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ABSTRACT

A Monte Carlo method is given for accurate determination of scattered photon energy in the distribution required by the Klein-Nishina cross section for Compton collisions. The relative error does not exceed 2.2% for all incident energies above 1 keV.

I. INTRODUCTION

In the Compton scattering of a photon of energy $\alpha(= E/mc^2)$ on a free electron at rest, the Klein-Nishina cross section requires that the probability distribution for the ratio $x = \alpha'/\alpha$ (of scattered to incident photon energy) be given by $P(x) = F(x)/F(\xi)$, $\xi \equiv (1 + 2\alpha)^{-1} \leqslant x \leqslant 1$, where $F(x) = \int_x^1 f(x)dx$, $f(x) = x + x^{-1} + \mu^2 - 1$, and $\mu = 1 + \alpha^{-1} - \alpha^{-1}x^{-1}$, as shown in LA-4448. Hence, sampling the distribution $P(x)$ for $x = \alpha'/\alpha$ provides a Monte Carlo method of obtaining the new energy α' and scattering cosine μ.

For an incident energy $\alpha > \alpha_0 > 2$, Section II shows that the relative error in replacing $P(x)$ by the simpler distribution $F_1(x)/F_1(\xi)$, $F_1(x) \equiv \int_x^1 (x + x^{-1})dx$, does not exceed $4/(\alpha_0 - 2)$. Consequently, with this accuracy, x may be found from the latter distribution by a standard device involving two random numbers and no further approximation.

For $0.002 \leqslant \alpha \leqslant \alpha_0$, we set a random number $r = P(x) = F(x)/F(\xi)$, and obtain $x = F^{-1}(rF(\xi)) \cong Q(rF(\xi))$, where $Q(y)$ is an approximation function for $F^{-1}(y)$. The function $Q(y)$, defined in Section III, is cubic on $[0,F(x_0)]$ and exponential on $[F(x_0),F(\xi)]$, x_0 being an α-dependent parameter subdividing the interval $(\xi,1)$.

Adopting the values of α_0 and $x_0(\alpha)$, specified in Section IV, insures that the relative error in x does not exceed 2.2% over the entire range $0.002 \leqslant \alpha < \infty$. The approximation function $Q(y)$ represents a considerable improvement over that proposed before,[1] due to the α-dependence of x_0. The tests used for accuracy are described, and a flow diagram included, in Section IV.

II. THE METHOD FOR $\alpha > \alpha_0$

The function $f_0(x) \equiv f(x) = x + x^{-1} + \alpha^{-2}(1 - x^{-1})(\xi^{-1} - x^{-1})$ may be written in the form

$$f_0(x) = f_1(x) - f_2(x), \qquad \xi \leqslant x \leqslant 1 \qquad (1)$$

where

$$f_1(x) = x^{-1} + x > 0$$

$$f_2(x) = \alpha^{-1}(x^{-1} - 1)[2 - \alpha^{-1}(x^{-1} - 1)] \geqslant 0 \quad . (2)$$

Since $0 \leqslant f_1(x) - f_0(x) = f_2(x) < 2\alpha^{-1}x^{-1} < 2\alpha^{-1}f_1(x)$, hence also $f_0(x) = f_1(x) - f_2(x) > f_1(x) - 2\alpha^{-1}f_1(x) = (1 - 2\alpha^{-1})f_1(x)$, we have the inequality

$$0 \leqslant f_1(x) - f_0(x) < 2f_0(x)/(\alpha - 2) \ , \quad \alpha > 2 \ . \quad (3)$$

For the integrals $F_i(x) = \int_x^1 f_i(x)dx$ therefore,

$$0 \leq F_1(x) - F_0(x) < 2F_0(x)/(\alpha - 2) \ , \quad \xi \leq x \leq 1 \quad (4)$$

in particular

$$0 < F_1 - F_0 < 2F_0/(\alpha - 2) \quad (5)$$

where $F_i \equiv F_i(\xi)$.

Consequently, the relative error $\varepsilon(x)$ in replacing $F_0(x)/F_0$ by the simpler distribution $F_1(x)/F_1$ satisfies

$$\varepsilon(x) = \left|\frac{F_1(x)}{F_1} - \frac{F_0(x)}{F_0}\right| \bigg/ \left(\frac{F_0(x)}{F_0}\right)$$

$$\leq [F_0|F_1(x) - F_0(x)| + F_0(x)|F_1 - F_0|] \big/ F_1F_0(x)$$

$$< \left[F_0\left(\frac{2}{\alpha - 2}\right)F_0(x) + F_0(x)\left(\frac{2}{\alpha - 2}\right)F_0\right] \bigg/ F_1F_0(x)$$

$$= \frac{4}{\alpha - 2}\left(\frac{F_0}{F_1}\right) < \frac{4}{\alpha - 2} \quad . \quad (6)$$

Similarly, one may show

$$\varepsilon'(x) \equiv \left|\frac{f_1(x)}{F_1} - \frac{f_0(x)}{F_0}\right| \bigg/ \left(\frac{f_0(x)}{F_0}\right) < \frac{4}{\alpha - 2}$$

for the relative error in the corresponding densities at each point. Note that $\varepsilon(x) < 4/(\alpha_0 - 2)$ for all $\alpha > \alpha_0$, and $\varepsilon(x) \to 0$ uniformly as $\alpha \to \infty$.

Since the function $F_1(x)$ has an inverse difficult to fit, we resort to the following well-known strategy. The variable x has distribution $F_1(x)/F_1$ iff it has density $f_1(x)/F_1$. We write $f_1(x) = a_1(x) + a_2(x)$, where $a_1(x) \equiv x^{-1}$ and $a_2(x) \equiv x$. Setting $A_i(x) = \int_x^1 a_i(x)dx$ and $A_i = A_i(\xi)$ this x density may be expressed in the form

$$\frac{f_1(x)}{F_1} = \left(\frac{A_1}{F_1}\right)\frac{a_1(x)}{A_1} + \left(\frac{A_2}{F_1}\right)\frac{a_2(x)}{A_2} \quad .$$

Hence, choosing the auxiliary density $a_i(x)/A_i$ with probability A_i/F_1, and x in the corresponding distribution $A_i(x)/A_i$, yields x with the required density $f_1(x)/F_1$.

Setting a random number $r = A_i(x)/A_i$ in the usual way gives

$$x = \exp[r \ln \xi] \quad \text{or} \quad x = [1 - r(1 - \xi^2)]^{1/2}$$

in the two cases. For the probabilities A_i/F_1 one requires the values $A_1 = \ln \xi^{-1}$, $A_2 = (1/2)(1 - \xi^2)$, and $F_1 = A_1 + A_2$.

<u>Note</u>: The inversion involved in the square root value of x above 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.[2]

III. APPROXIMATION OF $F^{-1}(x)$, $0.002 \leq \alpha \leq \alpha_0$

The function $f(x) = x + x^{-1} + \alpha^{-2}(1 - x^{-1})(\xi^{-1} - x^{-1})$, $\xi \leq x \leq 1$, has the integral $F(x) = \int_x^1 f(x)dx = (1/2)(1 - x^2) + \alpha^{-2}[\xi^{-1}(1 - x) + (x^{-1} - 1)] + (1 - 2\alpha^{-1} - 2\alpha^{-2}) \ln(1/x)$. As before,[1] we define

$$G \equiv F(\xi) = \frac{2\alpha(\alpha + 1)}{(2\alpha + 1)^2} + 4\alpha^{-1}$$

$$+ (1 - 2\alpha^{-1} - 2\alpha^{-2}) \ln(2\alpha + 1) \quad . \quad (7)$$

For an <u>arbitrary</u> point x_0 of $(\xi,1)$, we find that

$$F \equiv F(x_0) = K_1 + K_2\alpha^{-2} + K_3\alpha^{-2} \quad ,$$

$$f \equiv f(x_0) = N_1 + N_2\alpha^{-1} + N_3\alpha^{-2} \quad (8)$$

where

$$K_1 = \tfrac{1}{2}(1 - x_0^2) - \ln x_0 \qquad N_1 = x_0 + x_0^{-1}$$

$$K_2 = 2(\ln x_0 + (1 - x_0)) \qquad N_2 = 2(1 - x_0^{-1})$$

$$K_3 = x_0^{-1} - x_0 + 2 \ln x_0 \qquad N_3 = (1 - x_0^{-1})^2 \quad .$$

If, on the interval $[\xi,x_0]$, we assume the approximation[1] $f(x) \cong Cx^{-1}$, where $C = (G - F)/\ln(x_0/\xi)$, we shall have there also

$$y = F(x) = \int_x^{x_0} f(x)dx + F(x_0)$$

$$\cong L(x) \equiv F + C \ln (x_0/x)$$

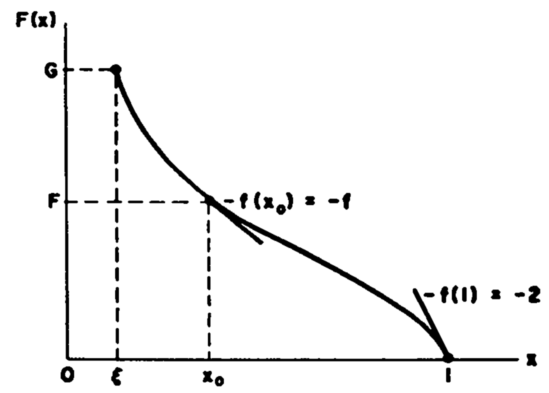
with $F(\xi) = L(\xi)$ and $F(x_0) = L(x_0)$. This leads to the approximation $x = F^{-1}(y) \cong Q(y) \equiv L^{-1}(y)$, where

$$Q(y) = x_0 \exp\left[-\frac{y-F}{G-F}\ln(x_0/\xi)\right] \quad , \quad F \leq y \leq G \quad ,$$

which is exact at the end points.

In practice therefore, for a random number r such that $J \equiv (F/G) \leq r \leq 1$, we find from $r = F(x)/G$ the approximation $x = F^{-1}(rG) \cong Q(rG) = x_0 \exp[-\Lambda(r - J)]$ where $\Lambda = \ln(x_0/\xi)/(1 - J)$.

On the interval $0 \leq y \leq F$, we assume a cubic approximation $F^{-1}(y) \cong Q(y) = a_0 + a_1 y + a_2 y^2 + a_3 y^3$, and demand that Q and Q' be exact at the end points. Since $F(1) = 0$, $F'(1) = -f(1) = -2$, and $F(x_0) = F$, $F'(x_0) = -f(x_0) = -f$, this requires that $Q(0) = 1, Q'(0) = -1/2$, and $Q(F) = x_0$, $Q'(F) = -1/f$. It follows that the cubic Q(y) has the form $Q(y) = 1 + a(y/F) + b(y/F)^2 + c(y/F)^3$, $0 \leq y \leq F$ where $a = -F/2$, $b = F + F/f - 3(1 - x_0)$, $c = -F/2 - F/f + 2(1 - x_0)$. Hence for a random number on $0 \leq r \leq J = F/G$, we take $x = F^{-1}(rG) \cong Q(rG) = 1 + a(r/J) + b(r/J)^2 + c(r/J)^3$. The essential features of F(x) are shown schematically in the figure below, and further details may be found in the earlier report[1], which was based on the fixed $x_0 = 0.3$.



IV. ACCURACY TESTS AND FLOW DIAGRAM

We adopt the value $\alpha_0 = 202$ insuring a steadily decreasing maximal relative error $\leq 4/(\alpha_0 - 2) = 0.02$ for all $\alpha \geq \alpha_0$ ($\cong$ 101 MeV), in the sense of Section II.

The general method used in testing the accuracy of the Section III approximation $x' = Q(y) \cong x = F^{-1}(y)$ for a particular α_h on [0.002, 202] and x_{hi} on $[\xi,1]$ consisted in computing the exact value of $F(x_{hi}) = y_{hi}$, the corresponding approximation $Q(y_{hi}) = x'_{hi} \cong x_{hi}$, and the relative error $\varepsilon_{hi} = (x'_{hi} - x_{hi})/x_{hi}$.

The α-interval [0.002, 2.002] was tested in this way for the 101 energies $\alpha_h = 0.002, 0.022, \cdots, 2.002$, using the α-dependent division point $x_0 = \xi + \phi(1 - \xi)$ for each of the values $\phi = 0.15, 0.17, 0.20, 0.25$, the interval $[\xi, x_0]$ 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 $\alpha_h = 2, 2.5, \cdots, 52$ for $\phi = 0.15, 0.20, 0.25$ and [52,202] at $\alpha_h = 52, 53.5, \cdots, 202$ for $\phi = 0.25$. The results showed the maximal relative error $|\varepsilon|$ to be minimal for the correlated α-ranges and φ values tabulated below. The accuracy could be still further improved, but the present bounds are sufficiently good for our purposes.

TABLE I

$0.002 \leq \alpha < 0.962$	$\phi = 0.25$	$\lvert\varepsilon\rvert = 0.0211$
$0.962 \leq \alpha < 1.642$	$\phi = 0.20$	$\lvert\varepsilon\rvert = 0.0218$
$1.642 \leq \alpha < 2.002$	$\phi = 0.17$	$\lvert\varepsilon\rvert = 0.0218$
$2.002 \leq \alpha < 10$	$\phi = 0.15$	$\lvert\varepsilon\rvert = 0.0213$
$10 \leq \alpha < 52$	$\phi = 0.25$	$\lvert\varepsilon\rvert = 0.0177$
$52 \leq \alpha < 202$	$\phi = 0.25$	$\lvert\varepsilon\rvert = 0.0194$

These choices of parameters may be incorporated into the following schematic flow diagram for Monte Carlo determination of x, for a given incident energy $\alpha \geq 0.002$.

FLOW DIAGRAM

Determination of x in Distribution $F(x)/F(\xi)$.

$(\alpha_0 \equiv 202)$

1. $\eta = 1 + 2\alpha$
2. $\xi = 1/\eta$
3. $N = \ln \eta$
4. $\alpha > \alpha_0 \rightarrow (5), \alpha \leq \alpha_0 \rightarrow (11)$
5. $T = 1 - \xi^2$
6. $F_1 = N + (1/2)T$
7. Generate r, r'
8. $F_1 r' < N \rightarrow (9)$, $F_1 r' \geq N \rightarrow (10)$
9. $x = +\exp(-Nr)$ EXIT
10. $x = \sqrt{1 - rT}$ EXIT (See Note, Part II)
11. $\beta = 1/\alpha$
12. Set $\phi = \phi(\alpha)$. (See Table I)

13. $x_0 = \xi + \phi\,(1 - \xi)$

14. $M = \ln x_0$

15. $K_1 = (1/2)(1 - x_0^2) - M$

16. $K_2 = 2(M + 1 - x_0)$

17. $K_3 = x_0^{-1} - x_0 + 2M$

18. $F = K_1 + \beta(K_2 + \beta K_3)$

19. $G = \dfrac{2\alpha(\alpha + 1)}{\eta^2} + 4\beta + [1 - 2\beta(1 + \beta)]N$

20. $J = F/G$

21. Generate r

22. $r \leq J \rightarrow (23)$, $r > J \rightarrow (32)$

23. $R = r/J$

24. $N_1 = x_0 + x_0^{-1}$

25. $N_2 = 2(1 - x_0^{-1})$

26. $N_3 = (1 - x_0^{-1})^2$

27. $f = N_1 + \beta(N_2 + \beta N_3)$

28. $a = -F/2$

29. $b = F + F/f - 3(1 - x_0)$

30. $c = -F/2 - F/f + 2(1 - x_0)$

31. $x = 1 + R[a + R(b + Rc)]$ EXIT

32. $\Lambda = \dfrac{M + N}{1 - J}$

33. $x = x_0 \exp - \Lambda\,(r - J)$ EXIT

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

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