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ON A FUNCTION, J(x,y), OCCURRING IN PROBLEMS OF SOLUTE TRANSPORT WITH NON-EQUILIBRIUM INTERPHASE MASS TRANSFER

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ABSTRACT

The function, J(x,y), which has appeared frequently in analytical solutions of a variety of technical problems, is described and its applications briefly reviewed. Two detailed examples of applications are given. Tabulations of functions related to J(x,y) are listed, and relationships of J(x,y) to these functions are stated. Methods of computation of J(x,y), suitable for use with digital computers, are described.

1. INTRODUCTION

Analytical solutions of the partial differential equations of mass or heat transport in porous media with time-dependent (non-equilibrium) transfer of mass or heat between fluid and solid phases may include certain irreducible integrals in which the integrands are, in general, products of exponential functions and Bessel functions. These integrals have appeared frequently in the literature on heat and mass transport, as well as in that describing other phenomena, and in recent years have been abbreviated by use of the functional designation $J(x,y)$. Aside from purely mathematical interest, knowledge of the properties of the function $J(x,y)$ is required for its numerical evaluation in a variety of technical applications. Here we briefly review properties and applications of the function $J(x,y)$, describe published (and unpublished) tabulations of related functions, and discuss methods for numerical evaluation of $J(x,y)$.

2. DEFINITIONS AND PROPERTIES OF J(x,y)

The function J(x,y) can be defined (Goldstein, 1953) by:

$$J(x, y) = 1 - e^{-y} \int_0^x e^{-\xi} I_0(2\sqrt{y\xi})\, d\xi, \quad x \geq 0, \; y \geq 0, \tag{1}$$

where $I_0(z)$ is the modified Bessel function of the first kind, of order zero, with argument z. The form (1) appears to have been used most frequently in technical applications. Other, equivalent forms have been derived by Anzelius (1926):

$$J(x, y) = 1 - e^{-y} \int_0^x e^{-\xi} J_0(2i\sqrt{y\xi})\, d\xi, \tag{2}$$

and by Terazawa (1922) and Goldstein (1932, 1953):

$$J(x, y) = 1 - x^{1/2} \int_0^\infty e^{-\xi} J_0(2\sqrt{y\xi})\, J_1(2\sqrt{x\xi})\, \xi^{-1/2} d\xi, \tag{3}$$

where $J_0(z)$ and $J_1(z)$ are the Bessel functions of the first kind, of orders zero and one respectively, with argument z. Vermeulen and Hiester (1952) appear to have been the first to use the symbol J(x,y) for this function.

Mathematical properties of J(x,y) have been summarized by Goldstein (1953) and, more extensively, by Luke (1962). Some of the more useful properties derivable from (1) are listed below, where subscripts x and y indicate partial differentiation.

$$J(x, y) + J(y, x) = 1 + e^{-x-y} I_0(2\sqrt{xy}), \tag{4}$$

$$J(x, x) = \frac{1}{2} + \frac{1}{2}e^{-2x} I_0(2x) \tag{5}$$

$$J_x(x, y) = - e^{-x-y} I_0(2\sqrt{xy})$$

$$J_y(x, y) = e^{-x-y} \left(\frac{x}{y}\right)^{1/2} I_1(2\sqrt{xy})$$

$$J(x,0) = e^{-x}$$

$$J(0,y) = 1$$

$$\lim_{x\to\infty} J(x,y) = 0$$

$$\lim_{y\to\infty} J(x,y) = 1$$

$$\lim_{x\to\infty} J(x,x) = \frac{1}{2}$$

Figures 1-4 show the variations of $J(x,y)$ over limited ranges of the arguments x and y.

3. APPLICATIONS

The function J(x,y) and related functions occur in the analytical solutions of a variety of technical problems. A sampling of such problems is given below with two detailed examples; the reader is referred to the original literature for detailed statements of other problems, including governing differential equations, initial conditions, and boundary conditions.

(1) heat exchange and heat transport:

Anzelius, 1926; Brinkley, 1947; Hougen and Marshall, 1948; Klinkenberg, 1948; Carslaw and Jaeger, 1959 (pp. 259-260, 393-396).

(2) hydrodynamics:

Terazawa, 1922 (p. 99); Goldstein, 1932 (pp. 66-72).

(3) probability and statistics:

Bose, 1947; Brinkley and Brinkley, 1947; Masters, 1955.

(4) fluid flow in pipes, electric current in cables:

Binnie and Miller, 1955.

(5) mass transport in porous media with interphase mass transfer:

(a) convective transport only:

Thomas, 1944, 1948, 1949; Walter, 1945; Hiester and Vermeulen, 1952; Vermeulen and Hiester, 1952; Goldstein, 1953; Opler and Hiester, 1954; Gardner and Brooks, 1957 .

(a) convective and dispersive transport:

Lapidus and Amundson, 1952; Ogata, 1961, 1964, 1969, 1970, 1976; Banks and Igbal, 1964; Eldor and Dagan, 1972; Lindstrom and Narasimhan, 1973; Lindstrom, 1976; Cameron and Klute, 1977; deSmedt and Wierenga, 1979a, 1979b; Carnahan and Remer, 1981.

Two detailed examples of applications of the function J(x,y) in problems concerning mass transport with interphase mass transfer are set forth below. The first example considers purely convective transport with a nonlinear expression for the rate of mass transfer. The second example considers convective and dispersive transport with a linear rate expression.

Hiester and Vermeulen (1952) considered a fixed-bed ion exchange process in which an ionic solute, A, in the feed solution exchanges with another solute previously sorbed on the solid phase (resin) occupying a packed column. The material balance relation for solute A at a given cross section of the column is (with minor changes of notation):

$$-\left(\frac{\partial c}{\partial v}\right)_V = \rho\left(\frac{\partial q}{\partial V}\right)_v + f\left(\frac{\partial c}{\partial V}\right)_v \qquad (6)$$

where c is the number of equivalents of A per unit volume of fluid phase, q is the number of equivalents of A per unit mass of dry resin, ρ is the bulk density of dry resin, f is the porosity of the column, v is the total column volume from inlet to cross section, and V is the volume of fluid fed to the column. The rate expression for ion exchange is:

$$\frac{dq}{d\tau} = k\left[c(q_\infty - q) - \frac{1}{K}\,q(c_o - c)\right] \qquad (7)$$

where τ is time, k is a rate constant, K is the selectivity coefficient for the ion-exchange reaction, q_∞ is the exchange capacity of the resin, and c_o is the total solute concentration in the fluid phase. The problem is recast by use of the dimensionless variables, r, s, and t,

where $r = K^{-1}$

$s = kv\rho q_\infty R^{-1}$

$t = k(V-fv)c_o R^{-1} = k\,(\tau - fvR^{-1})c_o$

and R is the volumetric rate of flow of feed solution. With this notation (6) and (7) become, respectively,

$$-\left[\frac{\partial(c/c_o)}{\partial s}\right]_t = \left[\frac{\partial(q/q_\infty)}{\partial t}\right]_s$$

$$\left[\frac{d(q/q_\infty)}{dt}\right]_v = \frac{c}{c_o}\left(1-\frac{q}{q_\infty}\right)-r\frac{q}{q_\infty}\left(1-\frac{c}{c_o}\right)$$

with the boundary conditions:

$c/c_o = 1$ at $s = 0$

$q/q_\infty = 0$ at $t = 0$

The resulting solutions are

$$\frac{c}{c_o} = \frac{J(rs,t)}{J(rs,t) + e^{(r-1)(t-s)}\left[1-J(s,rt)\right]} \tag{8}$$

and

$$\frac{q}{q_\infty} = \frac{1 - J(t,rs)}{J(rs,t) + e^{(r-1)(t-s)}\left[1-J(s,rt)\right]} \tag{9}$$

where $J(x,y)$ is defined by (1).

Carnahan and Remer (1981) considered a three-dimensional porous medium with porosity ε supporting a flow of fluid with velocity v parallel to the z-axis and moving toward the positive direction. A solute is introduced at a constant rate, m_o mass units per unit time, at the origin of coordinates and is subjected to convective transport with hydrodynamic dispersion, the dispersion being characterized by coefficients D_L and D_T in directions parallel and perpendicular, respectively, to the direction of fluid flow. If c is the solute mass per unit volume of fluid and q is the sorbed solute mass per unit volume of solid phase, the mass balance equation at a point (x,y,z) at time $t > 0$ is

$$\frac{\partial c}{\partial t} + \alpha \frac{\partial q}{\partial t} = D_T\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) + D_L \frac{\partial^2 c}{\partial z^2} - v \frac{\partial c}{\partial z} \tag{10}$$

where

$$\alpha = \frac{1-\varepsilon}{\varepsilon}$$

The rate expression for sorption is assumed to be linear and takes the form

$$\frac{\partial q}{\partial t} = k_1 c - k_2 q \tag{11}$$

where k_1 and k_2 are forward and backward rate constants. The linear rate expression used here corresponds to "Langmuir" sorption in which q is much smaller than the sorptive capacity of the solid. Initial conditions are:

$$c = 0,\ q = 0 \text{ for all } (x,y,z) \text{ at } t=0 \tag{12}$$

and the boundary conditions are

$$\lim_{x,y,z \to \infty} c = 0,\ t > 0 \tag{13}$$

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\ \left[\varepsilon c + (1-\varepsilon) q\right] = m_o t, \quad t > 0 \tag{14}$$

The solutions to (10) and (11) satisfying (12) - (14) were found to be:

$$c = Q\int_0^t e^{-\frac{x^2+y^2}{4D_T\tau} - \frac{(z-v\tau)^2}{4D_L\tau}} J\left[\alpha k_1\tau, k_2(t-\tau)\right] \frac{d\tau}{\tau^{3/2}} \tag{15}$$

$$q = \frac{k_1}{k_2} Q \int_0^t e^{-\frac{x^2+y^2}{4D_T\tau} - \frac{(z-v\tau)^2}{4D_L\tau}} \left\{1-J\left[k_2(t-\tau), \alpha k_1\tau\right]\right\} \frac{d\tau}{\tau^{3/2}} \tag{16}$$

where

$$Q = \frac{m_o}{8\pi^{3/2} D_T D_L^{1/2} \varepsilon} .$$

Although solutions (8) and (9) could be evaluated by use of tables of the function $J(x,y)$, it is evident that numerical evaluation of the irreducible integrals in (15) and (16) requires an efficient computational scheme for $J(x,y)$.

4. TABULATIONS

Although the function $J(x,y)$ as defined by (1)-(3) does not appear to have been tabulated in the published literature, tabulations of several related functions have been published or reported.

(1) Bose (1947) has tabulated the function $L(P,p,\lambda)$ where

$$L(P,p,\lambda) = \int_0^P \eta^{p/2}\, \lambda^{1-p/2}\, e^{-(\eta^2+\lambda^2)/2} I_{(p-2)/2}(\lambda\eta)\,d\eta$$

For the case $p = 2$,

$$J(x,y) = 1 - L\,(\sqrt{2x},\ 2, \sqrt{2y})$$

(2) Brinkley and Brinkley (1947) reported an unpublished table of the probability, $p(r,R)$, that the point of impact of a missile aimed at the origin of coordinates will lie within a circle of radius r whose center is distance R from the origin; $p(r,R)$ is sometimes called the offset circular probability function, and was defined by

$$p(r,R) = e^{-R^2} \int_0^{r^2} e^{-t} I_0(2R\sqrt{t})\ dt$$

Then,

$$J(x,y) = 1 - p\ (\sqrt{x}, \sqrt{y})$$

(3) The Rand Corporation (1951) has tabulated the offset circular probability function $q(R,r)$, where

$$q(R,r) = \int_R^{\infty} te^{-(t^2+r^2)/2} I_0(rt)dt \qquad (17)$$

(17)

Then,

$$J(x,y) = q(\sqrt{2x}. \sqrt{2y})$$

(4) Wilson (1951) and the Admiralty Research Laboratory (1953) have published tabulations of the Function F (β,ρ) where

$$F(\beta,\rho) = \frac{2e^{-\rho^2}}{\sqrt{\pi}\beta^2} \int_0^{\beta} e^{-\eta^2} I_0(2\rho\eta)\eta d\eta$$

Then,

$$J(x,y) = 1 - \sqrt{\pi} x \; F(\sqrt{x},\sqrt{y})$$

(5) Brinkley, Edwards, and Smith (1952) reported an unpublished table of the function $\phi_0(x,y)$ applicable to exchange of heat between a fluid and a porous solid, where

$$\phi_0(x,y) = e^x \int_0^x e^{-t} I_0(2\sqrt{yt})\, dt$$

Then,

$$J(x,y) = 1 - e^{-x-y}\phi_0(x,y)$$

(6) Masters (1955) tabulated the offset circular probability function, $P(z/\sigma, R/\sigma)$, and indicated the utility of this function in problems of nuclear particle scattering and heat conduction. $P(z/\sigma, R/\sigma)$ was defined by:

$$P(z/\sigma,\; R/\sigma) = \frac{e^{-R^2/2\sigma^2}}{\sigma^2} \int_0^z e^{-r^2/2\sigma^2} I_0(rR/\sigma^2) r dr$$

and is related to $J(x,y)$ by:

$$J(x,y) = 1 - P\;(\sqrt{2x}, \sqrt{2y})$$

5. COMPUTATIONAL METHODS

The tabulations of functions related to the function $J(x,y)$ are not suitable for repeated, numerical evaluations of $J(x,y)$ required for many practical applications. However, several computational methods are available.

Walter (1945) and Klinkenberg (1948) have given an analytical approximation to $J(x,y)$, based on the error function and applicable for large values of the arguments (x,y). Hastings and Wong (1953) have provided twenty-two analytical approximations to the function $q(R,r)$ defined by (17); their approximations are valid for a variety of ranges of argument values and exhibit a variety of accuracies.

An asymptotic expansion in a series of Bessel functions was attributed to L. Onsager and was described by Thomas (1944, 1948). Asymptotic expansions which are more easily implemented numerically have been derived by Goldstein (1953).

The available analytical approximations are not accurate enough for evaluation of expressions such as (15) and (16), where $J(x,y)$ appears as part of the integrand in integrals which must be evaluated by numerical methods. The remainder of this section describes methods which have been implemented at the Lawrence Berkeley Laboratory for computation of $J(x,y)$ as part of a study of mass transport in porous media (Carnahan and Remer, 1981).

One method uses an iterative Simpson's rule routine to evaluate the integral $S(x,y)$, where

$$S(x,y) = \int_0^1 e^{-x\xi}\ I_0(2\sqrt{xy\xi})d\xi$$

Approximations to $S(x,y)$ are made on successively smaller subintervals of $\Delta\xi$

until the absolute fractional error between successive approximations is less than an assigned value. The modified Bessel function is computed using polynomial approximations given by Olver (1965). If argument $x \leq 10$, or if $x>10$ while $x \leq y$, $J(x,y)$ is formed from:

$$J(x,y) = 1 - xe^{-y}S(x,y)$$

If $x>10$ while $x>y$, the routine computes $S(y,x)$, and $J(x,y)$ is formed from:

$$J(x,y) = ye^{-x}S(y,x) + e^{-x-y}I_0(2\sqrt{xy})$$

This method produces results which have relative errors of about 1×10^{-6}.

Another method uses infinite series expansions of $J(x,y)$. If the modified Bessel function in (1) is expanded in the series (Olver, 1965)

$$I_0(z) = \sum_{k=0}^{\infty} \frac{(z^2/4)^k}{(k!)^2} \tag{18}$$

and the integration is performed term by term, the following result is obtained:

$$J(x,y) = e^{-x-y} \sum_{n=0}^{\infty} \frac{y^n}{n!} \sum_{m=0}^{n} \frac{x^m}{m!} \tag{19}$$

This or equivalent results have been stated by Thomas (1944, 1948), Walter (1945), and deSmedt and Wierenga (1979a, 1979b). An alternative form, stated by deSmedt and Wierenga (1979a, 1979b), can be derived by using (19) to write $J(y,x)$ and finding $J(x,y)$ by use of (4) and (18). The result is:

$$J(x,y) = 1-e^{-x-y} \sum_{n=1}^{\infty} \frac{x^n}{n!} \sum_{m=0}^{n-1} \frac{y^m}{m!} \tag{20}$$

In principle, (19) and (20) can be used to compute $J(x,y)$ to any desired degree of accuracy. We have found that, for a given degree of accuracy, (19) requires fewer computational steps if $x > y$, while (20) is faster in this sense if $y > x$. In practice, large values of x and y require a large number of computations because of the slow rate of convergence of the double sum in the two expressions. Also, the numerical value of the double sum may exceed the range of the computing device for very large argument values. For example, assume that the computation is carried to a number of terms so that the contribution of the next term in the summation over n, relative to the double sum computed thus far, is less than 1×10^{-6}. Then if both x and y equal 116, the double sum equals about 10^{100}, and if both x and y equal 372, the double sum equals about 10^{322}, which is the upper limit of the range of real constants allowed by the CDC-7600 computer in use at this laboratory. In both examples, the value of $J(x,x)$ is about 0.5.

The problems of slow convergence and out-of-range computations encountered in use of (19) and (20) can be minimized by application of available asymptotic expansions of the function $J(x,y)$. We have adapted several expansions given by Goldstein (1953) to computations of $J(x,y)$ with large values of the arguments, our principal modification being the substitution of an asymptotic expansion of the modified Bessel function of the first kind of order zero wherever the Bessel function occurs in Goldstein's equations. We have also derived recursion relations for the coefficients occurring in the expansions.

The asymptotic expansion of the modified Bessel function of the first kind of order zero with argument z is (Goldstein, 1953):

$$I_0(z) \sim \frac{e^z}{\sqrt{2\pi z}} \sum_{m=0}^{\infty} \frac{A_m}{(2z)^m} \tag{21}$$

where $A_0 = 1$, $A_1 = \frac{1}{4}, \ldots, A_m = \frac{1^2 \cdot 3^2 \ldots (2m-1)^2}{4^m m!}$

The recurrence relation for the coefficient A_m is

$$A_m = \frac{(2m-1)^2}{4m} A_{m-1} \tag{22}$$

The expansion (21) can be used in (5) to derive an asymptotic expansion of $J(x,x)$:

$$J(x,x) \sim \frac{1}{2} + \frac{1}{4\sqrt{\pi x}} \sum_{m=0}^{\infty} \frac{A_m}{(4x)^m} \tag{23}$$

The following computational scheme provides $J^{(n)}(x,x)$, the approximation of $J(x,x)$ including terms through $m = n$:

$$Q_0(x) = \frac{1}{4\sqrt{\pi x}}, \ldots, Q_m(x) = \frac{(2m-1)^2}{16mx} Q_{m-1}(x)$$

$$J^{(n)}(x,x) = \frac{1}{2} + \sum_{m=0}^{n} Q_m(x) = J^{(n-1)}(x,x) + Q_n(x)$$

Define the relative difference, R_n, between successive approximations $J^{(n)}(x,y)$ by

$$R_n = \left| \frac{J^{(n)}(x,y) - J^{(n-1)}(x,y)}{J^{(n-1)}(x,y)} \right|$$

In this case,

$$R_n = \left| \frac{Q_n(x)}{J^{(n-1)}(x,x)} \right|$$

The computational scheme for $J(x,x)$ gives $R_n = 5x10^{-8}$ for $x = 100$ and $n = 2$, and $R_n = 8 \times 10^{-7}$ for $x = 10$ and $n = 3$. In contrast, use of (19) requires 152 terms in the outer summation to achieve $R_n = 8 \times 10^{-7}$ with $x = y = 100$. It is noted that (23) begins to diverge ($Q_m > Q_{m-1}$) at a value of m approximately equal to $4x + 1$, and if a desired R_n value has not been achieved by this step, it never will be achieved. For this reason, use of (23) is not advised for argument values less than $x = 4$ if $R_n < 10^{-7}$.

If the arguments of $J(x,y)$ are unequal, the asymptotic expansions given in the following paragraphs can be used. Using Goldstein's notation, the following variables are defined:

$$\xi = 2\sqrt{xy}, \ \eta = \sqrt{\frac{y}{x}} \ , \quad z = (\sqrt{y} - \sqrt{x})^2$$

If ξ is large while $\xi/z < 1/2$, we have

$$J(x,y) \sim \frac{e^{-z}}{2\sqrt{2\pi\xi}} \quad S_\infty(x,y) \ \text{for} \ \eta < 1$$

$$J(x,y) \sim 1 + \frac{e^{-z}}{2\sqrt{2\pi\xi}} \quad S_\infty(x,y) \ \text{for} \ \eta > 1$$

where

$$S_\infty(x,y) = \sum_{m=0}^{\infty} \frac{A_m}{(2\xi)^m} \quad \left[1 + \frac{1+\eta}{1-\eta} \quad \beta_m(\xi,z)\right]$$

A_m is defined by (22), and $\beta_m(\xi,z)$ is defined by

$$\beta_0(\xi,z) = 1, \ \beta_m(\xi,z) = 1 + \sum_{k=1}^{m} B_{m,k}(\xi,z) \qquad (24)$$

$$B_{m,k}(\xi,z) = (-)^k \frac{2m(2m-2)\ldots(2m-2k+2)}{(2m-1)(2m-3)\ldots(2m-2k+1)} \left(\frac{2\xi}{z}\right)^k$$

The following computational scheme provides $J^{(n)}(x,y)$:

$$B_{m,1}(\xi,z) = -\frac{2m}{2m-1}\left(\frac{2\xi}{z}\right), \quad B_{m,k}(\xi,z) = -\frac{2m+2-2k}{2m+1-2k}\left(\frac{2\xi}{z}\right) B_{m,k-1}(\xi,z)$$

Compute $\beta_m(\xi,z)$ according to (24).

$$C_0 = 1 + \frac{1+\eta}{1-\eta}, \quad C_m = 1 + \frac{1+\eta}{1-\eta} \beta_m(\xi,z)$$

$$D_0 = C_0, \quad D_m = \frac{(2m-1)^2}{8m\xi} \cdot \frac{C_m}{C_{m-1}} \cdot D_{m-1}$$

$$S_n = \sum_{m=0}^{n} D_m = S_{n-1} + D_n$$

$$J^{(n)}(x,y) = \frac{e^{-z}}{2\sqrt{2\pi\xi}} S_n \quad \text{for } \eta < 1$$

$$J^{(n)}(x,y) = 1 + \frac{e^{-z}}{2\sqrt{2\pi\xi}} S_n \quad \text{for } \eta > 1$$

$$R_n = \left|\frac{D_n}{S_{n-1}}\right| \quad \text{for } \eta < 1$$

$$R_n = \frac{e^{-z}}{2\sqrt{2\pi\xi}} \left|\frac{D_n}{J^{(n-1)}(x,y)}\right| \quad \text{for } \eta > 1$$

Using arguments $x = 100$, $y = 0.1$, this scheme produces $J^{(10)}(x,y) = 3.13601 \times 10^{-42}$ with $R_{10} = 0.99 \times 10^{-6}$.

If ξ is large while $\xi/z > 1$, we have

$$J(x,y) \sim F(\xi,z) + \frac{1}{2} e^{-z} \sum_{m=1}^{\infty} \left[G_m(\xi) + H_m(\xi,z) \right]$$

where

$$F(\xi,z) = \frac{e^{-z}}{2\sqrt{2\pi\xi}} + \frac{1}{2}(1 \mp \operatorname{erf}\sqrt{z}), \operatorname{erf}\sqrt{z} = \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{z}} e^{-u^2} du \tag{25}$$

$$G_m(\xi) = \frac{A_m}{\sqrt{2\pi\xi}(2\xi)^m}$$

$$H_m(\xi,z) = \pm \frac{\alpha_m T_m(z)}{(2\xi+z)^m} \sqrt{\frac{z}{\pi}} \tag{26}$$

and A_m is defined in (22).

In (25) and (26) the upper signs are used if $\eta < 1$, and the lower signs are used if $\eta > 1$. In (26), note that $2\xi + z = (\sqrt{x} + \sqrt{y})^2$. α_m and $T_m(z)$ are defined by:

$$\alpha_m = \frac{1 \cdot 3 \cdot 5 \ldots (2m-1)}{2 \cdot 4 \cdot 6 \ldots (2m)}$$

$$T_1(z) = 1, \ T_2(z) = z + \frac{1}{2}, \ T_3(z) = z^2 + z + \frac{3}{4},$$

$$T_m(z) = z^{m-1} + \frac{1}{2}(m-1)z^{m-2} + \frac{1}{2} \cdot \frac{3}{2} \cdot \frac{(m-1)(m-2)}{2!} z^{m-3} + \cdots$$

$$+ \frac{1}{2} \cdot \frac{3}{2} \cdots (k - \frac{1}{2}) \cdot \frac{(m-1)(m-2)\ldots(m-k)}{k!} z^{m-k-1} + \ldots + \frac{1}{2} \cdot \frac{3}{2} \ldots (m - \frac{3}{2})$$

The following computational scheme provides $J^{(n)}(x,y)$:

$$G_1(\xi) = (8\xi\sqrt{2\pi\xi})^{-1}, \quad G_m(\xi) = \frac{(2m-1)^2}{8m\xi} G_{m-1}(\xi)$$

$$T_m(z) = \sum_{k=0}^{m-1} C_{m,k} z^{m-k-1}$$

$$\text{where } C_{m,0} = 1, \quad C_{m,k} = \frac{(k-\frac{1}{2})\,(m-k)}{k} \cdot C_{m,k-1}$$

$$H_1(\xi,z) = \pm \frac{\sqrt{z}}{2(2\xi+z)\sqrt{\pi}}, \quad H_m(\xi,z) = \frac{2m-1}{2m} \cdot \frac{T_m(z)}{T_{m-1}(z)} (2\xi+z)^{-1} H_{m-1}(\xi,z)$$

$$S_n = \sum_{m=1}^{n} \left[G_m(\xi) + H_m(\xi,z)\right] = S_{n-1} + G_n(\xi) + H_n(\xi,z)$$

$$J^{(n)}(x,y) = F(\xi,z) + \frac{1}{2} e^{-z} S_n$$

$$R_n = \frac{e^{-z}}{2} \left| \frac{G_n(\xi)+H_n(\xi,z)}{J^{(n-1)}(x,y)} \right|$$

Using arguments $x = 100$, $y = 10$, this scheme produces $J^{(10)}(x,y) = 3.61548 \times 10^{-22}$ with $R_{10} = 2.3 \times 10^{-7}$.

The following asymptotic expansion is useful when ξ is large and z is neither very large nor very small relative to ξ, in particular when $\xi \leqslant z \leqslant 2\xi$:

$$J(x,y) \sim M(\xi,z) + \frac{e^{-z}}{2\sqrt{2\pi\xi}} \sum_{m=1}^{\infty} \left[L_m(\xi) + K_m(\xi,z)\right] \text{ for } \eta < 1$$

$$J(x,y) \sim 1 + M(\xi,z) + \frac{e^{-z}}{2\sqrt{2\pi\xi}} \sum_{m=1}^{\infty} \left[L_m(\xi) + K_m(\xi,z)\right] \quad \text{for } \eta > 1$$

where

$$L_m(\xi) = \frac{A_m}{(2\xi)^m}$$

$$M(\xi,z) = \frac{e^{-z}}{2\sqrt{2\pi\xi}} \pm \frac{\sqrt{x}+\sqrt{y}}{2\sqrt{2\xi}} \operatorname{erfc}\sqrt{z} \quad , \quad \operatorname{erfc}\sqrt{z} = \frac{2}{\sqrt{\pi}} \int_{\sqrt{z}}^{\infty} e^{-u^2} du \tag{27}$$

$$K_m(\xi,z) = \frac{(x-y)\alpha_m S_m(z)}{(2\xi)^m}$$

and A_m and α_m remain as defined previously.

In (27) the plus sign is to be used if $\eta < 1$, and the minus sign if $\eta > 1$. Goldstein (1953) defines the function $S_m(z)$ by

$$S_m(z) = \frac{\Gamma(m-\frac{1}{2})}{\Gamma(\frac{1}{2})} - \frac{\Gamma(m-\frac{3}{2})}{\Gamma(\frac{1}{2})} z + \frac{\Gamma(m-\frac{5}{2})}{\Gamma(\frac{1}{2})} z^2 - \ldots$$

$$+ (-)^m \frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{1}{2})} z^{m-2} + (-)^{m-1} z^{m-1} + (-)^m z^{m-1} \sqrt{\pi z}\, e^z \operatorname{erfc}\sqrt{z}$$

$$S_1(z) = 1 - \sqrt{\pi z}\; e^z \operatorname{erfc}\sqrt{z}$$

and gives a recurrence relation which we write as

$$S_m(z) + zS_{m-1}(z) = \frac{\Gamma(m-\frac{1}{2})}{\Gamma(\frac{1}{2})} \qquad (m>1)$$

$\Gamma(\zeta)$ is the gamma function with argument ζ and has the property (Davis, 1965):

$$\frac{\Gamma(m-\frac{1}{2})}{\Gamma(\frac{1}{2})} = \frac{1\cdot3\cdot5\cdot7\cdots(2m-3)}{2^{m-1}} \qquad (m>1)$$

The following computational scheme provides $J^{(n)}(x,y)$:

$$L_1(\xi) = \frac{1}{8\xi}, \quad L_m(\xi) = \frac{(2m-1)^2}{8m\xi} L_{m-1}(\xi)$$

$$S_1(z) = 1 - \sqrt{\pi z}\, e^z \operatorname{erfc}\sqrt{z}$$

$$S_m(z) = N_m - zS_{m-1}(z)$$

where $N_1 = 1$, $N_m = \frac{2m-3}{2} N_{m-1}$

$$K_1(\xi,z) = \frac{(x-y)S_1(z)}{4\xi}$$

$$K_m(\xi,z) = \frac{2m-1}{4m\xi} \cdot \frac{S_m(z)}{S_{m-1}(z)} K_{m-1}(\xi,z)$$

$$J^{(n)}(x,y) = M(\xi,z) + \frac{e^{-z}}{2\sqrt{2\pi\xi}} \sum_{m=1}^{n} \left[L_m(\xi) + K_m(\xi,z)\right], \eta<1$$

$$J^{(n)}(x,y) = 1 + M(\xi,z) + \frac{e^{-z}}{2\sqrt{2\pi\xi}} \sum_{m=1}^{n} \left[L_m(\xi) + K_m(\xi,z)\right], \eta>1$$

$$R_n = \frac{e^{-z}}{2\sqrt{2\pi\xi}} \left| \frac{L_n(\xi) + K_n(\xi,z)}{J^{(n-1)}(x,y)} \right|$$

Using arguments $x = 100$, $y = 4$, this scheme produces $J^{(5)}(x,y) = 1.26273 \times 10^{-29}$ with $R_5 = 8.8 \times 10^{-8}$.

The computational routines for the asymptotic expansions given here can be performed on a desk-top electronic calculator, provided certain functions such as $\operatorname{erf}\sqrt{z}$, $\operatorname{erfc}\sqrt{z}$, and $e^{-z}/(2\sqrt{2\pi\xi})$ are calculated or obtained from tables and stored beforehand. For implementation with a digital computer, software routines are usually available for calculation of the error function or its complement; alternatively, rational approximations and asymptotic expansions are available and are easily coded (see, for example, Gautschi, 1965).

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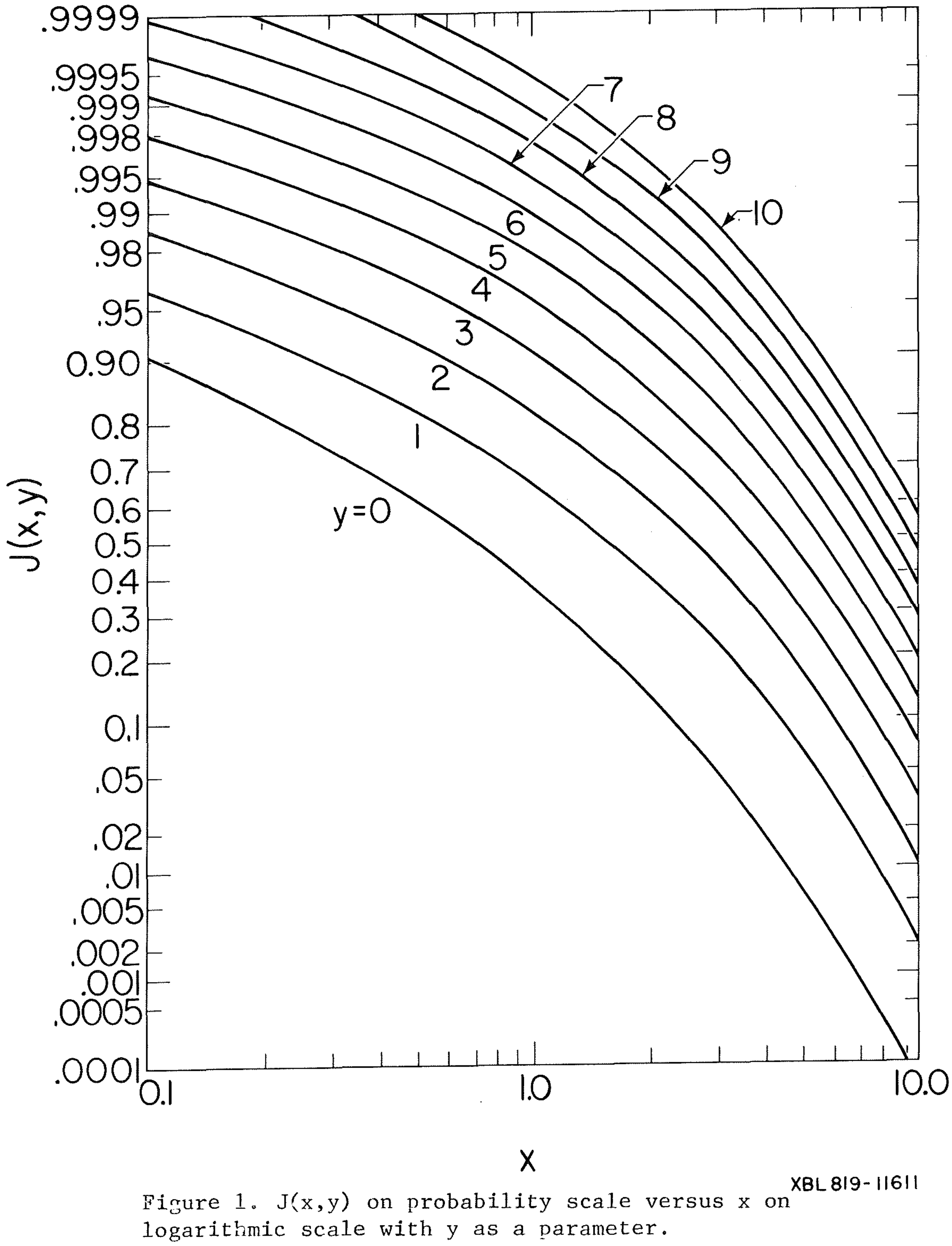

Figure 1. J(x,y) on probability scale versus x on logarithmic scale with y as a parameter.

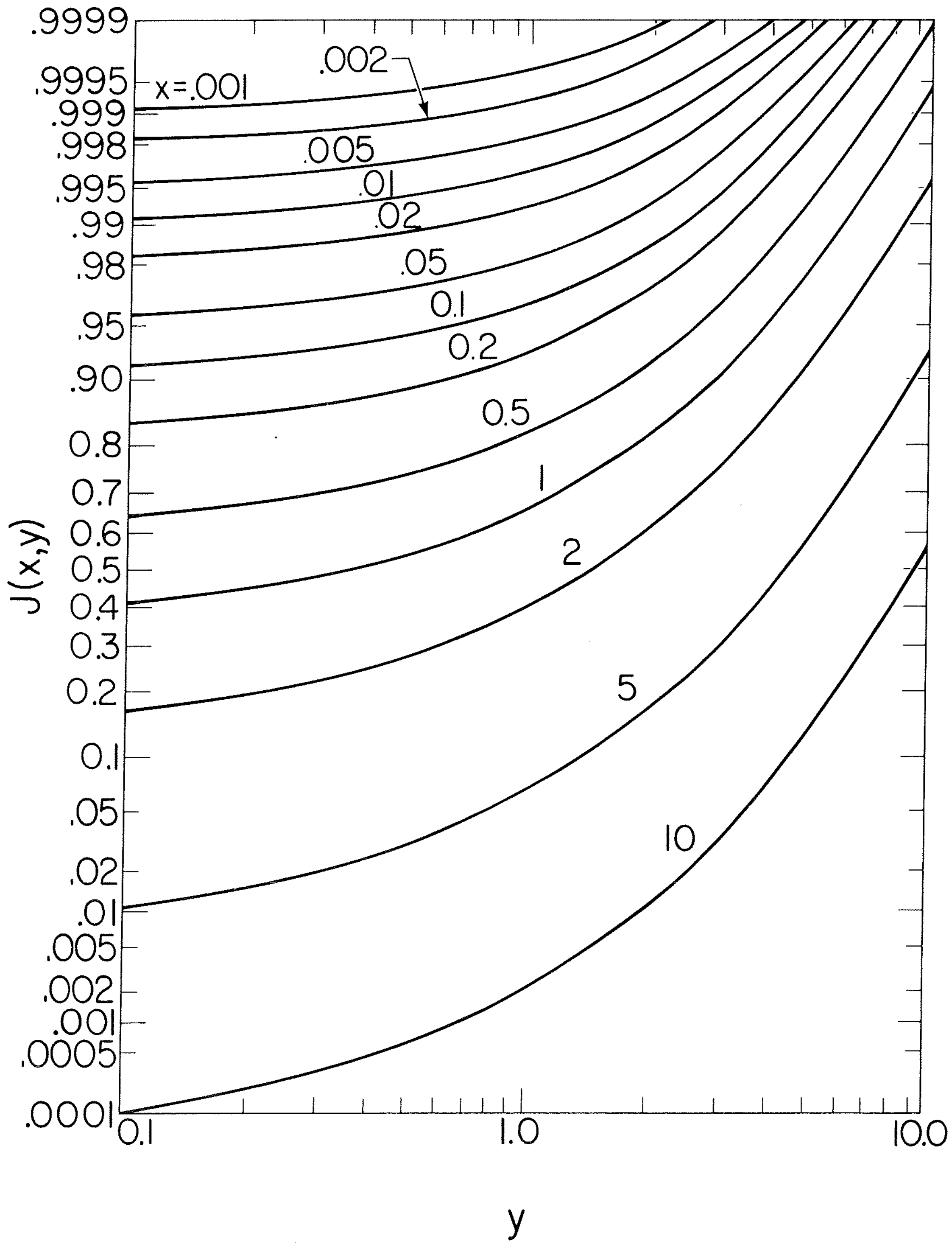

Figure 2. J(x,y) on probability scale versus y on logarithmic scale with x as a parameter.

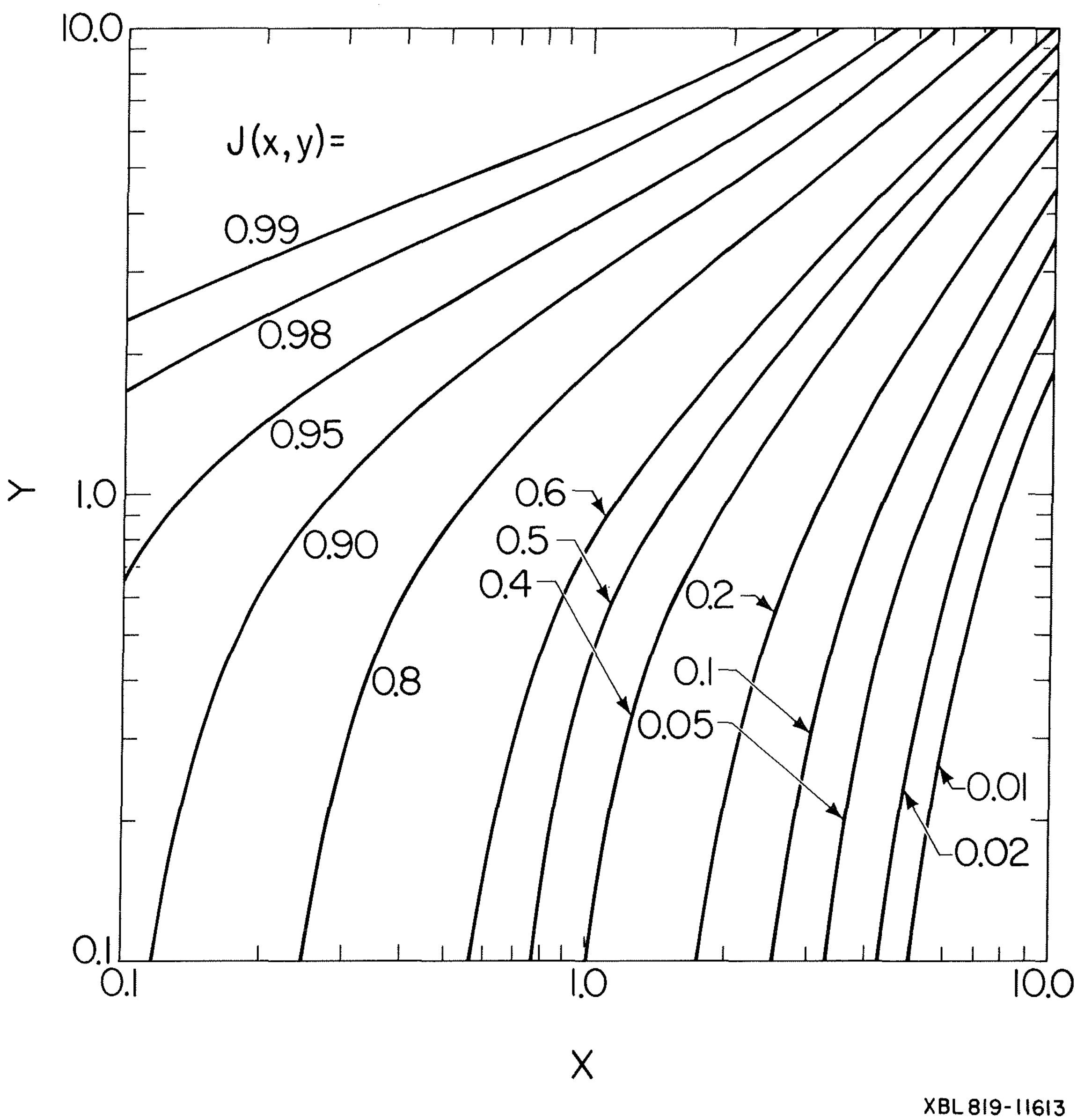

Figure 3. Curves of constant J(x,y) as functions of arguments x and y.

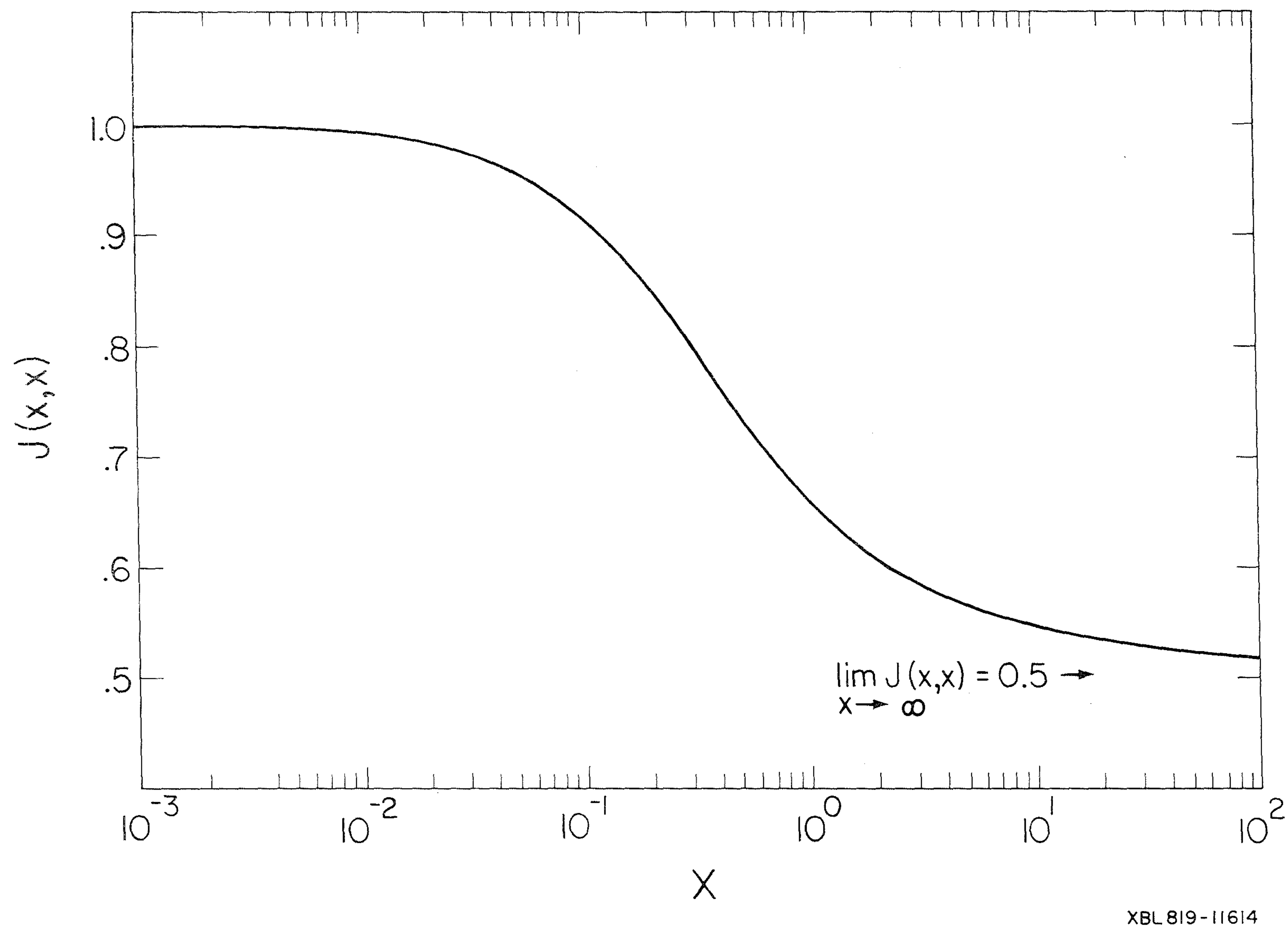

Figure 4. J(x,x) versus x.