} \text{DISLAN}(X, I) &= 0 \quad \text{for } X < -3.5, \quad I = 0, 1, \\ &0 \quad \text{for } X > 230, \quad I = 0, \\ &1 \quad \text{for } X > 230, \quad I = 1. \end{aligned}$$

(2) *DINLAN*(X). This is a function subprogram, which gives the value of the inverse of the conditional distribution function at the point X . It uses eqs. (5.12)–(5.13) with $S = 0.99$ and $T' = 85.46782$. The Fourier coefficients are given in a DATA statement. *DINLAN* is independent of any other subroutine. It is defined for all X with $0 \leq X \leq 1$. In particular,

$$\begin{aligned} \text{DINLAN}(0.) &= -3.5, \\ \text{DINLAN}(1.) &= 85.46782. \end{aligned}$$

If $X = \text{RNDM}$ is a random number, uniformly distributed over $(0, 1)$, *DINLAN*(X) yields a random number according to the conditional Landau distribution.

7.2. Vavilov distribution

(3) *DISVAV*(X, I). This function subprogram computes with the help of eqs. (2.3)–(2.6) the value of the density function if $I = 0$, and the value of the distribution function if $I = 1$. Before *DISVAV*(X, I) is used in a program the subroutine *COEDIS*($\text{RKA}, \text{BE2}, I, J$) (see (5)) must be called. *DISVAV* is defined for all real X . In particular

$$\begin{aligned} \text{DISVAV}(X, I) &= 0 \quad \text{for } X < T_-, \quad I = 0, 1, \\ &0 \quad \text{for } X > T_+, \quad I = 0, \\ &1 \quad \text{for } X > T_+, \quad I = 1. \end{aligned}$$

(4) *DINVAV*(X). This function subprogram uses (5.12) to compute the value of the inverse of the conditional distribution function. Before *DINVAV*(X) is used in a program the subroutine *COEDIN*($\text{RKA}, \text{BE2}, J$) (see (6)) must be called. *DINVAV* is defined for all X with $0 \leq X \leq 1$. In particular

$$\begin{aligned} \text{DINVAV}(0.) &= T_-, \\ \text{DINVAV}(1.) &= T', \end{aligned}$$

where T_- is computed in COEDIS and T' in COEDIN. As in (2), if $X = \text{RNDM}$ is a random number uniformly distributed over $(0, 1)$, $\text{DINVAV}(X)$ generates a random number according to the conditional Vavilov distribution.

(5) *COEDIS(RKA, BE2, I, J)*. In this subroutine eqs. (3.6)–(3.9) are used to compute T_{\pm} for all $\text{RKA} = \kappa$ and $\text{BE2} = \beta^2$ satisfying (1.11). Furthermore, the Fourier coefficients are computed. Any error messages which may arise during the execution of COEDIS are written on logical unit J as are the values of T_{\pm} . If J is replaced by $-J$, the values of T_{\pm} are suppressed.

(6) *COEDIN(RKA, BE2, J)*. This is a subroutine in which T' , defined in Section 5, is computed. In addition it expands the integrals (5.13) by the trapezoidal rule to compute the Fourier coefficients for the inverse of the conditional distribution function. The three arguments required by COEDIN are precisely the 1st, 2nd and 4th arguments of COEDIS; this subroutine is called from COEDIN.

7.3. The auxiliary routines

(7) *FCN(X, RKA, BE2)*. This function subroutine contains the three auxiliary functions which are used in COEDIS and COEDIN to compute T_+ , the number, N , of Fourier coefficients, and T' .

(8) *EXPINT(X)*. This is a function subprogram written by Kölbig [9] to compute the value of the exponential integral (3.8). The numerical method which is used was proposed by Cody and Thacher [10, 11].

(9) *CSINTL(X, L)*. This is a function subprogram which computes for $L = 1$ the sine integral (4.2), and for $L = 2$ the cosine integral (4.3), at the point X . It was published in ALGOL by Burlisch [12] and translated into FORTRAN by Kölbig [13].

(10) *RZERO(A, B, X, RKA, BE2, LU)*. This is a slightly modified version of a subroutine written by Pomentale [14]. It computes the root X of the equation $\text{FCN}(X) = 0$ [see (7)] in the interval (A, B) , where RKA and BE2 have the same meaning as in COEDIS, and LU is the number of the logical unit onto which any error messages will be written. The numerical method to find the root is based on Müller's method [15].

8. Usage of the routines

For the user who wants to compute the density function, or the distribution function, or the inverse of the conditional distribution functions, only the routines

$\text{DISLAN}, \text{DINLAN}, \text{DISVAV}, \text{DINVAV}$

are of immediate interest. The remaining routines

$\text{COEDIS}, \text{COEDIN}, \text{FCN}, \text{EXPINT}, \text{CSINTL}, \text{RZERO}$

are only auxiliary routines for DISVAV and DINVAV, although the last three are of general interest.

In the case of the Landau distribution the use of $\text{DISLAN}(X, 0)$ in an arithmetical expression yields the density, that of $\text{DISLAN}(X, 1)$ the distribution function, and $\text{DINLAN}(X)$ results in the inverse of the conditional distribution function, described in Section 5. DISLAN and DINLAN are independent of each other and of any other routine. DINLAN can be used to generate random numbers, as has already been described in ref. [2], Section 7.

The case of the Vavilov distribution is more complicated. Firstly, the user always has to specify $\text{RKA}(=\kappa)$ and $\text{BE2}(=\beta^2)$ in the range

$$0.01 \leq \kappa \leq 10 \quad \text{and} \quad 0 \leq \beta^2 \leq 1.$$

Secondly,

DISVAV requires: $\text{COEDIS}, \text{FCN}, \text{EXPINT}, \text{CSINTL}, \text{RZERO}$;

DINVAV requires: $\text{DISVAV}, \text{COEDIS}, \text{COEDIN}, \text{FCN}, \text{EXPINT}, \text{CSINTL}, \text{RZERO}$.

Finally, before DISVAV can be used for the first time, COEDIS must be called. Moreover, COEDIS must be called again whenever one of the arguments RKA , BE2 or I changes. For instance, to calculate values of the density function and the distribution function for a range of values X , the following coding could be used

```
CALL COEDIS(RKA, BE2, 0, J)
DO 1 I = 1, N
1 DENSIT(I) = DISVAV(X(I), 0)
  CALL COEDIS(RKA, BE2, 1, J)
DO 2 I = 1, N
2 DISFUN(I) = DISVAV(X(I), 1).
```


Similarly, a call must be made to COEDIN before DINVAV is used. COEDIN itself calls COEDIS with $I = 1$. Therefore, having called COEDIN, the function DISVAV can be called for $I = 1$ without calling again COEDIS. However, if DISVAV is used with $I = 0$, COEDIS has to be called first.

Similarly to the routines for the Landau distribution DISVAV(X, 0) yields the density function, DISVAV(X, 1) the distribution function and DINVAV(X) the inverse of the conditional distribution function. Again DINVAV can be used to generate corresponding random numbers.

9. Test runs

The results of the test runs are self-explanatory. However, we should mention two things. Firstly, the abscissae to the values of column 2 of the test runs are the corresponding values of column 5 divided by the appropriate S (see Section 5). Secondly, the trailing zeros of the values taken from Seltzer—Berger [4] are not significant.

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OUTPUT FROM LANDAU TEST

TEST VALUES FOR THE LANDAU DISTRIBUTION

| ABSCISSA | INVERSE CONDITIONAL DISTR. FUNCT. | DENSITY FUNCTION (DISLAN) | DENSITY FUNCTION (BORSCH-SUPAN) | DISTRIBUTION FUNCTION |
|----------|---|---------------------------------|---------------------------------------|--------------------------|
| -3,500 | -3,473 | .00008 | .00001 | .00005 |
| -2,500 | -2,599 | .00974 | .00964 | .00197 |
| -1,500 | -1,489 | .10045 | .10055 | .04995 |
| 0,000 | 0,002 | .17894 | .17886 | .28698 |
| 5,000 | 4,996 | .03920 | .03917 | .77332 |
| 10,000 | 10,007 | .01196 | .01198 | .88338 |
| 20,000 | 20,016 | .00296 | .00300 | .94417 |
| 30,000 | 29,981 | .00136 | .00130 | .96423 |
| 50,000 | 49,982 | .00046 | .00045 | .98000 |
| 80,000 | 80,282 | .00027 | .00017 | .98694 |

OUTPUT FROM VAVILOV TEST

TEST VALUES FOR THE VAVILOV DISTRIBUTION

KAPPA = .01 BETA**2 = 0.0

| ABSCISSA | INVERSE CONDITIONAL DISTR. FUNCT. | DENSITY FUNCTION (DISVAV) | DENSITY FUNCTION (SELTZER-BERGER) | DISTRIBUTION FUNCTION |
|----------|---|---------------------------------|---|--------------------------|
| -3,000 | -3,025 | .00068 | .00068 | .00002 |
| -2,000 | -1,979 | .04442 | .04440 | .01417 |
| -1,000 | -.995 | .15291 | .15300 | .11469 |
| 0,000 | 0,016 | .18065 | .18100 | .28965 |
| 5,000 | 5,000 | .03956 | .03960 | .78074 |
| 10,000 | 10,007 | .01210 | .01210 | .89176 |
| 15,000 | 15,006 | .00546 | .00546 | .93253 |
| 20,000 | 20,000 | .00304 | .00304 | .95290 |
| 30,000 | 29,990 | .00131 | .00131 | .97288 |
| 34,000 | 34,005 | .00101 | .00101 | .97747 |

TEST VALUES FOR THE VAVILOV DISTRIBUTION

KAPPA = 4.00 BETA**2 = .5

| ABSCISSA | INVERSE CONDITIONAL DISTR. FUNCT. | DENSITY FUNCTION (DISVAV) | DENSITY FUNCTION (SELTZER-BERGER) | DISTRIBUTION FUNCTION |
|----------|---|---------------------------------|---|--------------------------|
| -3,500 | -3,623 | .00950 | .00945 | .00088 |
| -3,250 | -3,265 | .06881 | .06880 | .00879 |
| -3,000 | -2,999 | .26406 | .26400 | .04682 |
| -2,750 | -2,749 | .59997 | .60000 | .15324 |
| -2,500 | -2,499 | .88127 | .88100 | .34233 |
| -2,250 | -2,250 | .89520 | .89500 | .57079 |
| -2,000 | -2,000 | .66268 | .66300 | .76888 |
| -1,750 | -1,750 | .37256 | .37300 | .89754 |
| -1,500 | -1,500 | .16442 | .16400 | .96237 |
| -1,250 | -1,251 | .05852 | .05850 | .98843 |