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Monte Carlo Selection of Energy Loss and Scattering Angle via Edgeworth Series

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1 Introduction

Use of the Edgeworth series to predict energy loss and scattering angle in Monte Carlo calculations of particle transport through thick targets is described in [1]. As mentioned therein, accurate calculation of energy loss and angular distribution involves—besides the Edgeworth series—simulating individual events above some threshold in energy loss or angle. While the underlying algorithms are quite straightforward, their practical application results in rather complicated code. When treating such code as a 'black box' this poses no problem, but delving into computational details or making modifications to it may be more daunting. Yet, modifications may be necessitated, e.g., by implementing a different physical model for energy loss and/or scattering or going to higher orders of the Edgeworth series.

'Gaussians-with-tails' arise in many other problems, notably when random variables are summed over a sample which falls short of the asymptotic Gaussian limit. As long as the underlying processes are well understood and the random variables under study are additive over a series of events problems of this type might benefit from a similar approach. For such cases a detailed account of the Monte Carlo procedure for the present applications might be useful.

This note describes in some detail the routines which select energy loss and angular distribution for Monte Carlo muon transport in a thick tar-

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get using the algorithms of [1]. The routines are intended for application to muon ionization cooling but—with little modification—can be used to transport other charged particles as well. These algorithms are analog simulations, i.e., they do *not* introduce weights as part of the procedure. They are therefore suited equally to analog-type calculations, which mimic complete events in the computer, as to weighted ones where emphasis is on estimating averaged properties. Below, in Secs. 2 and 3, energy loss and angular selection routines are described in turn. The series associated with these two processes differ only in the practical sense that for the scattering application entire orders vanish—along with many terms of the remaining orders—due to the symmetry about zero of the (projected) angular distribution. Such symmetry is absent in the energy loss problem. For comparable computational effort the multiple scattering series might be pursued to much higher order than the energy loss series. For each process, a brief review of the physical model is followed by a description of the Monte Carlo procedure in sufficient detail to interpret the code. Large energy losses and angular deflections are simulated individually. Since they form part of the program the algorithms for this are briefly described here even if they do not rely on the Edgeworth series. Complications arising from transport through targets made of compounds and mixtures are dealt with in Sec. 4. Sec. 5 compares methods of calculating the cumulants of the energy loss and scattering angle distribution. In conclusion, Sec. 6 offers a few brief remarks. Some mathematical details are relegated to the Appendices.

2 Energy Loss

The series used here is the full Edgeworth series, obtained via the method outlined in [2] and briefly sketched in App. 1. The series is reproduced here to order presently incuded in the routines [3]:

$$
\begin{aligned}
f(x) = G(x) \Bigg\{ & 1 + \left[\frac{\kappa_3}{3!\kappa_2^{3/2}} H_3(x)\right] + \left[\frac{\kappa_4}{4!\kappa_2^2} H_4(x) + \frac{\kappa_3^2}{2!3!^2\kappa_2^3} H_6(x)\right] \qquad (1) \\
+ & \left[\frac{\kappa_5}{5!\kappa_2^{5/2}} H_5(x) + \frac{2\kappa_3\kappa 4}{2!3!4!\kappa_2^{7/2}} H_7(x) + \frac{\kappa_3^3}{3!^4\kappa_2^{9/2}} H_9(x)\right] \\
+ & \left[\frac{\kappa_6}{6!\kappa_2^3} H_6(x) + \left(\frac{\kappa_4^2}{2!4!^2} + \frac{2\kappa_3\kappa_5}{2!3!5!}\right)\frac{H_8(x)}{\kappa_2^4} + \frac{3\kappa_3^2\kappa_4}{3!^3 4!\kappa_2^5} H_{10}(x) + \frac{\kappa_3^4}{3!^4 4!\kappa_2^6} H_{12}(x)\right] \\
+ & \Bigg[\frac{\kappa_7}{7!\kappa_2^{7/2}} H_7(x) + \left(\frac{2\kappa_3\kappa_6}{2!3!6!} + \frac{2\kappa_4\kappa_5}{2!4!5!}\right)\frac{H_9(x)}{\kappa_2^{9/2}} + \left(\frac{3\kappa_3^2\kappa_5}{3!^3 5!} + \frac{3\kappa_3\kappa_4^2}{3!^2 4!^2}\right)\frac{H_{11}(x)}{\kappa_2^{11/2}}
\end{aligned}
$$

$$
\begin{aligned}
&\qquad\qquad + \frac{4\kappa_3^3\kappa_4}{3!^3 4!^2 \kappa_2^{13/2}} H_{13}(x) + \frac{\kappa_3^5}{3!^5 5! \kappa_2^{15/2}} H_{15}(x) \Bigg] \\
&+ \Bigg[\frac{\kappa_8}{8!\kappa_2^4} H_8(x) + \left(\frac{\kappa_5^2}{2!5!^2} + \frac{2\kappa_3\kappa_7}{2!3!7!} + \frac{2\kappa_4\kappa_6}{2!4!6!} \right) \frac{H_{10}(x)}{\kappa_2^5} + \Bigg(\frac{\kappa_4^3}{3!4!^3} + \frac{3\kappa_3^2\kappa_6}{3!^3 6!} \\
&\qquad\qquad + \frac{6\kappa_3\kappa_4\kappa_5}{3!^2 4!5!} \Bigg) \frac{H_{12}(x)}{\kappa_2^6} + \left(\frac{4\kappa_3^3\kappa_5}{3!^3 4!5!} + \frac{6\kappa_3^2\kappa_4^2}{3!^2 4!^3} \right) \frac{H_{14}(x)}{\kappa_2^7} \\
&\qquad\qquad + \frac{5\kappa_3^4\kappa_4}{3!^4 4!5! \kappa_2^8} H_{16}(x) + \frac{\kappa_3^6}{3!^6 6! \kappa_2^9} H_{18}(x) \Bigg] \quad \Bigg\}
\end{aligned}
$$

where $G(x)$ is the normal distribution, the $H_i(x)$ are the Hermite polynomials (see App. 2) and x represents a standardized random variable, $(\Delta E - \overline{\Delta E})/\sigma_{\Delta E}$, where ΔE is energy lost in a Monte Carlo step. The κ_i in Eq. 1 are the cumulants of the probability distribution of x. As shown in [1], in Vavilov's approach [4] the moments (about the origin) of *individual* events times their expected number are essentially equivalent to the cumulants of the joint distribution. The cumulants may be more accurately evaluated using formulae which follow directly from their definition. See, e.g., ref. [2], where cumulants are expressed in terms of the moments, or App. 3 for a more convenient representation in terms of both moments and cumulants of lower order. As discussed below and in Sec. 5, the moments approximation yields quite accurate results for typical applications. The user must specify the desired order of the Edgeworth series, i.e., how far to go in Eq. 1. Each of the square brackets represents such an order, beginning with the zeroth-order plain Gaussian. In general, all terms of the same order should either be included or neglected [2], although this principle has not been tested in these problems. As a practical matter a minimum order of *three* is assumed, i.e., the first three square brackets of Eq. 1 are included automatically. At present the maximum order is *six*, i.e., the entire Eq. 1. If yet higher orders are desired they must be added to the program. As Eq. 1 shows quite graphically, increasing amounts of coding and CPU time are required to include these higher orders for what are, typically, decreasing gains in relative accuracy.

2.1 Physical Model

The distribution of energy transfer, ϵ, in *free* μ–e scattering is given by Bhabha's formula [5]:

$$w(\epsilon) = \frac{\xi}{\epsilon^2}\left[1 - \beta^2\frac{\epsilon}{\epsilon_{max}} + \frac{\epsilon^2}{2E_0^2}\right] \tag{2}$$

where ϵ_{max} is the maximum energy transfer, E_0 is the incident muon's total energy, $\xi = 2\pi N_{Av} Z^2 r_e^2 m_e/(A\beta^2)$ with r_e the classical electron radius, m_e its mass, and with the usual meaning for the other symbols. When energy transfer is large compared to electron binding energies, Eq. 2 may be assumed to hold and the electron target may be taken as stationary. For smaller energy transfers motion of the bound electrons and the quantized nature of atomic energy levels complicate matters considerably.

In [1] the simplifying assumption is made that Eq. 2 holds for ϵ above the *average* ionization potential, ϵ_i, while below ϵ_i it is conjectured that:

$$w_<(\epsilon) = \frac{\xi\epsilon_i}{\epsilon^3}. \tag{3}$$

It is further assumed that there exists a *minimum* energy transfer, ϵ_{min}, below which $w(\epsilon) = 0$, as must be true below the lowest excited state of the atom (neglecting a small ϵ resulting from atomic recoil). As a practical matter, ϵ_{min} is determined here by equating the average energy loss as determined by Eqs. 2 and 3 with that obtained from the Bethe-Bloch formula. The average energy loss for individual losses below some arbitrary upper limit, ϵ_c, (less than ϵ_{max}) is called the *restricted* energy loss, $(dE/dx)_R$, and is described by a variant of the Bethe-Bloch formula [6]:

$$\left(\frac{dE}{dx}\right)_R = \xi\left[\ln\left(\frac{2m_e\ \beta^2\gamma^2\epsilon_c}{\epsilon_i^2}\right) - \beta^2\left(1 + \frac{\epsilon_c}{\epsilon_{max}}\right) - \delta + \frac{\epsilon_c^2 - \epsilon_i^2}{4E_0^2}\right] \tag{4}$$

where δ is the density effect correction. The value of ϵ_{min}, which depends on muon energy, then becomes [7]:

$$\epsilon_{min} = \epsilon_i\left[1 + \ln\left(\frac{2m_e\beta^2\gamma^2}{\epsilon_i}\right) - \beta^2\left(1 + \frac{\epsilon_i}{\epsilon_{max}}\right) - \delta\right]^{-1}. \tag{5}$$

The value of ϵ_{min} thus obtained is about one tenth that of ϵ_i. This appears more reasonable than the very small ϵ_{min} which results if one assumes that

Eq. 2 holds throughout, the latter being closer to the Vavilov approximation [4]. Note that use of the Bethe-Bloch formula is a matter of choice and—if preferred—one could use other formulae or even tabulated values for dE/dx. For large energy transfer complete μ–e events are simulated. The minimum energy transfer for individual simulation coincides with the maximum transfer for those events included in the collective distribution, denoted by ϵ_c as in Eq. 4.

In summary, there are thus three regimes of energy transfer in this model:

1. $\epsilon_{min} < \epsilon < \epsilon_i$, with scattering law given by Eq. 3.

2. $\epsilon_i < \epsilon < \epsilon_c$, with scattering law as per Eq. 2. The κ for processes (1) and (2) may be combined:

$$\kappa_i = \overline{N}_c \left(\int_{\epsilon_{min}}^{\epsilon_i} \epsilon^i w_<(\epsilon) d\epsilon + \int_{\epsilon_i}^{\epsilon_c} \epsilon^i w_>(\epsilon) d\epsilon \right) \tag{6}$$

   where $\overline{N}_c$ is the expected number of encounters, in a step.

3. $\epsilon > \epsilon_c$, the number of such collisions is determined on a random basis from a Poisson distribution and ϵ for each such μ–e collision is directly sampled from Eq. 2 assuming a free and stationary electron target.

Combining the first two ϵ-regimes to determine the κ of the collective regime is contrary to [1] where they were kept apart and angular deflections associated with each energy loss regime were evaluated separately. In the present program this angular deflection is determined jointly as well, see below. The Edgeworth series approach easily accommodates either model.

2.2 Monte Carlo Strategy

As mentioned in connection with Eq. 1, x is a standardized random variable:

$$x = \frac{\Delta E - (dE/dx)_R}{\sigma} \tag{7}$$

where $(dE/dx)_R$ is the restricted average energy loss ($\epsilon \leq \epsilon_c$). Integrating Eq. 1 term-by-term over all x shows that only the normal distribution contributes: for odd order Hermite polynomials (with odd powers of x only) the contributions above and below $x = 0$ cancel, while for the even orders they are separately equal to zero. Likewise, integrals of the first moment are zero for each term. Therefore, to any order, the x-distribution is properly

normalized and is guaranteed to yield the correct average—in this case the (restricted) Bethe-Bloch prediction. (Integrals connected with the Edgeworth series, here and below, use infinite limits in spite of the finite range for energy loss or scattering angle. This is not strictly necessary but simplifies matters enormously and is not expected to introduce significant error.) The strategy for Monte Carlo selection from Eq. 1 is:

- First choose randomly between positive and negative parts of the x-domain by comparing the integrals of Eq. 1 above and below zero.
- Given the x-domain, a particular term of the type $b_k x^k G(x)$ is selected from among the positive ones in that domain: odd power terms with negative coefficient for $x < 0$ but with positive coefficient for $x > 0$, even power terms with positive coefficients on both sides. The selection probability for a given term is proportional to its integral over the domain.
- Given a term of the type $x^k G(x)$ and its x-domain, a particular value of x is selected from such a (normalized) distribution.
- At the chosen value of x, the sums of *all* positive terms (f_+) terms and of all negative terms (f_-) of Eq. 1 are evaluated. (Negative terms arise solely because of the $H_i(x)$ since the coefficients displayed in Eq. 1 are all positive). The value of x is accepted if a uniform random number is less than $(f_+(x) + f_-(x))/f_+(x)$ at that x. If not, one starts over from the step where $x^k G(x)$-term is selected.

2.3 Monte Carlo Selection

From Eqs. 2 and 3 the average energy loss (below ϵ_c) is:

$$\left(\frac{dE}{dx}\right)_R = \xi \left(\frac{\epsilon_i}{\epsilon_{min}} - 1 + \ln \frac{\epsilon_c}{\epsilon_i} - \beta^2 \frac{\epsilon_c - \epsilon_i}{\epsilon_{max}} + \frac{\epsilon_c^2 - \epsilon_i^2}{4E_0^2} \right) \tag{8}$$

while

$$\sigma^2 = \kappa_2 = \xi \left(\epsilon_i \ln \frac{\epsilon_i}{\epsilon_{min}} + \epsilon_c - \epsilon_i - \beta^2 \frac{\epsilon_c^2 - \epsilon_i^2}{2\epsilon_{max}} + \frac{\epsilon_c^3 - \epsilon_i^3}{6E_0^2} \right) - \left(\frac{dE}{dx}\right)_R^2 / \overline{N}_c \tag{9}$$

where $\overline{N}_c$ is the number of collisions in the step:

$$\overline{N}_c = \xi \left[\epsilon_i \left(\frac{1}{\epsilon_{min}^2} - \frac{1}{\epsilon_i^2} \right) + \left(\frac{1}{\epsilon i} - \frac{1}{\epsilon_c} \right) - \frac{\beta^2}{\epsilon_{max}} \ln \frac{\epsilon_c}{\epsilon_i} + \frac{\epsilon_c - \epsilon_i}{2E_0^2} \right]. \tag{10}$$

Both $(dE/dx)_R$ and σ are needed to determine a random ϵ as per Eq. 7. This differ slightly from [1] where σ^2 was taken as the second moment (about the origin) times $\overline{N}_c$. See Sec. 5 for further discussion of this point.

The coefficients of the Hermite polynomials, $C_{i,j}$, in Eq. 1:

$$f(x) = G(x) \sum_i \sum_j C_{i,j} H_k(x) \tag{11}$$

up to the desired order of approximation, are readily expressed in terms of $u_j = \kappa_j / j! \kappa_2^{j/2}$. In Eq. 11, index i represents the order of approximation (successive square brackets of Eq. 1) while j counts the number of Hermite polynomials, $H_k(x), (k = i + 2j)$ within the ith order. For example, up to third order:

$$\begin{aligned} C_{1,1} &= u_3 & k = 3 \\ C_{2,1} &= u_4 & k = 4 \\ C_{2,2} &= u_3^2/2! & k = 6 \\ C_{3,1} &= u_5 & k = 5 \\ C_{3,2} &= u_3 u_4 & k = 7 \\ C_{3,3} &= u_3^3/3! & k = 9. \end{aligned} \tag{12}$$

In the program the higher u_j are calculated recursively.

2.3.1 Domain

The first step selects the domain of x—above or below zero. The probability for $x > 0$ is obtained by integrating Eq. 1 from zero to infinity (only odd orders of $H_i(x)$ contribute):

$$\begin{aligned} P(x > 0) &= \frac{1}{2} - \frac{C_{1,1}}{\sqrt{2\pi}} + \frac{3C_{3,1} - 15C_{3,2} + 105C_{3,3}}{\sqrt{2\pi}} \\ &+ \frac{-15C_{5,1} + 105C_{5,2} - 945C_{5,3} + 10\,395C_{5,4} - 135\,135C_{5,5}}{\sqrt{2\pi}} \end{aligned} \tag{13}$$

where the first and second terms of Eq. 13 apply, respectively, to 0th and 1st order, respectively. The third term applies only if the desired order of approximation is greater than *three* and the fourth only when the order is *five* or larger.

2.3.2 Term Selection

Next a particular term of the type $b_k x^k G(x)$ is chosen, one which is positive in the chosen domain. The b_k are determined by collecting, within each order of approximation, coefficients of the x^k which derive jointly from the $C_{i,j}$ and the Hermite polynomials. To yield the selection probabilities, terms which are positive in the chosen domain are integrated over that domain. For $k = 0$ and $k = 1$ the integrals of $x^k G(x)$ equal $1/2$ and $1/\sqrt{2\pi}$, respectively. For *even* powers of $x (k \geq 2)$

$$B_k = \int_0^\infty b_k x^k G(x) dx = \frac{b_k}{2}(k-1)!! \tag{14}$$

while for the *odd* powers of $x (k \geq 3)$

$$B_k = \int_0^\infty b_k x^k G(x) dx = \frac{b_k}{\sqrt{2\pi}}(k-1)!! \tag{15}$$

where $m!!$ indicates the product $m \cdot (m-2) \cdot \ldots$ The B_k, up to *third* order, are listed below for even powers—common to both positive and negative x:

$$\begin{aligned} B_0 &= \frac{1}{2}(1 + 3C_{2,1}) \\ B_2 &= \frac{1}{2} 45 C_{2,2} \\ B_4 &= \frac{3!!}{2} C_{2,1} \\ B_6 &= \frac{5!!}{2} C_{2,2}. \end{aligned} \tag{16}$$

For odd powers in the $x < 0$ domain:

$$\begin{aligned} B_1 &= \frac{1}{\sqrt{2\pi}}(3C_{1,1} + 105C_{3,2}) \\ B_3 &= \frac{2!!}{\sqrt{2\pi}}(10C_{3,1} + 1260C_{3,3}) \\ B_5 &= \frac{4!!}{\sqrt{2\pi}} 21 C_{3,2} \\ B_7 &= \frac{6!!}{\sqrt{2\pi}} 36 C_{3,3} \end{aligned} \tag{17}$$

while for odd powers in the $x > 0$ domain:

$$B_1 = \frac{1}{\sqrt{2\pi}}(15C_{3,1} + 945C_{3,3}) \tag{18}$$

$$
\begin{aligned}
B_3 &= \frac{2!!}{\sqrt{2\pi}}\left(C_{1,1} + 105C_{3,2}\right) \\
B_5 &= \frac{4!!}{\sqrt{2\pi}}\left(C_{3,1} + 378C_{3,3}\right) \\
B_7 &= \frac{6!!}{\sqrt{2\pi}}C_{3,2} \\
B_9 &= \frac{8!!}{\sqrt{2\pi}}C_{3,3}
\end{aligned}
$$

with similar expressions for higher orders. In the given the domain, a term $x^k G(x)$ is selected by comparing a uniform random number *versus* successive values of $\sum_0^k B_j / \sum_0^n B_j$ where n is the total number of terms for the given order of approximation [8].

2.3.3 Select x

Given a particular term, the x-selection procedure depends on whether x in the selected term is to an even or odd power [9]. For even powers:

$$
x = \left(-2\ln\prod_1^{i/2} r_u + r_G^2\right)^{1/2} \tag{19}
$$

where r_u is a uniform $(0 < r_u < 1)$ random number and r_G is a normally distributed $(\overline{r_G} = 0, \sigma_{r_G} = 1)$ random variate. while for odd powers:

$$
x = \left(-2\ln\prod_1^{(i+1)/2} r_u\right)^{1/2} \tag{20}
$$

where i represents the chosen power of x in both equations.

2.3.4 Accept or Reject

Finally, the positive and negative contributions to $f(x)$ are evaluated at that x to the specified order. If $r_u < (f_+(x) + f_-(x))/f_+(x) = f(x)/f_+(x)$ the value of x is accepted. Otherwise one starts over by selecting a new $x^k G(x)$ term since the probabilty used to determine whether x is above or below zero already takes negative contributions to $f(x)$ into account.

2.4 Associated Angular Deflection

The (random) energy loss in a given step is $\Delta E = (dE/dx)_R + x\sigma$. There is an *ms* angular deflection associated with this energy loss (from collective μ–e interactions) which is estimated to be:

$$\vartheta^2 = \frac{2m_e \Delta E}{p_0^2 - E_0 \Delta E} \tag{21}$$

where p_0 is the incident muon energy [1]. No distinction is made in this regard between the two energy regimes—contrary to [1] where the low energy-transfer regime is lumped together with multiple scaterring for estimating angular deflection. The latter overestimates the contribution of electrons to angular deflection since most of the energy transfer is spent on excitation of the atom rather than on imparting transverse momentum to it. Dropping the distinction in kinematic treatment allows the two regimes to be combined and simplifies energy loss selection. This matter probably deserves more attention than is devoted to it here because the large difference in Eq. 21 between using m_e and M_A can lead to significant differences in $\langle \vartheta^2 \rangle^{1/2}$. It is clear, however, that the algorithm can accomodate either model and more sophisticated ones as well.

The distribution is assumed to be Gaussian in projected angle with parameters $(0, \vartheta/\sqrt{2})$ with ϑ from Eq. 21. In principle, higher moments could also be estimated and a random angle determined using the Edgeworth procedure as for multiple scattering off nuclei, see below. However, these angles are typically smaller than from scattering off a nucleus—and larger angles are determined individually—while the cross section is lower by a factor of Z^{-1}, so the Gaussian assumption appears justified.

2.5 Large Losses

Above the cut-off energy, ϵ_c, events are fully simulated individually. This permits keeping track of energy-angle correlations due to μ–e interactions and—where needed—determine the trajectory of the struck electron (δ-ray). In convenient but roundabout fashion ϵ_c is determined from a specified (approximate) number of collisions to be treated individually. Then, given ϵ_c, the precise average number of collisions is calculated and a random number of collisions is selected from a Poisson distribution. If non-zero then for each collision a random energy loss is determined from Eq. 2 by selecting an energy loss ($\epsilon_c < \epsilon < \epsilon_{max}$) from a ϵ^{-2} distribution and taking account of the factor in square brackets by rejection. The angles associated with the event follow from two-body kinematics.

In terms of CPU-time, an optimum value of $\overline{N}_>$, the number of events to be simulated individually, appears to lie around two to five. Increasing the number of individual simulations is easily seen to be time consuming, while lowering $\overline{N}_>$ increases rejection rates in the Edgeworth algorithm and renders it less efficient.

3 Multiple Scattering

The additive quantities for multiple scattering are the *projected* angles, θ_x and θ_y. In contrast to energy loss, their domain includes negative as well as positive real numbers with probabilities independent of the sign of θ_x or θ_y. As a result all *odd* κ vanish along with many terms in the series of Eq. 1. The procedure of [2] (see App. 1) simplifies considerably if the odd indexed κ are ignored from the start. Using the abbreviation: $u_k = \kappa_k/k!\kappa_2^{k/2}$ introduced above, one obtains:

$$
\begin{aligned}
f(x) = G(x) \quad & \Bigg\{ \; 1 + [u_4 H_4(x)] + \left[u_6 H_6(x) + \frac{1}{2!} u_4^2 H_8(x) \right] \qquad (22) \\
+ \; & \left[u_8 H_8(x) + \frac{1}{2!} 2 u_4 u_6 H_{10}(x) + \frac{1}{3!} u_4^3 H_{12}(x) \right] \\
+ \; & \Bigg[u_{10} H_{10}(x) + \frac{1}{2!} \left(2 u_4 u_8 + u_6^2 \right) H_{12}(x) \\
& \qquad + \frac{1}{3!} 3 u_4^2 u_6 H_{14}(x) + \frac{1}{4!} u_4^4 H_{16}(x) \Bigg] \\
+ \; & \Bigg[u_{12} H_{12}(x) + \frac{1}{2!} \left(2 u_4 u_{10} + u_6^2 \right) H_{14}(x) + \frac{1}{3!} \left(3 u_4^2 u_8 + 3 u_4 u_6^2 \right) H_{16}(x) \\
& \qquad + \frac{1}{4!} 4 u_4^3 u_6 H_{18}(x) + \frac{1}{5!} u_4^5 H_{20}(x) \Bigg] \Bigg\} \quad .
\end{aligned}
$$

Again successive orders (evens only here) are grouped within square brackets. In terms of the full Edgeworth series, Eq. 22—and the program—runs through the 10th order. Comparison with the lower orders of Eq. 1 shows that terms containing *only even* κ survive to contribute to Eq. 22. It is assumed that *four* is the minimum order (first line of Eq. 22).

3.1 Physical Model

As with energy loss, a cut-off angle is chosen below which scattering is treated collectively while above it individual events are fully simulated. Be-

low cut-off the number of muons at projected angle, θ_x, after a Monte Carlo step of length Δ is represented by [10]:

$$v(\theta_x) = \frac{\pi}{2}\frac{N_{Av}\rho}{A}\left(\frac{2Ze^2}{p_0\beta}\right)^2 \frac{\theta_c}{\sqrt{\theta_0^2+\theta_c^2}}\frac{\Delta}{(\theta_x^2+\theta_0^2)^{\frac{3}{2}}} = \frac{\theta_c}{\sqrt{\theta_0^2+\theta_c^2}}\frac{K\Delta}{p_0^2\beta^2\,(\theta_x^2+\theta_0^2)^{\frac{3}{2}}} \tag{23}$$

where θ_c is the cut-off angle. The angle θ_0 is associated with screening of the nuclear charge by electrons and is based on tables of atomic form factors by Hubbell et al. [11]. Eq. 23 differs slightly from its counterpart in [10]: (1) $(\theta_x^2+\theta_0^2)^{\frac{3}{2}}$ in the denominator, instead of θ_x^3, as follows from assuming $(\theta^2+\theta_0^2)^{-2}$ instead of θ^{-4} for the polar angular dependence in Rutherford's formula, and (2) a factor $\frac{\theta_c}{\sqrt{\theta_0^2+\theta_c^2}}$ due to cutting off the θ_y distribution at $\pm\theta_c$ since an event with $|\theta_x| < \theta_c$ but $|\theta_y| > \theta_c$ is treated as an individual event. This extra factor, typically very close to unity, is the ratio of the integral of the distribution between $\pm\theta_c$ to that between $\pm\infty$. There is a similar distribution for θ_y independent of $v(\theta_x)$. For small angles, Eq. 23 is preferred for simplicity over the more precise Rosenbluth-type formula with atomic form factor. In this regime it has been shown to be in quite close agreement [12] with the latter.

3.2 Monte Carlo Strategy

The x from Eq. 22 is again a standardized random variable:

$$x = \frac{\vartheta_x}{\sigma} \tag{24}$$

where ϑ_x indicates $\sum\theta_x$ over a Monte Carlo step, and $\overline{\vartheta}_x = 0$ here. The strategy is essentially the same as for energy loss selection, but now the domain is over all reals, with ϑ_x and $-\vartheta_x$ equiprobable. Therefore sign selection can be saved for last—after a satisfactory value of $|\vartheta_x|$ has been chosen. The entire procedure is repeated for ϑ_y.

3.3 Monte Carlo Selection

The σ in Eq. 24 is readily obtained from Eq. 23:

$$\sigma = \kappa_2 = K\Delta\left[\frac{\theta_c}{\sqrt{\theta_0^2+\theta_c^2}}\ln\left(\frac{\sqrt{\theta_c^2+\theta_0^2}+\theta_c}{\sqrt{\theta_c^2+\theta_0^2}-\theta_c}\right) - \frac{2\theta_c^2}{\theta_c^2+\theta_0^2}\right] \tag{25}$$

where the first equality holds for any distribution. The higher order κ are obtained recursively. By partial integration:

$$\int \frac{\theta_x^n}{\left(\theta_x^2+\theta_0^2\right)^{3/2}} d\theta_x = -\frac{\theta_x^{n-1}}{\left(\theta_x^2+\theta_0^2\right)^{1/2}} + (n-1)\int \frac{\theta_x^{n-2}}{\left(\theta_x^2+\theta_0^2\right)^{1/2}} d\theta_x. \tag{26}$$

After some manipulation this leads to:

$$\kappa_n = \frac{2K\Delta\,\theta_c^n}{(n-2)\left(\theta_0^2+\theta_c^2\right)} - \frac{n-1}{n-2}\theta_0^2\kappa_{n-2}. \tag{27}$$

Since only κ_n with even n are required, this permits for quick generation of the series of Eq. 22 to any order, with Eq. 25 as the starting point.

The x selection procedure is much like for the energy loss case:

- The positive terms of the series are identified and their integrals are obtained.
- A term of the type $b_k x^k G(x)$ is selected among them.
- An x-value is chosen in accordance with this distribution. Since k is always even, only Eq. 19 applies.
- At that x, positive and negative contributions to $f(x)$ are evaluated—with x accepted only if $r_u < (f_+(x)+f_-(x))/f_+(x)$. Otherwise a new $b_k x^k G(x)$ is selected.
- An equi-probable sign of x is chosen.

3.4 Associated Energy Loss

The energy loss associated with (nuclear) multiple scattering through angle $\vartheta = \sqrt{\vartheta_x^2+\vartheta_y^2}$ in a given step is estimated to be

$$\Delta\epsilon = \frac{p_0^2\vartheta^2}{2M_A} \tag{28}$$

where M_A is the nuclear mass of the target. This follows from equating the momentum transfers to the target nucleus and to the muon in each individual event:

$$2M_A\Delta\epsilon = p_0^2\theta^2 \tag{29}$$

and summing over all events in a step, p_0 being treated as constant. Eq. 28 corresponds to the average energy loss for a given multiple scattering angle. Fluctuations about this value are ignored since $\Delta\epsilon$ is expected to be small compared to losses due to electron scattering.

3.5 Large Deflections

Scattering with angles larger than θ_c in a single event is simulated individually. The cross sections adopted here for these processes are discussed in [12]. For targets other than hydrogen this includes both coherent and incoherent (wherein a nucleon is liberated) scattering. As with large energy losses, a cut-off angle is determined by specifying an approximate number of events to be treated individually. Then, given this cut-off angle, an *upper limit* to the average number of collisions is determined and a random number of events is selected from a Poisson distribution. Upper limit here refers to the average number as determined from a simplified formula which represents a strict upper bound to the cross section. In the Monte Carlo procedure this upper limit reduces to the proper value by rejection. At present, the (simplified) cross sections are calculated for each step. Savings in CPU time would result by precalculating the cross sections and relying on interpolation during the Monte Carlo. The number of collisions to be treated individually is again a compromise between extra time spent on simulating collisions and increased rejection rates for the collective treatment. But it can be set much lower here than for energy loss: in the 0.05 to 0.5 range.

One concern is the demarcation between collective—expressed in terms of *projected* angles—and individual scattering regime which relies on *polar* angles. A convenient strategy, adopted here, is to select individual (polar) θ on the $\theta > \theta_c$ domain and collective (projected) θ_x, θ_y on the domain $-\theta_c < \theta_{x,y} < \theta_c$. In the $\theta_{x,y}$ plane these domains overlap in the corners of a $2\theta_c \times 2\theta_c$ square. Therefore when, in an individual (coherent) scattering, θ_x and θ_y are each less than θ_c (but $\theta_x^2 + \theta_y^2 > \theta_c^2$, as assured by selection), the event is rejected without reprise.

3.5.1 Hydrogen

For hydrogen the cross section is assumed as given by Berestetskii et al. [13]:

$$\begin{aligned} \frac{d\sigma}{dt} &= \frac{\pi\alpha^2}{p_0^2 t^2}\Bigg\{ \; G_E^2 \left[\frac{(4ME_0 - t)^2}{(4M^2 + t)} + t \right] \\ &+ \frac{t}{4M^2} G_M^2 \left[\frac{(4ME_0 - t)^2}{(4M^2 + t)} - \left(4m^2 - t\right) \right] \Bigg\} F_A(t) \end{aligned} \tag{30}$$

where m and M are the muon and proton mass and G_E and G_M are the proton electric and magnetic form factor, respectively. Contrary to [12] t is the *negative* 4-momentum transfer (and thus a positive quantity) here as well as in the program. Selection proceeds as follows:

- The average number of collisions is based on an upper limit of Eq. 30 given by:

$$\begin{aligned} \frac{d\sigma}{dt} &= \frac{\pi\alpha^2}{p_0^2}\left\{\frac{1}{t^2}\left[\frac{(4ME_0-t_c)^2}{(4M^2+t_c)}-t_c\right]\right. \\ &+ \left.\frac{2.79^2}{4M^2t}\left[\frac{(4ME_0-t_c)^2}{(4M^2+t_c)}-\left(4m^2-t_c\right)\right]\right\} \end{aligned} \tag{31}$$

  in which the square brackets of Eq. 30 are replaced by their maximum values occurring at $t = t_c$. The constant 2.79 represents the ratio G_E/G_M assumed to be independent of t here.

- For *each term* associated with the square brackets of Eq. 31 the average number of collisions is determined and a random number to be simulated is selected from a Poisson distribution.

- If that number is nonzero then t is chosen, either $\propto t^{-2}$ or $\propto t^{-1}$, depending on the term.

- This t is accepted if a uniform random number is less than the ratio of the square bracket of Eq. 30 pertaining to the term selected, times the atomic form factor, to the corresponding bracket of Eq. 31—all evaluated at the chosen t.

- If the selected t is rejected *no* collision takes place.

Above typical cut-off angles the atomic form factor will be very close to unity and could be neglected. In most applications the approximation $t = p_0^2\theta^2$ should be sufficient to determine θ.

3.5.2 Coherent Nuclear

For nuclear targets, the coherent cross section assumed is [12]:

$$\frac{d\sigma}{dt} = \frac{Z^2\pi\alpha^2}{4M^2p_0^2t^2}\left[(4ME_0-t)^2-\left(4M^2+t\right)t\right]F_N^2(t)F_A(t). \tag{32}$$

Here M is the nuclear mass while F_N and F_A are the nuclear and atomic form factors, respectively. With only one term present, selection is simplified *vs* μ–p but otherwise proceeds along the same lines. Eq. 32 is correct only for a spin zero nucleus. For some of the lighter nuclei considered here with nonzero spin, such as lithium and boron, the magnetic term may still contribute although at a much reduced level relative to hydrogen (after scaling by Z^2) [14]. For these materials, it is thus likely that Eq. 32 underestimates large angle scattering somewhat.

3.5.3 Incoherent Nuclear

Using the model of [12] for incoherent scattering, the program calculates—for each nuclear species present—upper limits to the probabilities for the muon to undergo incoherent scattering with a nuclear constituent: (a) proton (1st or E-term), (b) proton (2nd or M-term), or (c) neutron (M-term), in the manner of Sec. 3.5.1. Each probability is further split in two according to whether the nucleus remains bound or not. These probabilities are taken to correspond to integrals of Eq. 31 between t-limits derived from energy systematics for each nuclear species. Selection of t and subsequent rejection test are again as above. An empirical 'geometric' factor (< 1)multiplies the cross section to take 'shadowing' into account. This factor is taken as the ratio of the (high-energy) nuclear inelastic cross section to the sum of the inelastic cross sections of the individual nucleons.

4 Composite Targets

Since interest is mainly in light nuclei, specific nuclear (and atomic) data are provided in the program for the elements with $Z = 1$–8 as well as for five low-Z compounds of potential interest to muon cooling: LiH, B_4C, BeO, H_2O, and *air* (represented as 80% N_2, 20% O_2). This appears preferable since generic nuclear models are almost exclusively applicable only to heavier nuclei. For *energy loss*, average ionization potentials and density effect parameters for many compound targets (including those listed above) are given by Sternheimer et al. [15] and Monte Carlo simulation thus can proceed exactly as for monatomic targets. For *multiple scattering*, the angular distribution may be written as a sum over elemental targets $\sum_i v_i(\theta_x)$, as per Eq. 23. Likewise, the κ may be evaluated as a sum over terms, with common cut-off angle θ_c:

$$\begin{aligned} \kappa_j &= \int_{-\theta_c}^{\theta_c} \theta_x^j \sum_i^n v_i(\theta_x) d\theta_x \qquad (33) \\ &= 2\pi \frac{N_{Av}\rho e^4}{p_0^2 \beta^2 W} \Delta \sum_i^n n_i Z_i^2 \frac{\theta_c}{\sqrt{\theta_{0,i}^2 + \theta_c^2}} \int_{-\theta_c}^{\theta_c} \frac{\theta_x^n d\theta_x}{\left(\theta_x^2 + \theta_{0,i}^2\right)^{3/2}} \end{aligned}$$

where W is the molecular weight, n_i the number of atoms of type i belonging to the compound, and $\theta_{0,i}$ are the screening angles of species i, precalculated and stored in the program. With these κ the angular distribution is again represented by Eq. 22. For mixtures n_i is taken proportional to the relative

number of atoms present while $W = \sum_i n_i A_i$. In evaluating energy losses associated with multiple scattering, M_A in in Eq. 28 is replaced by a weighted average:

$$M_A = \frac{\sum n_j Z_j^2}{\sum n_j Z_j^2 / M_{A_j}}. \tag{34}$$

5 Cumulant Calculation

The parameters of Eqs. 1 and 23 are expressed entirely in terms of the κ which are approximated by the moments of the single event distribution. For energy loss, the validity of this is demonstrated in [1] for the Landau-Vavilov differential equation and for a similar equation governing multiple scattering. However, in general the κ differ from the moments about the origin by a set of terms (of both signs, expressed in terms of the lower moments) which increase rapidly in number with k [2]. More convenient expressions for the κ, written in terms of both moments and lower order κ, are listed in App. 3. The Vavilov approach essentially assumes that $\overline{N}_c$ in Eq. 9 can be taken to be infinite—on account of $\epsilon_{min} \to 0$ in Eq. 10—so that at least the second cumulant and second moment about zero can be taken to be equal in this case. Under this assumption dominance of the highest moment is likely for the higher cumulants as well. Alternatively, in the more general approach (finite $\overline{N}_c$), the κ can be calculated from the moments of the single event distribution (Eqs. 2 or 3) and then—on the basis of additivity of the cumulants—multiplied by the number of events expected in a Monte Carlo step. This is somewhat more cumbersome, particularly for higher orders. Comparisons show both methods give close to the same results and typical differences may be compared to those between successive orders of the Edgeworth series.

For example, in calculating the *energy loss* distribution, for 0.2 GeV/c muons incident on 1 cm of beryllium, and with *five* collisions to be treated individually, the relative *rms* difference between the *sixth* order in the Edgeworth series and the third, fourth, and fifth orders are about $2 \cdot 10^{-2}$, $1.1 \cdot 10^{-2}$, and $4 \cdot 10^{-3}$, respectively, averaged over a domain between -3.5σ and 7σ. (Relative to peak value, probabilities at $-3.5\ \sigma$ and at $7\ \sigma$ are reduced by $5 \cdot 10^{-5}$ and $3 \cdot 10^{-7}$, respectively. Below around $-3.5\ \sigma$ the distribution rapidly falls to zero.) For the same conditions, the relative *rms* difference between using the full κ_k and using the kth moments about the origin is $7.5 \cdot 10^{-3}$. Using Eq. 9 for κ_2, instead of the 2nd moment about zero, this measure improves to $5 \cdot 10^{-4}$. The comparison is even better ($1.5 \cdot 10^{-4}$)

if one uses Eq. 9 only in the Gaussian part of Eq. 1. These last results are approximately the same for orders three through six. It is interesting to note that the κ, calculated both ways in the above example, differ by a few parts per thousand while agreement of the $\kappa_k/\kappa_2^{k/2}$ ratios varies from $1.5 \cdot 10^{-3}$ to about 2%. The better agreement of the probability densities suggests that some cancellations occur which lead to (approximately) the same underlying expression either with the full κ or with the moments in the Edgeworth series.

For *multiple scattering*, approximating the κ by the second moments appears *a priori* even better justified. Since $\overline{\vartheta_x} = \overline{\vartheta_y} = 0$, κ_2 coincides with the second moment about zero. However, for κ_k, $k \geq 4$ differences appear and this will lead to differences in the distribution. As with the Edgeworth series, the vanishing odd moments result in much fewer terms for higher order κ. Using the same example as for energy loss, but with a large angle cut-off equivalent to 0.2 scatterings to be treated individually, the relative *rms* differences between the *tenth* order result and that of the fourth, sixth, eight order are, respectively, $7 \cdot 10^{-6}$, $7 \cdot 10^{-7}$, and $1.1 \cdot 10^{-7}$ averaged over a domain of $\pm 3.5\ \sigma$. The same differences averaged over $\pm 7\ \sigma$ are $8 \cdot 10^{-3}$, $1.7 \cdot 10^{-3}$, and $1.0 \cdot 10^{-4}$. (Probabilities at $\pm 3.5\ \sigma$ and $\pm 7\ \sigma$ are down to $2.5 \cdot 10^{-4}$ and $4 \cdot 10^{-11}$, respectively, from peak value.) For orders four through ten of the Edgeworth series, the two methods of estimating the cumulants produce agreement in the angular distribution to within about $1 \cdot 10^{-5}$ averaged over $\pm 3.5\ \sigma$ and $1 \cdot 10^{-4}$ over $\pm 7\ \sigma$. For $k \geq 4$ relative *rms* difference of the κ_k evaluated both ways range form 0.2 to 1.5%, with roughly the same differences for the $\kappa_k/\kappa_2^{k/2}$. As in the energy loss example, the probability distributions again agree better than do the κ or $\kappa_k/\kappa_2^{k/2}$ on which they are based.

Nevertheless, when dominance of the higher moments is not well established full calculation of the cumulants may be necessary. However, since smaller higher moments imply quicker convergence to a Gaussian, lower orders of the Edgeworth series will be sufficient for such cases. In this connection, there are presently three options in the program: (1) assume the kth moments about zero for κ_k throughout, (2) ditto, but use the square root of the second moment about the mean for scaling the standardized random Gaussian variate determined by the Monte Carlo, (Eq. 7), and (3) work with the fully evaluated κ throughout. Note that options (1) and (2) are identical for the angular distribution. Options (2) and (3) do not require any extra effort on the part of the user when a different distribution is introduced.

6 Concluding Remarks

In [1] comparisons are presented which demonstrate the validity of the method detailed here. The main focus there is energy loss and by going to 5th order excellent comparisons with analytic calculations are produced. Higher orders require progressively more code and more computation time for lesser gains in accuracy. Therefore, for present applications, the orders of the series included—up to 6th in the energy loss calculation, 10th in the multiple scattering—should be more than sufficient. If still higher orders are desired the program must be augmented via the methods sketched in App. 1.

An important advantage of the present method is demonstrated above: an energy loss cross section defined differently in two energy regimes still results in a single energy loss distribution [16]. Likewise multiple scattering in a compound or mixture, with different parameters for each component, results in a single angular distribution. In each instance more work is required to generate the distribution but, after that, the calculation is the same as for a single energy regime or for a monatomic target. The energy– and angular distributions—though rather formidable looking, see Eqs 1 and 22—are nonetheless relatively easily sampled.

A tempting shortcut is to precalculate and store certain quantities as a function of muon energy for each material present. Then, during execution, to rely on interpolation with respect to muon energy to save CPU time. Since the same energy range and materials are common to many problems such precalculated tables could be used repeatedly. It is important to note, however, that different orders of the Edgeworth series scale differently with respect to steplength—which may vary during a Monte Carlo simulation. Ordinarily, at each step, the precise steplength is used to evaluate the coefficients of the Edgeworth series and related quantities. When an interpolation scheme is used, a standard steplength is adopted in the initialization, then during simulation interpolated values of each order are rescaled to the correct steplength and recombined. Such scaling is exact—with the usual caveats that a step must be small enough to be well represented by a straight line segment and that variation of the coefficients over its length is negligible. At present, an interpolation version is not included as an option. To accommodate steplength scaling, each order must be pretabulated separately, tables must be spaced sufficiently close, and the interpolation scheme must be sufficiently powerful to yield accurate results. This demand on computer resources makes interpolation less attractive. After brief experimentation with the energy loss algortihm, savings in CPU time compared

with the 'long' version did not seem significant enough to proceed further—although this should be further examined. Precalculation and interpolation of the more complicated formulae for large angle scattering may also be worth studying. A more thorough study of the cumulant estimation problem of Sec. 5 as well as intercomparison of various orders of the series might yield better insight and provide valuable practical information with regard to optimizing the program to the problem at hand.

Another area of potential investigation lies in the selection scheme of the Edgeworth series. The one offered here suffers from high rejection rate when the threshold is set high. For energy loss or multiple scattering one can always resort to simulating more individual events but this may be more troublesome in other applications if the distributions corresponding to single events are not that simple. Perhaps some precalculation/interpolation scheme may likewise be useful here. Series similar to Edgeworth's, such as Gram-Charlier, which also approximate distributions based on a Gaussian-plus-Hermite-polynomials should also be examined. While the Edgeworth series is preferred in principle [2], others may well outperform it if computational considerations are included.

The Edgeworth series permits negative values contrary to what is required for a probability density. At higher orders such 'negative probabilities' occur over narrow intervals where the true probability is very small. In the Monte Carlo this creates no practical difficulties: selection is done everywhere from positive terms and if negative terms predominate in some interval an initial selection in that neighborhood will invariably be rejected resulting in zero probability. Since the algorithm always selects one outgoing particle for every incoming one the distribution is effectively renormalized by uniformly multiplying the positive regions of the Edgeworth series by an appropriate factor close to unity.

For convenience in making modifications or applications to other problems, the calculation of the moments is done in a routine separate from Monte Carlo selection based on them. The user thus provides the moments calculation to suit a particular model or application while the Monte Carlo selection routine—with the given moments—remains 'content-free'. Similarly, if complete evaluation of the cumulants is desired this is performed in a separate routine which is independent of the application. In principle, the same routine could be used for both energy loss and scattering but, as a practical matter, the vanishing odd order moments of the angular distribution invites going to higher orders which would either become unwieldy for the energy loss problem or cause a lot of wasteful operations in the scattering case. Since in other applications the elementary probability may or

may not be an even function of its argument, it may be useful to have both sets of routines available.

In summary, the method generates a statistical distribution of a random variable summed over many events directly from the moments of the probability distribution for individual events. The domain of the variable may include positive as well as negative values. It must be strictly additive over all events—which is why it wouldn't work, e.g., for *polar* angles in the multiple scattering problem. The distribution obtained is particularly attractive for Monte Carlo selection. When evaluated to reasonably high order the approximation does quite well [1]. While its analytical representation in terms of the Hermite polynomials is rather unwieldy, it may nevertheless also serve to generate the distribution in numerical or graphical form—perhaps with 'negative probabilities' smoothed over. This may be useful even where an analytic expression for the statistical distribution exists since it may be quite complicated and tied to a specific—often simplified—model of the underlying interaction. Such is indeed the case for both the energy loss and scattering examples discussed here since neither the distribution of Vavilov or of Moliere is a closed form expression and evaluation requires considerable numerical work. It is hoped that the detailed look provided here at these examples might encourage use of this method in other applications.

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Appendix 1

The derivations of the Edgeworth series for both energy loss, Eq. 1, and angular distribution, Eq. 22, are briefly sketched below.

Energy Loss

According to [2] (top p.228, sec 17.7):

$$e^{t^2/2}\Psi(t) = \sum_{h=0}^{\infty} \frac{(it)^{2h}}{h!} \left[\sum_{\nu=1}^{\infty} \frac{\lambda'_{\nu+2}}{(\nu+2)!} \left(\frac{it}{\sqrt{n}} \right)^{\nu} \right]^h \tag{35}$$

where $\Psi(t)$ is the characteristic function associated with the probability density, $f(x)$, one wishes to approximate. The RHS of Eq. 35 is expanded and terms up to the desired power (the *sixth* here) of $n^{-1/2}$ are retained. Physically, the n in Eq. 35 corresponds to the average number of encounters in a Monte Carlo step. Up to sixth order, with the abbreviation $y_j =$

$\lambda'_j (it)^{j-2}/j!$ and with terms grouped according to successive values of sum index h:

$$
\begin{aligned}
e^{t^2/2}\Psi(t) &= 1 + \frac{(it)^2}{1!}\left[\frac{y_3}{n^{1/2}} + \frac{y_4}{n} + \frac{y_5}{n^{3/2}} + \frac{y_6}{n^2} + \frac{y_7}{n^{5/2}} + \frac{y_8}{n^3} + ...\right] \\
&+ \frac{(it)^4}{2!}\left[\frac{y_3^2}{n} + \frac{2y_3y_4}{n^{3/2}} + \frac{y_4^2}{n^2} + \frac{2y_3y_5}{n^2} + \frac{2y_3y_6}{n^{5/2}} + \frac{2y_4y_5}{n^{5/2}} + \frac{y_5^2}{n^3} + \frac{2y_3y_7}{n^3}\right. \\
&\qquad \left. + \frac{2y_4y_6}{n^3} + ...\right] \\
&+ \frac{(it)^6}{3!}\left[\frac{y_3^3}{n^{3/2}} + \frac{3y_3^2y_4}{n^2} + \frac{3y_3^2y_5}{n^{5/2}} + \frac{3y_3y_4^2}{n^{5/2}} + \frac{y_4^3}{n^3} + \frac{3y_3^2y_6}{n^3} + \frac{6y_3y_4y_5}{n^3} + ...\right] \\
&+ \frac{(it)^8}{4!}\left[\frac{y_3^4}{n^2} + \frac{4y_3^3y_4}{n^{5/2}} + \frac{4y_3^3y_5}{n^3} + \frac{6y_3^2y_4^2}{n^3} + ...\right] \\
&+ \frac{(it)^{10}}{5!}\left[\frac{y_3^5}{n^{5/2}} + \frac{5y_3^4y_4}{n^3} + ...\right] \\
&+ \frac{(it)^{12}}{6!}\left[\frac{y_3^6}{n^3} + ...\right].
\end{aligned}
\tag{36}
$$

Re-grouped according to power of $n^{-1/2}$, and with the y expressed in terms of the λ', this becomes:

$$
\begin{aligned}
& e^{t^2/2}\Psi(t) = 1 + \frac{1}{n^{1/2}}\left[\frac{\lambda'_3}{3!}(it)^3\right] + \frac{1}{n}\left[\frac{\lambda'_4}{4!}(it)^4 + \frac{\lambda'^2_3}{2!3!^2}(it)^6\right] \\
+ & \frac{1}{n^{3/2}}\left[\frac{\lambda'_5}{5!}(it)^5 + \frac{2\lambda'_3\lambda'_4}{2!3!4!}(it)^7 + \frac{\lambda'^3_3}{3!^4}(it)^9\right] \\
+ & \frac{1}{n^2}\left[\frac{\lambda'_6}{6!}(it)^6 + \left(\frac{\lambda'^2_4}{2!4!^2} + \frac{2\lambda'_3\lambda'_5}{2!3!5!}\right)(it)^8 + \frac{3\lambda'^2_3\lambda'_4}{3!^3 4!}(it)^{10} + \frac{\lambda'^4_3}{4!3!^4}(it)^{12}\right] \\
+ & \frac{1}{n^{5/2}}\left[\frac{\lambda'_7}{7!}(it)^7 + \left(\frac{2\lambda'_3\lambda'_6}{2!3!6!} + \frac{2\lambda'_4\lambda'_5}{2!4!5!}\right)(it)^9\right. \\
& \quad \left. + \left(\frac{3\lambda'^2_3\lambda'_5}{3!^3 5!} + \frac{3\lambda'_3\lambda'^2_4}{3!^2 4!^2}\right)(it)^{11} + \frac{4\lambda'^3_3\lambda'_4}{3!^3 4!^2}(it)^{13} + \frac{\lambda'^5_3}{5!3!^5}(it)^{15}\right] \\
+ & \frac{1}{n^3}\left[\frac{\lambda'_8}{8!}(it)^8 + \left(\frac{\lambda'^2_5}{2!5!^2} + \frac{2\lambda'_3\lambda'_7}{2!3!7!} + \frac{2\lambda'_4\lambda'_6}{2!4!6!}\right)(it)^{10}\right. \\
& \quad + \left(\frac{\lambda'^3_4}{3!4!^3} + \frac{3\lambda'^2_3\lambda'_6}{3!^3 6!} + \frac{6\lambda'_3\lambda'_4\lambda'_5}{3!^2 4!5!}\right)(it)^{12} + \\
& \quad \left. + \left(\frac{4\lambda'^3_3\lambda'_5}{3!^3 4!5!} + \frac{6\lambda'^2_3\lambda'^2_4}{3!^2 4!^3}\right)(it)^{14} + \frac{5\lambda'^4_3\lambda'_4}{3!^4 4!5!}(it)^{16} + \frac{\lambda'^6_3}{6!3!^6}(it)^{18}\right] .
\end{aligned}
\tag{37}
$$

Ref [2] writes both characteristic function and probability density in terms of the coefficients $b_{i,j}$, belonging to the powers of it as well as to the Gaussian

derivatives:

$$\Psi(t) = e^{-t^2/2}\left[1+\sum_{\nu=1}^{\infty}\frac{b_{\nu,\nu+2}(it)^{\nu+2}+b_{\nu,\nu+4}(it)^{\nu+4}+...+b_{\nu,3\nu}(it)^{3\nu}}{n^{\nu/2}}\right] \quad (38)$$

$$f(x) = G(x)+\sum_{\nu=1}^{\infty}(-1)^{\nu}\frac{b_{\nu,\nu+2}G^{(\nu+2)}(x)+b_{\nu,\nu+4}G^{(\nu+4)}(x)+...+b_{\nu,3\nu}G^{(3\nu)}(x)}{n^{\nu/2}}$$

where $G^m(x) = (-1)^m H_m(x)G(x)$ is the mth derivative of $G(x)$, the Gaussian probability density. The $b_{i,j}$ in the first member of Eqs. 38 may now be identified with the corresponding coefficients of the powers of n and it in Eq. 37 and then introduced into the second member. Using the relations $\lambda'_\nu = \kappa'_\nu/\sigma'^\nu$, $\sigma'^2 = \kappa_2/n$, $\kappa_k = n\kappa'_k$ as per Eqs.17.6.7 and 8 of [2]—and substituting for the $G^m(x)$—Eq. 1 is obtained. (Here primed quantities pertain to the single events while unprimed ones pertain to the composite distribution.)

Angular Distribution

The series used for multiple scattering could be derived from the full Edgeworth series by continuing the above procedure up to 10th order and then setting all odd κ_i equal to zero. It is more readily obtained by keeping only the *even* subscripted λ'_ν in Eq. 35. Going to 10th order, or to n^{-5}, one obtains:

$$\begin{aligned} e^{t^2/2}\Psi(t) &= \frac{(it)^2}{1!}\left[\frac{y_4}{n}+\frac{y_6}{n^2}+\frac{y_8}{n^3}+\frac{y_{10}}{n^4}+\frac{y_{12}}{n^5}+...\right] \quad (39)\\ &+ \frac{(it)^4}{2!}\left[\frac{y_4^2}{n^2}+\frac{2y_4y_6}{n^3}+\frac{2y_4y_8}{n^4}+\frac{y_6^2}{n^4}+\frac{2y_6y_8}{n^5}+\frac{2y_4y_{10}}{n^5}+...\right]\\ &+ \frac{(it)^6}{3!}\left[\frac{y_4^3}{n^3}+\frac{3y_4^2y_6}{n^4}+\frac{3y_4^2y_8}{n^5}+\frac{3y_4y_6^2}{n^5}+...\right]\\ &+ \frac{(it)^8}{4!}\left[\frac{y_4^4}{n^4}+\frac{4y_4^3y_6}{n^5}+...\right]\\ &+ \frac{(it)^{10}}{5!}\left[\frac{y_4^5}{n^5}+...\right]. \end{aligned}$$

Steps similar to those for the series used for energy loss now lead to Eq. 22.

Appendix 2

The Hermite polynomials, $H_i(x)$, needed here are reproduced below for convenience. They differ from those defined in some places by an overall factor

$H = H'/2^{i/2}$ and a scaling factor $x = x'/\sqrt{2}$, the unprimed quantities being associated with the definition of [2] and adopted here.

$$
\begin{aligned}
H_1(x) &= x \qquad (40)\\
H_2(x) &= x^2 - 1\\
H_3(x) &= x^3 - 3x\\
H_4(x) &= x^4 - 6x^2 + 3\\
H_5(x) &= x^5 - 10x^3 + 15x\\
H_6(x) &= x^6 - 15x^4 + 45x^2 - 15\\
H_7(x) &= x^7 - 21x^5 + 105x^3 - 105x\\
H_8(x) &= x^8 - 28x^6 + 210x^4 - 420x^2 + 105\\
H_9(x) &= x^9 - 36x^7 + 378x^5 - 1260x^3 + 945x\\
H_{10}(x) &= x^{10} - 45x^8 + 630x^6 - 3150x^4 + 4725x^2 - 945\\
H_{11}(x) &= x^{11} - 55x^9 + 990x^7 - 6930x^5 + 17\,325x^3 - 10\,395x\\
H_{12}(x) &= x^{12} - 66x^{10} + 1485x^8 - 13\,860x^6 + 51\,975x^4 - 62\,370x^2 + 10\,395\\
H_{13}(x) &= x^{13} - 78x^{11} + 2145x^9 - 25\,740x^7 + 135\,135x^5 - 270\,270x^3\\
&+ \quad 135\,135x\\
H_{14}(x) &= x^{14} - 91x^{12} + 3003x^{10} - 45\,045x^8 + 315\,315x^6 - 945\,945x^4\\
&+ \quad 945\,945x^2 - 135\,135\\
H_{15}(x) &= x^{15} - 105x^{13} + 4095x^{11} - 75\,075x^9 + 675\,675x^7 - 2837\,835x^5\\
&+ \quad 4729\,725x^3 - 2027\,025x\\
H_{16}(x) &= x^{16} - 120x^{14} + 5460x^{12} - 120\,120x^{10} + 1351\,350x^8 - 7567\,560x^6\\
&+ \quad 18\,918\,900x^4 - 16\,216\,200x^2 + 2027\,025\\
H_{18}(x) &= x^{18} - 153x^{16} + 9180x^{14} - 278\,460x^{12} + 4594\,590x^{10} - 41\,351\,310x^8\\
&+ \quad 192\,972\,780x^6 - 413\,513\,100x^4 + 310\,134\,825x^2 - 34\,459\,425\\
H_{20}(x) &= x^{20} - 190x^{18} + 14\,535x^{16} - 581\,400x^{14} + 13\,226\,850x^{12}\\
&- 174\,594\,420x^{10} + 1309\,458\,150x^8 - 5237\,832\,600x^6 + 9820\,936\,125x^4\\
&- 6547\,290\,750x^2 + 654\,729\,075\,.
\end{aligned}
$$

Appendix 3

The cumulants, κ_k, are usually expressed in terms of the moments either about the origin, μ'_i, or about the mean [2], e.g., in [17] they are listed in this fashion up to 10th order. The cumulants simplify considerably if the RHS are expressed in terms of *both* μ'_i and lower order κ_k. They are listed below in this manner, to order needed here. For energy loss where all orders

must be included:

$$
\begin{aligned}
\kappa_2 &= \mu_2' - \mu_1'^2 \\
\kappa_3 &= \mu_3' - 2\kappa_2\mu_1' - \mu_1'\mu_2' \\
\kappa_4 &= \mu_4' - 3\kappa_3\mu_1' - 3\kappa_2\mu_2' - \mu_1'\mu_3' \\
\kappa_5 &= \mu_5' - 4\kappa_4\mu_1' - 6\kappa_3\mu_2' - 4\kappa_2\mu_3' - \mu_1'\mu_4' \\
\kappa_6 &= \mu_6' - 5\kappa_5\mu_1' - 10\kappa_4\mu_2' - 10\kappa_3\mu_3' - 5\kappa_2\mu_4' - \mu_1'\mu_5' \\
\kappa_7 &= \mu_7' - 6\kappa_6\mu_1' - 15\kappa_5\mu_2' - 20\kappa_4\mu_3' - 15\kappa_3\mu_4' - 6\kappa_2\mu_5' - \mu_1'\mu_6' \\
\kappa_8 &= \mu_8' - 7\kappa_7\mu_1' - 21\kappa_6\mu_2' - 35\kappa_5\mu_3' - 35\kappa_4\mu_4' - 21\kappa_3\mu_5' - 7\kappa_2\mu_6' - \mu_1'\mu_7'.
\end{aligned}
\tag{41}
$$

Eqs. 41 permit confident extrapolation to higher orders:

$$
\kappa_n = \mu_n' - \sum_{i=1}^{n-1} \binom{n-1}{i} \kappa_{n-i}\mu_i' \tag{42}
$$

something which seems much harder to do when the κ_k expressed solely in terms of the moments. For the angular distribution all odd μ_i' and κ_k vanish and only even κ_k are needed:

$$
\begin{aligned}
\kappa_2 &= \mu_2' \\
\kappa_4 &= \mu_4' - 3\mu_2'^2 \\
\kappa_6 &= \mu_6' - 10\kappa_4\mu_2' - 5\mu_4'\mu_2' \\
\kappa_8 &= \mu_8' - 21\kappa_6\mu_2' - 35\kappa_4\mu_4'^2 - 7\mu_6'\mu_2'^2 \\
\kappa_{10} &= \mu_{10}' - 36\kappa_8\mu_2' - 126\kappa_6\mu_4' - 84\kappa_4\mu_6' - 9\mu_8'\mu_2' \\
\kappa_{12} &= \mu_{12}' - 55\kappa_{10}\mu_2' - 330\kappa_8\mu_4' - 462\kappa_6\mu_6' - 165\kappa_4\mu_8' - 11\mu_{10}'\mu_2'
\end{aligned}
\tag{43}
$$

In the program the κ_k can thus be evaluated recursively. As Eqs 41 and 43 indicate, full evaluation of the higher order cumulants adds to computation time—though perhaps not prohibitively so for most applications.

References

[1] A. Van Ginneken, Nucl. Inst. Meth. **B160**, 460 (2000).

[2] H. Cramér, *Mathematical Methods of Statistics*, Princeton Univ. Press (1945).

[3] This also affords the opportunity to straighten out a misprint in [1]. As in the preprint, each order in the series written there was supposed to appear on a separate line as mentioned in the text. Alas, this was not realized in the printed article.

[4] P. V. Vavilov, Zh. Eksp. Teor. Fiz., **32**, 920 (1957) (in Russian),—Sov. Phys. JETP, **5**, 749 (1957) (Engl. transl.).

[5] H. J. Bhabha, Proc. Roy. Soc. Lond., **164**, 257 (1938).

[6] D. E. Groom et al., Eur. Phys. J. **C 15**, 1 (2000). The last term inside the square brackets is omitted in Groom et al. as well as in most other reviews (it would make the formula spin dependent). However, this term is needed here for consistency with Eq. 2. It is not expected to cause significant differences in overall dE/dx.

[7] Eq. 14 of [1], which bears on this point, contains two misprints: the upper limit of the integral is ϵ_i, not ϵ_c. Likewise ϵ_c in the numerator inside the second parentheses RHS should be replaced by ϵ_i.

[8] Care must be taken when a (single precision) random number is used in the comparisons. In the program a new random number, between zero and the remaining total probability, is generated when the latter is small ($< 10^{-4}$).

[9] C. J. Everett and E.D. Cashwell, *A Third Monte Carlo Sampler*, LA-9721-MS (1983).

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[15] R. M. Sternheimer et al., Atomic Data and Nuclear Data Tables **30**, 261 (1984).

[16] Where it is advantageous to do so, one could sample each regime separately—using its own Edgeworth series—and combine the results to obtain the same energy loss distribution.

[17] A. Stuart and J. K. Ord, *Kendall's Advanced Theory of Statistics, Vol. 1*, John Wiley & Sons (1994).