Written: May 1970
Distributed: June 1970

LA-4448
UC-32, MATHEMATICS
AND COMPUTERS
TID-4500

LOS ALAMOS SCIENTIFIC LABORATORY
of the
University of California
LOS ALAMOS • NEW MEXICO

Approximation for the Inverse of the Klein-Nishina Probability Distribution

by

C. J. Everett
E. D. Cashwell

APPROXIMATION FOR THE INVERSE OF THE KLEIN-NISHINA PROBABILITY DISTRIBUTION

by

C. J. Everett

E. D. Cashwell

ABSTRACT

Approximate formulas, convenient for machine computation, and required in Monte Carlo practice, are given for the inverse of the Klein-Nishina probability distribution, permitting the direct determination of the energy E' of a Compton-scattered photon, from a uniformly distributed random number. The relative error does not exceed 3.2% over the range $0.001 \leq E < 100$ MeV of incident photon energies, and is usually much less, being at most 1%, for example, when $E' \geq .3E$ and $E/mc^2 > 4$.

---

1. Analysis of the Klein-Nishina cross section. The K-N cross section for scattering of a photon of "energy" $\alpha = E/mc^2$, on a free rest-electron, at an angle θ within $d\mu$ of $\mu = \cos\theta$ from its line of flight, is given by

$$\sigma(\alpha,\mu)d\mu = \pi r^2 \left(\frac{\alpha'}{\alpha}\right)^2 \left\{\frac{\alpha'}{\alpha} + \frac{\alpha}{\alpha'} + \mu^2 - 1\right\} d\mu, \quad -1 \leqq \mu \leqq 1,$$

where $\alpha' = \alpha/\{1+\alpha(1-\mu)\}$ is its final "energy" $\alpha' = E'/mc^2$, and $r = e^2/mc^2 \cong 2.82\times 10^{-13}$ cm is the electron "radius."

With α fixed throughout, we define $x = 1/\{1+\alpha(1-\mu)\}$, and $\tilde{\sigma}(\alpha,x)dx \equiv \sigma(\alpha,\mu)d\mu$. Thus $\mu = 1 + \alpha^{-1} - \alpha^{-1}x^{-1}$, $d\mu/dx = \alpha^{-1}x^{-2}$, and $\tilde{\sigma}(\alpha,x)dx = \pi r^2\alpha^{-1}\{x+x^{-1}+\mu^2-1\}dx$, with an associated probability density

$$p(x)dx = f(x)dx/F(\xi); \quad \xi \equiv \frac{1}{2\alpha+1} \leqq x \leqq 1,$$

where $f(x) = x+x^{-1}+\mu^2-1$, $\mu = 1+\alpha^{-1}-\alpha^{-1}x^{-1}$, and

$$F(\xi) = \int_\xi^1 f(x)dx \equiv G.$$

The Monte Carlo method of sampling for $x = \alpha'/\alpha$ consists of solving the equation

$$r = F(x)/G; \quad F(x) \equiv \int_x^1 f(x)dx$$

for x in terms of a random number r, equidistributed on [0,1]. Our object here is to approximate the inverse function $x = F^{-1}(y) \cong Q(y)$ of $y = F(x)$, and to take $x = F^{-1}(Gr) \cong Q(Gr)$.

Since $\mu - 1 = \alpha^{-1}(1-x^{-1})$ and $\mu + 1 = 2 + \alpha^{-1} - \alpha^{-1}x^{-1} = \alpha^{-1}(2\alpha+1-x^{-1}) = \alpha^{-1}(\xi^{-1}-x^{-1})$, we have

$$f(x) = x+x^{-1} + \alpha^{-2}(1-x^{-1})(\xi^{-1}-x^{-1}); \quad \xi \leqq x \leqq 1, \ \xi < 1 \quad (1)$$

with $f(\xi) = \xi + \xi^{-1} > 2 = f(1)$.

Differentiation yields

$$f'(x) = 1-x^{-2} + \alpha^{-2}x^{-2}(\xi^{-1}-2x^{-1}+1)$$

so $f'(\xi) = (1-\xi^{-1})(1+\xi^{-1}+\alpha^{-2}\xi^{-2}) < 0$ and $f'(1) = 2\alpha^{-1} > 0$.

Moreover, $f''(x) = 2\alpha^{-2}x^{-4}\{(\alpha^2-\xi^{-1}-1)x+3\} > 0$ on $[\xi,1)$, since $A(\alpha) \equiv \alpha^2 - \xi^{-1} - 1 = \alpha^2 - 2\alpha - 2 \geqq A(1) = -3$, and for $0 < \xi \leqq x \leqq 1$, one has $A(\alpha)x \geqq -3x \geqq -3$. Thus $f''(x) \geqq 0$, with equality iff $\alpha = 1$ and $x = 1$.

Finally, $f'''(x) = -6\alpha^{-2}x^{-5}\{A(\alpha)x+4\} < 0$ on $[\xi,1]$.

Integration of $f(x) = x+\alpha^{-2}\xi^{-1}+\alpha^{-2}A(\alpha)x^{-1}+\alpha^{-2}x^{-2}$ gives

$$F(x) = \tfrac{1}{2}(1-x^2)+\alpha^{-2}\xi^{-1}(1-x)+\alpha^{-2}A(\alpha)\log x^{-1} + \alpha^{-2}(x^{-1}-1) \quad (2)$$

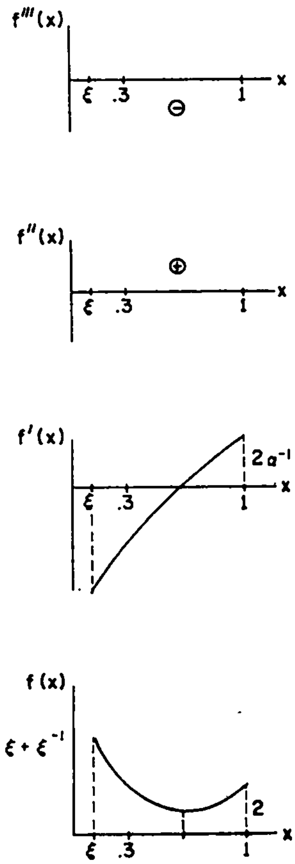
$$= (1-2\alpha^{-1}-2\alpha^{-2})\log x^{-1} + \tfrac{1}{2}(1-x^2)$$

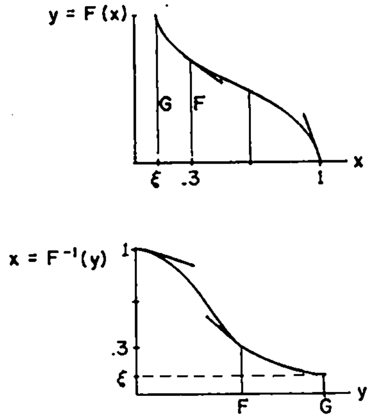
$$+ \alpha^{-2}\{\xi^{-1}(1-x)+(x^{-1}-1)\}.$$

Hence $F(\xi) = (1-2\alpha^{-1}-2\alpha^{-2})\log \xi^{-1} + \frac{\xi^2}{2}(\xi^{-2}-1) + 2\alpha^{-2}(\xi^{-1}-1)$, so

$$G \equiv F(\xi) = (1-2\alpha^{-1}-2\alpha^{-2})\log(2\alpha+1) + \frac{2\alpha(\alpha+1)}{(2\alpha+1)^2} + 4\alpha^{-1}; \quad F(1) = 0. \qquad (3)$$

These remarks show that $F(x)$ decreases from $F(\xi) = G$ to $F(1) = 0$, with $F'(x) = -f(x) < 0$, $F'(\xi) = -f(\xi) = -(\xi+\xi^{-1}) < -2 = -f(1) = F'(1)$, and has a unique inflection point at the minimum of $f(x)$, i.e., at the zero of $f'(x)$. Moreover, $F(x)$ is concave up to the left, and concave down to the right of the inflection point. The relations are indicated below in a qualitative way. (The 0.3 and F of the figures apply only in the case $\alpha > 7/6$ of Sec. 2.)





2. <u>The approximation Q(y)</u>. Case I. $(\alpha > 7/6)$. Guided by the graphs of Ref. 1, we assume $\log \sigma(E') \cong -\log E' + C_1$ for $\alpha > 7/6$ and $E' \leq 0.3E$, i.e., for $x \leqq 0.3$. Note that, for $\alpha > 7/6$, $\xi = 1/(2\alpha+1) < 0.3 < 1$ and 0.3 is on $(\xi,1)$. Since $\sigma(E') = C_2 f(x)$ and $E' = C_3 x$, this implies $\log f(x) \cong -\log x + C_4 = \log Cx^{-1}$, so that $f(x) \cong Cx^{-1}$ on $[\xi, 0.3]$. Hence

$$F(x) = \int_x^1 f(x)\,dx = \int_x^{0.3} + \int_{0.3}^1 \cong F(0.3) + \int_x^{0.3} Cx^{-1}dx,$$

and

$$y = F(x) \cong F + C\log(0.3/x); \quad \xi < x < 0.3,$$

where $F \equiv F(0.3)$, and the relation is exact at $x = 0.3$. We make it exact at $x = \xi$ also by defining

$$C = (G-F)/\log(0.3/\xi).$$

Hence we have $x = F^{-1}(y) \cong$

$$Q(y) \equiv 0.3\exp[-(y-F)\log(0.3/\xi)/(G-F)]; \quad \xi \leqq x \leqq 0.3,$$

$G \geqq y \geqq F$. In practice, therefore, we obtain from $r = F(x)/G$ the approximation $x \cong Q(Gr) = 0.3\exp[-\Lambda(r-J)]$, where $J \equiv F/G$, $\Lambda = \log(0.3/\xi)/(1-J)$, and $1 \geqq r \geqq J$. Substitution in Eq. (2) yields the required

$$F = F(0.3) = 1.65898 - 1.00796\alpha^{-1} + .62537\alpha^{-2},$$

while G is given by Eq. (3).

For $y = F(x)$ on $0.3 \leqq x \leqq 1$, we know $F(0.3) = F$, $F'(0.3) = -f(0.3) \equiv -f$, and $F(1) = 0$, $F'(1) = -f(1) = -2$. We assume a cubic $Q(y) = a_0+a_1y+a_2y^2+a_3y^3$, with $Q(F) = 0.3$, $Q'(F) = -1/f$, and $Q(0) = 1$, $Q'(0) = -1/2$. Thus Q and Q' are exact at the end points of $[0,F]$, and one finds $a_0 = 1$, $a_1 = -1/2$, $F^2a_2 = F+(F/f)-2.1$,

$F^3a_3 = -(F/2)-(F/f)+1.4$. We may therefore write Q in the convenient form

$$Q(y) = 1 - (F/2)(y/F) + (F^2a_2)(y/F)^2 + (F^3a_3)(y/F)^3.$$

We require from Eq. (1) the value

$$f \equiv f(0.3) = 3.63333 - 4.66667\alpha^{-1} + 5.44444\alpha^{-2}.$$

Thus for $r = F(x)/G$ on $J \geqq r \geqq 0$, we shall have

$$x = F^{-1}(Gr) \cong$$

$$Q(Gr) = 1-(F/2)(r/J)+(F^2a_2)(r/J)^2+(F^3a_3)(r/J)^3,$$

where $J = F/G$ as before.

Case II. $\alpha \leq 7/6$. Now $0.3 \leqq \xi < 1$, and we use a single, cubic approximation over the whole range which is exact, together with its derivative, at the end points. Demanding that $Q(y) = a_0+a_1y+a_2y^2+a_3y^3$, $Q(G) = \xi$, $Q'(G) = -1/f(\xi) \equiv -1/f$, and $Q(0) = 1$, $Q'(0) = -1/2$ determines $a_0 = 1$, $a_1 = -1/2$, $G^2a_2 = G+(G/f)-3(1-\xi)$, $G^3a_3 = -(G/2)-(G/f)+2(1-\xi)$, where now $f = \xi + \xi^{-1}$. Hence

$$Q(y) = 1-(G/2)(y/G)+(G^2a_2)(y/G)^2+(G^3a_3)(y/G)^3$$

and for arbitrary r on [0,1] we take $x = F^{-1}(Gr) \cong$

$$Q(Gr) = 1-(G/2)r+(G^2a_2)r^2+(G^3a_3)r^3.$$

3. Monte Carlo method for x in terms of r. These considerations lead to the following routine (page 4) for the approximate determination of $x = \alpha'/\alpha$ in terms of $r = F(x)/G$.

4. Test for accuracy of Q(y). In Case I ($\alpha > 7/6$) the method consisted of assigning to x the 15 values $x_i = 1, 0.9, 0.8, \cdots, 0.3; 0.3, 0.3-\delta, 0.3-2\delta, \cdots, 0.3-6\delta = \xi$, and computing for each $\alpha = 1.18, 1.20, 1.22, \cdots, 1.98; 2, 4, 6, \cdots, 200$, the exact value of $y_i = F(x_i)$ from Eq. (2), the corresponding approximation $x_i' = Q(y_i)$; and the relative error $e_i = (x_i'-x_i)/x_i$, where necessarily $e_1 = e_8 = e_9 = e_{15} = 0$. The same method was used in Case II, with $x_i = 1, 1-\delta, 1-2\delta, \cdots, 1-10\delta = \xi$ and $\alpha = 0.002, 0.022, 0.042, \cdots, 1.162$.

A machine computation by D. Turner showed all $|e_i| < 0.032$ in Case I, the maximum appearing at $\alpha = 1.422$, $x_i = 0.6$. For $\alpha \geqq 4$ and $x_i \geqq 0.3$ no $|e_i|$ exceeded 0.01, while for each $x_i \leqq 0.3$, each $|e_i|$ reached its maximum at $\alpha = 200$. In Case II, the maximal error $e = -0.031$ appeared at the center of the range for $\alpha = 0.842$. In both cases the average error is far less than the maximum.

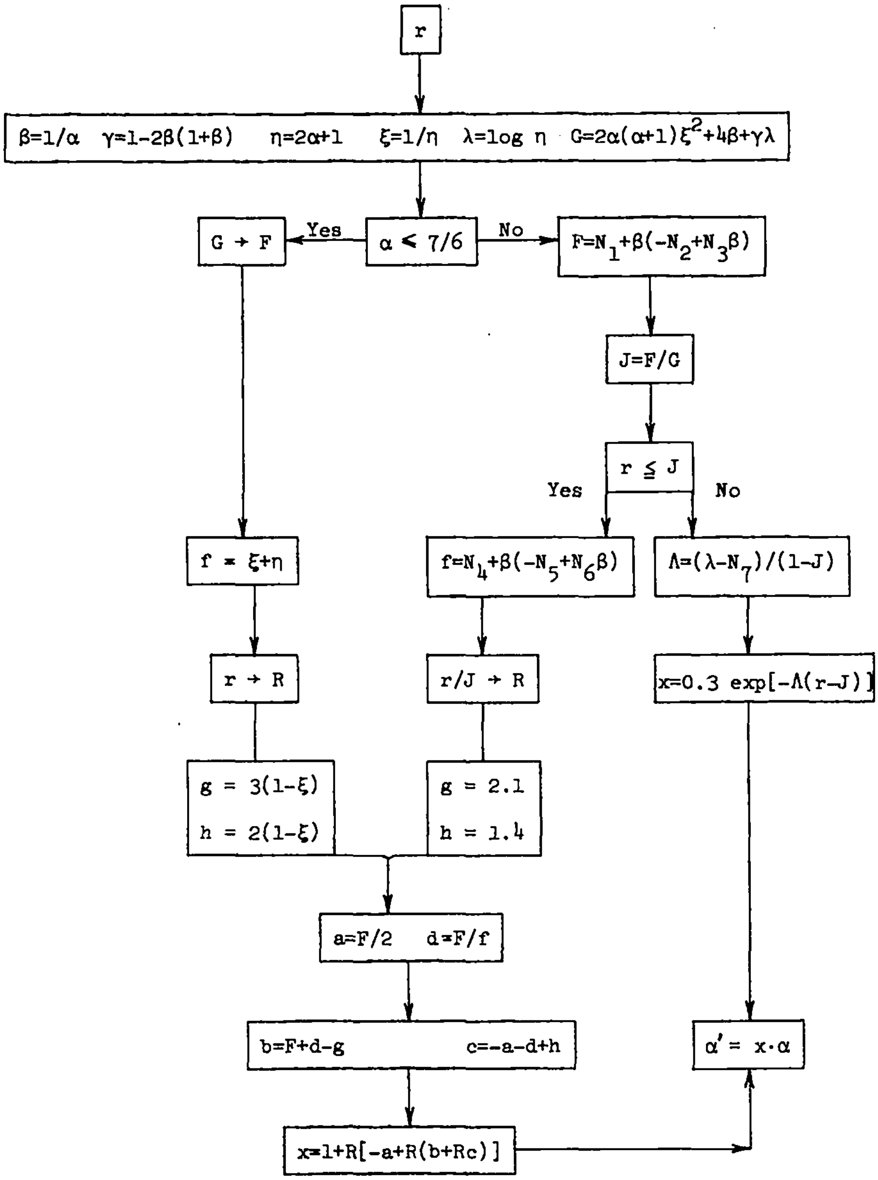
All previous Los Alamos photon routines have employed approximations for the inverse function by Carlson[2] for $\alpha \leq 4$ (maximum error ≅ 6%) and by E. D. Cashwell (cf. Ref. 3) for $4 < \alpha \leq 24$ (maximum error ≅ 4%). The present formulas permit efficient Monte Carlo treatment of Compton collisions from 1 keV up to 100 MeV, the extent of existing cross-section tables, with error, in the sense described, not exceeding 3.2%.

REFERENCES

1. A. T. Nelms, "Graphs of the Compton Energy-Angle Relationship and the Klein-Nishina Formula from 10 keV to 500 MeV," N.B.S. Circular 542, Aug. 28, 1953, Fig. VI.

2. B. Carlson, "The Monte Carlo Method Applied to a problem in γ-ray Diffusion," AECU-2857 (1953).

3. C. J. Everett, "A Relativity Notebook for Monte Carlo practice," LA-3839, (1968) p. 120.



$N_1 = 1.65898$

$N_2 = 1.00796$

$N_3 = 0.62537$

$N_4 = 3.63333$

$N_5 = 4.66667$

$N_6 = 5.44444$

$N_7 = 1.20397$