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A New Method of Sampling the Klein-Nishina Probability Distribution for All Incident Photon Energies Above 1 keV

(A Revised Complete Account)

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A NEW METHOD OF SAMPLING THE KLEIN-NISHINA PROBABILITY DISTRIBUTION FOR ALL INCIDENT PHOTON ENERGIES ABOVE 1 keV

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ABSTRACT

A Monte Carlo method is given for determination of the scattered photon energy in the distribution required by the Klein-Nishina differential cross section for Compton collision, with a relative error not exceeding 2.2% over the infinite range of incident energies above 1 keV. The present work is a self-contained account of the method and the underlying theory, and is intended to supersede earlier less complete reports. A somewhat revised flow chart is included which should help to reduce running time.

I. INTRODUCTION

The Klein-Nishina differential cross section for the scattering of a photon on a free electron at rest is given by

$$\sigma(\alpha;\mu)d\mu = \pi r^2(\alpha'/\alpha)^2 \{\alpha'/\alpha+\alpha/\alpha'+\mu^2-1\}d\mu; \ -1 \leq \mu \leq 1 \ , \qquad (1)$$

where $r=e^2/mc^2 \cong 2.82 \times 10^{-13}$ cm is the "radius" of the electron, α and α' are the incident and scattered photon energies in units of the electron rest energy mc^2, $\alpha' \equiv \alpha/\{1+\alpha(1-\mu)\}$, and $\mu = \cos\theta$, θ being the angle of scattering of the photon from its initial line of flight.

If, with α fixed throughout, we change variable from μ to

$$x = 1/\{1+\alpha(1-\mu)\};\ 1/(1+2\alpha) \equiv \xi \leq x \leq 1 \ , \tag{2}$$

we see that

$$\mu = 1+(1/\alpha)-(1/\alpha x);\ d\mu/dx = 1/\alpha x^2 \ , \tag{3}$$

and therefore the corresponding cross section is

$$\hat{\sigma}(\alpha;x)dx = \sigma(\alpha;\mu)(d\mu/dx)dx, \text{ or}$$

$$\hat{\sigma}(\alpha;x)dx = (\pi r^2/\alpha)(x+1/x+\mu^2-1)dx \ , \tag{4}$$

where $\mu = \mu(x)$ is given by (3). Defining the functions

$$f(x) = x+1/x+\mu^2-1,\ F(x)=\int_x^1 f(x)dx;\ \xi \leq x \leq 1 \ , \tag{5}$$

the probability density for x is seen to be

$$p(x) = f(x)/F(\xi);\ \xi \leq x \leq 1 \ , \tag{6}$$

with the (upper) distribution function

$$P(x) = F(x)/F(\xi);\ \xi \leq x \leq 1 \ . \tag{7}$$

Our object is to give a method of sampling the density $p(x)$ for x on $[\xi,1]$, and so obtaining the values of $\alpha' = \alpha x$, and $\mu = 1+1/\alpha-1/\alpha x$ for the scattered photon.

II. ANALYSIS OF THE FUNCTION $y = F(x)$

(a) We first note that

$$f(x) = (x+1/x)+\mu^2-1 \geq 2+0-1=1.$$

(b) We next write $f(x)$ explicitly in terms of x. From (3) we have

$$\mu-1 = \alpha^{-1}(1-x^{-1}),\ \mu+1 = 2+\alpha^{-1} - \alpha^{-1}x^{-1} = \alpha^{-1}(\xi^{-1}-x^{-1}),\ \text{whence}$$

$$f(x) = x+x^{-1}+\alpha^{-2}(1-x^{-1})(\xi^{-1}-x^{-1}) \ . \qquad (8)$$

In descending powers of x, this may be expressed as

$$f(x) = x+\alpha^{-2}\xi^{-1}+\alpha^{-2}A(\alpha)x^{-1}+\alpha^{-2}x^{-2} \ , \qquad (9)$$

$$\text{where } A(\alpha) = \alpha^2-2\alpha-2 \ . \qquad (10)$$

From (8) we find the end-point values

$$f(\xi) = \xi+\xi^{-1} > 2 = f(1) \qquad (11)$$

(c) Differentiating in (8) gives

$$f'(x) = 1-x^{-2}+\alpha^{-2}x^{-2}(1+\xi^{-1}-2x^{-1}) \qquad (12)$$

while from (9) we obtain

$$f'(x) = 1-\alpha^{-2}A(\alpha)x^{-2}-2\alpha^{-2}x^{-3} \qquad (13)$$

The slope end-point values from (12) are

$$f'(\xi) = 1-\xi^{-2}+\alpha^{-2}\xi^{-2}(1-\xi^{-1})=(1-\xi^{-1})(1+\xi^{-1}+\alpha^{-2}\xi^{-2}) < 0 \qquad (14)$$

$$f'(1) = \alpha^{-2}(1+1+2\alpha-2) = 2\alpha^{-1} > 0 \ . \qquad (15)$$

(d) Differentiation in (13) yields

$$f''(x) = 2\alpha^{-2}A(\alpha)x^{-3}+6\alpha^{-2}x^{-4} = 2\alpha^{-2}(A(\alpha)x+3)x^{-4} \geqslant 0 \ . \qquad (16)$$

For clearly $A(\alpha) \equiv \alpha^2-2\alpha-2 \geqq -3$, and $A(\alpha)x+3 \geqq$

$-3x+3 \geqslant 0$ since $0 < x \leqslant 1$. In fact, $f''(x)=0$ iff $\alpha=1$ and $x=1$.

(e) From (16) we have

$$f'''(x) = -6\alpha^{-2}A(\alpha)x^{-4}-24\alpha^{-2}x^{-5}$$
$$= -6\alpha^{-2}x^{-5}(A(\alpha)x+4) < 0 \quad , \qquad (17)$$

since $A(\alpha)x+3 \geq 0$ as noted above.

(f) Integration of (9) shows that

$$F(x) = \int_x^1 f(x)dx$$
$$=(1/2)(1-x^2)+\alpha^{-2}\xi^{-1}(1-x)+\alpha^{-2}A(\alpha)\log x^{-1}+\alpha^{-2}(x^{-1}-1)$$
$$=(1/2)(1-x^2)+\alpha^{-2}\{\xi^{-1}(1-x)+A(\alpha)\log x^{-1}+(x^{-1}-1)\} \quad . \qquad (18)$$

From this we obtain the end-point values

$$F(1) = 0 \quad , \qquad (19)$$

and, since $\xi = 1/(1+2\alpha)$,

$$F(\xi) = \frac{2\alpha(1+\alpha)}{(1+2\alpha)^2} + 4\alpha^{-1} + \alpha^{-2}A(\alpha)\log(1+2\alpha) \equiv G \quad . \qquad (20)$$

These remarks show that $y = F(x)$ decreases from

$$F(\xi) = G \text{ to } F(1) = 0, \text{ with } F'(x) = -f(x) < 0 \text{ on } [\xi,1],$$

and has end-point slopes

$$F'(\xi) = -f(\xi) = -(\xi+\xi^{-1}) < -2 = -f(1) = F'(1).$$

Moreover $F(x)$ has a unique inflection point at the minimum of $f(x)$, i.e., at the zero ζ of $f'(x)$, being concave up to the left and concave down to the right of the inflection point. The behavior of the several functions is indicated schematically in Fig. 1.

This analysis was made in Ref. 1 but omitted from Ref. 2.

III. APPROXIMATION OF $F^{-1}(y)$, $.002 \leq \alpha < \alpha_0 = 202$

A direct method of sampling the density p(x) of Eq. (6) for x on $[\xi,1]$ consists in solving the equation $r=P(x)=F(x)/F(\xi)$ for x in terms of a random number r uniformly distributed on [0,1]. We obtain in this section an approximating function Q(y) to the inverse $F^{-1}(y)$ of the function F(x) of Eq. (18), thus enabling us to obtain

$$x = F^{-1}(rF(\xi)) \cong Q(rF(\xi)) \quad ,$$

where $F(\xi)$ is computed exactly from Eq. (20).

For an arbitrary x_0 on $(\xi,1)$, we define a composite approximating function Q(y), $0 \leq y \leq G \equiv F(\xi)$, which is cubic on $0 \leq y \leq F_0 \equiv F(x_0)$, and exponential on $F_0 \leq y \leq G$. Moreover, Q(y) will coincide with $F^{-1}(y)$ at the end points of the second interval, and Q(y), $Q'(y)$ will coincide with $F^{-1}(y)$, $(F^{-1}(y))'$ at the end points of the first. (See Fig. 2.)

For this we require the value of G from Eq. (20), and formulas for $F(x_0)$ and $f(x_0)$ from (18) and (8), namely

$$F_0 \equiv F(x_0) = \tfrac{1}{2}(1-x_0^{\,2}) + \alpha^{-2}\{\xi^{-1}(1-x_0) + (x_0^{-1}-1)\} - \alpha^{-2}A(\alpha)\log x_0 \qquad (21)$$

$$f_0 \equiv f(x_0) = x_0+x_0^{-1} + \alpha^{-2}(1-x_0^{-1})(\xi^{-1}-x_0^{-1}) \quad . \qquad (22)$$

If we assume $f(x) \cong Cx^{-1}$ on $[\xi,x_0]$, we shall have

$$F(x) \equiv \int_x^{x_0} f(x)dx + \int_{x_0}^{1} f(x)dx \cong C\log x_0/x + F_0 \equiv L(x)$$

for x on that interval. Moreover, $F(x_0) = F_0 = L(x_0)$ necessarily and $F(\xi) = L(\xi)$ provided we define the constant

$$C = (G-F_0)/\log(x_0/\xi) \quad . \qquad (23)$$

Hence we obtain the approximation

$$Q(y) = L^{-1}(y) = x_0 \exp\left\{-\frac{y-F_0}{G-F_0}\log(x_0/\xi)\right\}; \; F_0 \leq y \leq G \quad . \qquad (24)$$

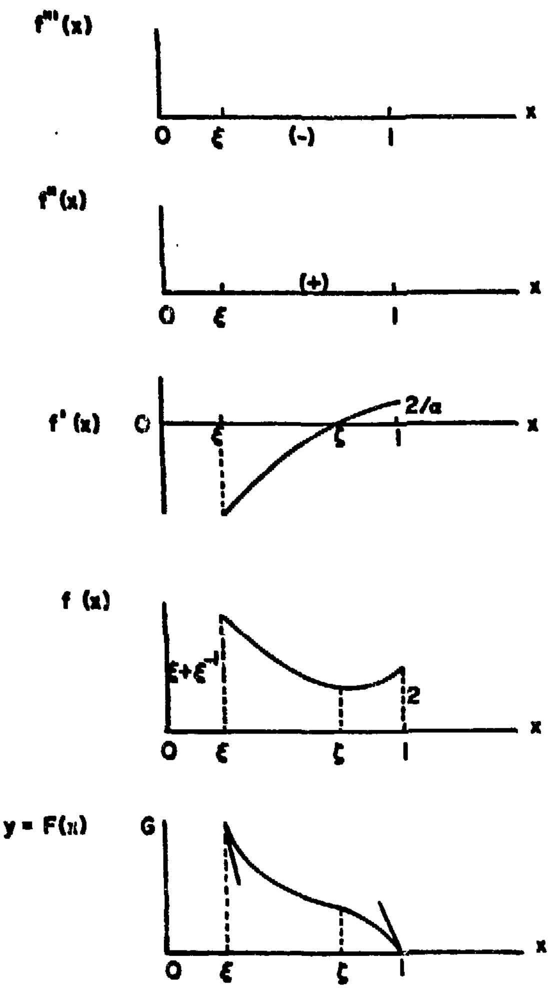

Fig. 1. The behavior of $y = F(x)$.

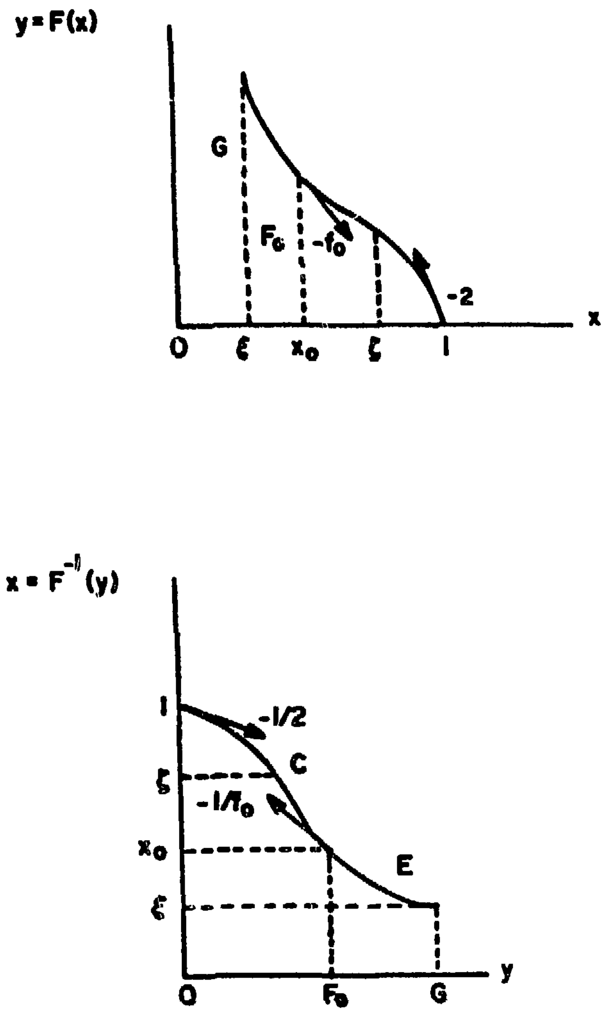

Fig. 2. The functions $y = F(x)$ and $x = F^{-1}(y)$.

In practice therefore, for a random number r such that $J_0 \equiv F_0/G \leqslant r \leqslant 1$, we take

$$x = F^{-1}(rG) \cong Q(rG) = x_0 \exp\{-\Lambda_0(r-J_0)\} \quad , \tag{25}$$

$$\text{where } \Lambda_0 \equiv \log(x_0/\xi)/(1-J_0),\ J_0 \equiv F_0/G \quad . \tag{26}$$

On the interval $0 \leqslant y \leqslant F_0$, we assume a cubic approximation $F^{-1}(y) \cong Q(y) = a_0+a_1y+a_2y^2+a_3y^3$, and demand that $Q(y), Q'(y)$ be exact at the end points of this interval. Since

$$F(1)=0 \qquad\qquad F(x_0)=F_0$$

$$F'(1)=-f(1)=-2 \qquad\qquad F'(x_0)=-f(x_0)=-f_0 \quad ,$$

this requires that

$$Q(0)=1 \qquad\qquad Q(F_0)=x_0$$

$$Q'(0)=-1/2 \qquad\qquad Q'(F_0)=-1/f_0 .$$

It follows that the cubic has the form

$$Q(y) = 1+A_0(y/F_0)+B_0(y/F_0)^2+C_0(y/F_0)^3;\ 0 \leqslant y \leqslant F_0 \tag{27}$$

$$A_0 = -F_0/2,\ B_0 = F_0+(F_0/f_0)-3(1-x_0),\ C_0 = -(F_0/2)-(F_0/f_0)+2(1-x_0) \quad . \tag{28}$$

Hence, for a random number r on $0 \leqslant r < J_0 = F_0/G$, we take $x = F^{-1}(rG) \cong Q(rG)$

$$=1+A_0(r/J_0)+B_0(r/J_0)^2+C_0(r/J_0)^3 \quad . \tag{29}$$

Although the above argument is valid for an arbitrary $\alpha > o$, we shall apply it only on the range $.002 \leqslant \alpha < 202$ (~103 MeV), with an α-dependent point of subdivision of the corresponding interval $(\xi,1)$, namely

$$x_0 = x_0(\alpha) = \xi+(1-\xi)\phi(\alpha) \quad , \tag{30}$$

where the values of $\phi(\alpha)$ are given in Table I.

The absolute relative errors $|\varepsilon|$ listed were obtained by a method described in Sec. VI.

IV. APPROXIMATION OF $F^{-1}(x)$, $\alpha_0 = 202 \leq \alpha < \infty$

We first show that, for any fixed $\alpha_0 > 2$ and arbitrary incident energy $\alpha \geq \alpha_0$, the relative error incurred in replacing the exact distribution P(x) of Sec. I by that based on the simple function $f_1(x) = x+x^{-1}$ does not exceed $4/(\alpha_0-2)$, which is .02 for the α_0=202 we have adopted.

From Eq. (8), it appears that the original function $f(x)$ may be written in the form

$$f(x) = f_1(x)-f_2(x), \; \xi \leq x \leq 1 \quad , \tag{31}$$

where $f_1(x) = x+x^{-1} \geq 2$ and

$$f_2(x) = \alpha^{-2}(x^{-1}-1)(\xi^{-1}-x^{-1}) = \alpha^{-1}(x^{-1}-1)(2-\alpha^{-1}(x^{-1}-1)) \geq 0 \quad . \tag{32}$$

Since $0 \leq x^{-1}-1 < x^{-1}$, and $0 \leq 2-\alpha^{-1}(x^{-1}-1) \leq 2$, we have

TABLE I

THE FUNCTION $\phi=\phi(\alpha)$

$.002 \leq \alpha < .962$	$\phi = .25$	$\lvert\varepsilon\rvert = .0211$
$.962 \leq \alpha < 1.642$	$\phi = .20$	$\lvert\varepsilon\rvert = .0218$
$1.642 \leq \alpha < 2.002$	$\phi = .17$	$\lvert\varepsilon\rvert = .0218$
$2.002 \leq \alpha < 10$	$\phi = .15$	$\lvert\varepsilon\rvert = .0213$
$10 \leq \alpha < 52$	$\phi = .25$	$\lvert\varepsilon\rvert = .0177$
$52 \leq \alpha < 202$	$\phi = .25$	$\lvert\varepsilon\rvert = .0194$

$$f_2(x) < \alpha^{-1}\ (x^{-1})(2) < (2/\alpha)\ f_1(x), \text{ or}$$

$$f_1(x) > (\alpha/2)\ f_2(x) \quad . \tag{33}$$

Consequently,

$$f(x) > (\alpha/2)f_2(x) - f_2(x) = (\alpha-2)f_2(x)/2, \text{ and since } \alpha \geqslant \alpha_0 > 2,$$

$$f_2(x) < 2f(x)/(\alpha-2) \quad . \tag{34}$$

Defining the integrals

$$F_1(x) = \int_x^1 f_1(x)dx,\ F(x) = \int_x^1 f(x)dx;\ \xi \leqslant x \leqslant 1 \quad , \tag{35}$$

we see that, for $x \neq 1$,

$$0 < F_1(x) - F(x) = \int_x^1 (f_1(x) - f(x))dx = \int_x^1 f_2(x)dx$$

$$< \frac{2}{\alpha-2} \int_x^1 f(x)dx = \frac{2}{\alpha-2} F(x) \quad , \tag{36}$$

and in particular

$$0 < G_1 - G < \frac{2}{\alpha-2} G \quad , \tag{37}$$

where $\qquad G_1 = F_1(\xi) \text{ and } G = F(\xi) \quad .$

Hence the relative error $\varepsilon(x)$ involved in replacing $F(x)/G$ by the simpler distribution $F_1(x)/G_1$ on the interval $\xi \leqslant x < 1$ satisfies

$$|\varepsilon(x)| \equiv \left| \frac{F_1(x)}{G_1} - \frac{F(x)}{G} \right| \Bigg/ \left(\frac{F(x)}{G}\right)$$

$$\leq \{G|F_1(x)-F(x)|+F(x)|G-G_1|\}/G_1F(x)$$

$$\leq \{\frac{2}{\alpha-2} GF(x)+ \frac{2}{\alpha-2} F(x)G\}/G_1F(x) = \frac{4}{\alpha-2} (\frac{G}{G_1}) < \frac{4}{\alpha-2} \quad . \tag{38}$$

Similarly one may show the same bound for the error in replacing the density $f(x)/G$ by $f_1(x)/G_1$, namely

$$|\hat{\varepsilon}(x)| \equiv \left|\frac{f_1(x)}{G_1} - \frac{f(x)}{G}\right| \Big/ (\frac{f(x)}{G}) < \frac{4}{\alpha-2} \quad . \tag{39}$$

Note that $|\varepsilon(x)| \leq 4/(\alpha_0-2)$ for all $\alpha \geq \alpha_0(> 2)$, and in fact $\varepsilon(x)\to 0$ uniformly in x as $\alpha \to \infty$.

Since inversion of the distribution function $F_1(x)/G_1$ is difficult, we resort to the following well-known device. We write $f_1(x) = a_1(x)+a_2(x)$, where $a_1(x) = x^{-1}$, $a_2(x) = x$. Setting

$A_i(x) = \int_x^1 a_i(x)dx$ and $A_i = A_i(\xi)$, the underlying density has

the form

$$f_1(x)/G_1 = \left(\frac{A_1}{G_1}\right) \frac{a_1(x)}{A_1} + \left(\frac{A_2}{G_1}\right) \frac{a_2(x)}{A_2} \quad . \tag{40}$$

Hence, choosing the auxiliary density $a_i(x)/A_i$ with probability A_i/G_1, and x in the corresponding distribution $A_i(x)/A_i$ yields x with the required density $f_1(x)/G_1$. Setting a random number $r = A_i(x)/A_i$ in the usual way gives

$$x = \exp(r \log \xi) \quad \text{or} \quad x = (1-r(1-\xi^2))^{1/2} \tag{41}$$

in the two cases. For the probabilities A_i/G_1 one requires the values

$$A_1 = \log \xi^{-1},\ A_2 = (1-\xi^2)/2,\ G_1 = A_1+A_2 \quad . \tag{42}$$

Note. The square root in (41) may be obviated, if desired, by setting

$$x = \xi + \max\{(1-\xi)r,\ (1+\xi)s-2\xi\}\ ,$$

where r,s are independent random numbers.[3,4]

V. A FLOW CHART

We include here a complete procedure for obtaining, from a given incident photon energy $\alpha = E(\text{MeV})/.511 \geq .002$, the value of x in the distribution $F(x)/F(\xi)$ of Sec. I. From x one obtains for the scattered photon the deflection cosine

$$\mu = \cos\theta = 1+(1/\alpha)-(1/\alpha x)$$

and the final energy $E' = .511\ \alpha'(\text{MeV})$, where $\alpha' = \alpha x$.

The value $\alpha_0 = 202$ is understood below.

1. $\eta = 1+2\alpha$
2. $\xi = 1/\eta$
3. $N = \log\eta$
4. $\alpha \geq \alpha_0 \rightarrow (5) \qquad \alpha < \alpha_0 \rightarrow (11)$
5. $T = 1-\xi^2$
6. $G_1 = N+(T/2)$
7. Generate r, r'
8. $G_1 r' < N \rightarrow (9) \qquad G_1 r' \geq N \rightarrow (10)$
9. $x = \exp(-Nr)$ Exit
10. $x = (1-rT)^{1/2}$ Exit (see Note, Sec. IV)
11. $\beta = 1/\alpha$
12. Set $\phi = \phi(\alpha)$ (see Table I, Sec. III)
13. $x_0 = \xi+\phi(1-\xi)$
14. $M = \log x_0$
15. $K_1 = 1-x_0$
16. $K_2 = 1/x_0$
17. $K_3 = 1-2\beta(1+\beta)$
18. $F_0 = K_1\{(1/2)(1+x_0)+\beta^2(\eta+K_2)\}-MK_3$
19. $G = 2\ \alpha(1+\alpha)\xi^2+4\beta+NK_3$
20. $J_0 = F_0/G$
21. Generate r

22. $r < J_0 \rightarrow (23)$ $r \geq J_0 \rightarrow (32)$

23. $R = r/J_0$

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27. $f_0 = x_0+K_2+\beta^2(1-K_2)(\eta-K_2)$

28. $A_0 = -F_0/2$

29. $B_0 = F_0+(F_0/f_0)-3K_1$

30. $C_0 = A_0-(F_0/f_0)+2K_1$

31. $x = 1+R\,\{A_0+R(B_0+RC_0)\}$ Exit

32. $\Lambda_0 = (M+N)/(1-J_0)$

33. $x = x_0 \exp\{-\Lambda_0(r-J_0)\}$ Exit

Note. This is essentially the method given earlier [2]. The few changes may serve to decrease computing time. Steps (24-26) are purposely omitted, and the previous numbering has been retained.

VI. THE RELATIVE ERROR ON $.002 \leq \alpha \leq 202$

This final section gives an account of the errors listed in Table I of Sec. III. The method used in testing the accuracy of the approximation $x' = Q(y) \cong x = F^{-1}(y)$ for a particular α_h on [.002, 202] and x_{hi} on $[\xi_h, 1]$ consisted in computing the exact value of $F(x_{hi}) = y_{hi}$ from Eq. (18), the corresponding approximation $Q(y_{hi}) = x'_{hi} \cong x_{hi}$ by the formulas of Sec. III, and the relative error $\varepsilon_{hi} = (x'_{hi}-x_{hi})/x_{hi}$.

The α interval [.002, 2.002] was tested in this way for the 101 energies α_h = .002, .022,..., 2.002, using the α - dependent division point $x_0 = \xi_h+\phi(1-\xi_h)$ for each of the values ϕ = .15, .17, .20, .25, the interval $[\xi_h, x_0]$ being subdivided into 6 equal intervals, and $[x_0, 1]$ into 7, by a sequence of test points x_{hi}. In the same way, the α interval [2, 52] was tested at α_h = 2. 2.5,..., 52 for ϕ = .15, .20, .25, and the interval [52, 202] at α_h = 52, 53.5,..., 202 for ϕ = .25. The results showed the maximal absolute relative error to be minimal for the correlated α ranges and ϕ values tabulated in Sec. III. The accuracy could be still further improved by more refined machine search, but the present bounds are sufficiently good for our purposes.

REFERENCES

1. C. J. Everett, E. D. Cashwell, "Approximation for the Inverse of the Klein-Nishina Probability Distribution," Los Alamos Scientific Laboratory report LA-4448 (1970).

2. C. J. Everett, E. D. Cashwell, G. D. Turner, "A New Method of Sampling the Klein-Nishina Probability Distribution for All Incident Photon Energies Above 1 keV," Los Alamos Scientific Laboratory report LA-4663 (1971).

3. C. J. Everett, E. D. Cashwell, G. D. Turner, "A Method of Sampling Certain Probability Densities Without Inversion of the Distribution Functions," Los Alamos Scientific Laboratory report LA-5407-MS (1973).

4. C. J. Everett, E. D. Cashwell, "A Monte Carlo Sampler," Los Alamos Scientific Laboratory report LA-5061-MS (1972), p.20, C9.