SIMULATION OF ENERGY LOSS STRAGGLING

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Abstract
This contribution describes how to deal with the statistical nature of ionisation energy loss, characterized by large fluctuations in the amount of energy deposited by a particle traversing an absorber element. Various models a reviewed.

1 INTRODUCTION

Due to the statistical nature of ionisation energy loss, large fluctuations can occur in the amount of energy deposited by a particle traversing an absorber element. Continuous processes such as multiple scattering and energy loss play a relevant role in the longitudinal and lateral development of electromagnetic and hadronic showers, and in the case of sampling calorimeters the measured resolution can be significantly affected by such fluctuations in their active layers. The description of ionisation fluctuations is characterised by the significance parameter κ, which is proportional to the ratio of mean energy loss to the maximum allowed energy transfer in a single collision with an atomic electron

$$\kappa = \frac{\xi}{E_{\max}}$$

$E_{\max}$ is the maximum transferable energy in a single collision with an atomic electron.

$$E_{\max} = \frac{2m_e\beta^2\gamma^2}{1 + 2\gamma m_e/m_x + (m_e/m_x)^2},$$

where $\gamma = E/m_x$, E is energy and m_x the mass of the incident particle, $\beta^2 = 1 - 1/\gamma^2$ and m_e is the electron mass. ξ comes from the Rutherford scattering cross section and is defined as:

$$\xi = \frac{2\pi z^2 e^4 N_{Av} Z\rho\delta x}{m_e\beta^2 c^2 A} = 153.4\frac{z^2}{\beta^2}\frac{Z}{A}\rho\delta x \quad \text{keV},$$

where

z	charge of the incident particle
N_{Av}	Avogadro's number
Z	atomic number of the material
A	atomic weight of the material
ρ	density
δx	thickness of the material

κ measures the contribution of the collisions with energy transfer close to $E_{\max}$. For a given absorber, κ tends towards large values if δx is large and/or if β is small. Likewise, κ tends towards zero if δx is small and/or if β approaches 1.

The value of κ distinguishes two regimes which occur in the description of ionisation fluctuations:

1. A large number of collisions involving the loss of all or most of the incident particle energy during the traversal of an absorber.
   As the total energy transfer is composed of a multitude of small energy losses, we can apply the central limit theorem and describe the fluctuations by a Gaussian distribution. This case is applicable to non-relativistic particles and is described by the inequality $\kappa > 10$ (i.e. when the mean energy loss in the absorber is greater than the maximum energy transfer in a single collision).

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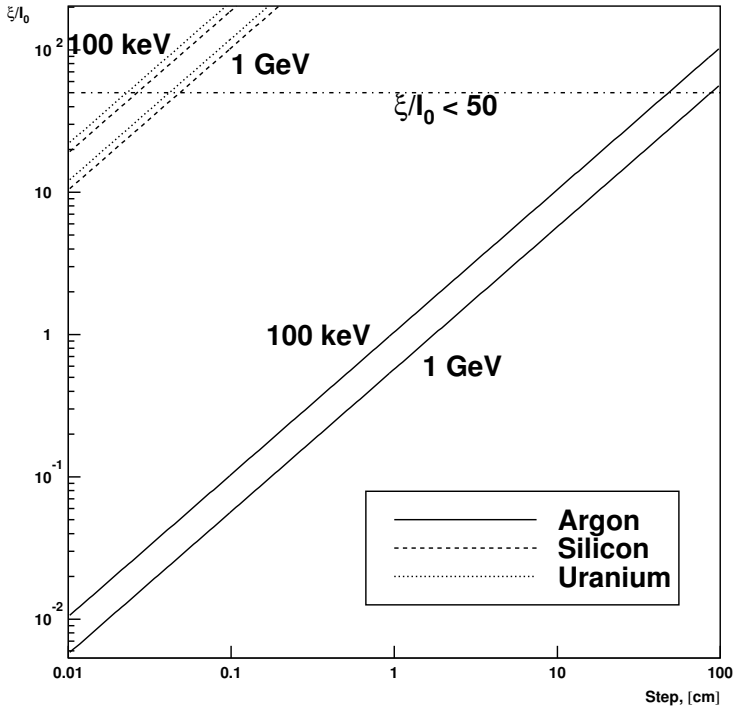

Fig. 1: The variable ξ/I_0 can be used to measure the validity range of the Landau theory. It depends on the type and energy of the particle, Z, A and the ionisation potential of the material and the layer thickness.

2. Particles traversing thin counters and incident electrons under any conditions.
   The relevant inequalities and distributions are $0.01 < \kappa < 10$, Vavilov distribution, and $\kappa < 0.01$, Landau distribution.

An additional regime is defined by the contribution of the collisions with low energy transfer which can be estimated with the relation ξ/I_0, where I_0 is the mean ionisation potential of the atom. Landau theory assumes that the number of these collisions is high, and consequently, it has a restriction $\xi/I_0 \gg 1$. In `GEANT` (see URL `http://wwwinfo.cern.ch/asdoc/geant/geantall.html`), the limit of Landau theory has been set at $\xi/I_0 = 50$. Below this limit special models taking into account the atomic structure of the material are used. This is important in thin layers and gaseous materials. Figure 1 shows the behaviour of ξ/I_0 as a function of the layer thickness for an electron of 100 keV and 1 GeV of kinetic energy in Argon, Silicon and Uranium.

In the following sections, the different theories and models for the energy loss fluctuation are described. First, the Landau theory and its limitations are discussed, and then, the Vavilov and Gaussian straggling functions and the methods in the thin layers and gaseous materials are presented.

2 LANDAU THEORY

For a particle of mass m_x traversing a thickness of material δx, the Landau probability distribution may be written in terms of the universal Landau function $\phi(\lambda)$ as [1]:

$$f(\epsilon, \delta x) \quad = \quad \frac{1}{\xi}\phi(\lambda)$$

where

$$\begin{aligned}
\phi(\lambda) &= \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \exp\left(u\ln u + \lambda u\right) du \qquad\qquad c \geq 0 \\
\lambda &= \frac{\epsilon - \bar{\epsilon}}{\xi} - \gamma' - \beta^2 - \ln\frac{\xi}{E_{\max}} \\
\gamma' &= 0.422784\cdots = 1 - \gamma \\
\gamma &= 0.577215\ldots \text{(Euler's constant)} \\
\bar{\epsilon} &= \text{average energy loss} \\
\epsilon &= \text{actual energy loss}
\end{aligned}$$

2.1 Restrictions

The Landau formalism makes two restrictive assumptions:

1. The typical energy loss is small compared to the maximum energy loss in a single collision. This restriction is removed in the Vavilov theory (see section 3).
2. The typical energy loss in the absorber should be large compared to the binding energy of the most tightly bound electron. For gaseous detectors, typical energy losses are a few keV which is comparable to the binding energies of the inner electrons. In such cases a more sophisticated approach which accounts for atomic energy levels [4] is necessary to accurately simulate data distributions. In `GEANT`, a parameterised model by L. Urbán is used (see section 5).

In addition, the average value of the Landau distribution is infinite. Summing the Landau fluctuation obtained to the average energy from the dE/dx tables, we obtain a value which is larger than the one coming from the table. The probability to sample a large value is small, so it takes a large number of steps (extractions) for the average fluctuation to be significantly larger than zero. This introduces a dependence of the energy loss on the step size which can affect calculations.

A solution to this has been to introduce a limit on the value of the variable sampled by the Landau distribution in order to keep the average fluctuation to 0. The value obtained from the `GLANDO` routine is:

$$\delta dE/dx = \epsilon - \bar{\epsilon} = \xi(\lambda - \gamma' + \beta^2 + \ln\frac{\xi}{E_{\max}})$$

In order for this to have average 0, we must impose that:

$$\bar{\lambda} = -\gamma' - \beta^2 - \ln\frac{\xi}{E_{\max}}$$

This is realised introducing a $\lambda_{\max}(\bar{\lambda})$ such that if only values of $\lambda \leq \lambda_{\max}$ are accepted, the average value of the distribution is $\bar{\lambda}$.

A parametric fit to the universal Landau distribution has been performed, with following result:

$$\lambda_{\max} = 0.60715 + 1.1934\bar{\lambda} + (0.67794 + 0.052382\bar{\lambda})\exp(0.94753 + 0.74442\bar{\lambda})$$

only values smaller than $\lambda_{\max}$ are accepted, otherwise the distribution is resampled.

3 VAVILOV THEORY

Vavilov [5] derived a more accurate straggling distribution by introducing the kinematic limit on the maximum transferable energy in a single collision, rather than using $E_{\max} = \infty$. Now we can write [2]:

$$f\left(\epsilon, \delta s\right) = \frac{1}{\xi}\phi_v\left(\lambda_v, \kappa, \beta^2\right)$$

where

$$\begin{aligned}
\phi_v\left(\lambda_v,\kappa,\beta^2\right) &= \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\phi\left(s\right)e^{\lambda s}ds \qquad\qquad c\geq 0\\
\phi\left(s\right) &= \exp\left[\kappa(1+\beta^2\gamma)\right]\ \exp\left[\psi\left(s\right)\right],\\
\psi\left(s\right) &= s\ln\kappa+(s+\beta^2\kappa)\left[\ln(s/\kappa)+E_1(s/\kappa)\right]-\kappa e^{-s/\kappa},
\end{aligned}$$

and

$$\begin{aligned}
E_1(z) &= \int_z^\infty t^{-1}e^{-t}dt \qquad \text{(the exponential integral)}\\
\lambda_v &= \kappa\left[\frac{\epsilon-\bar{\epsilon}}{\xi}-\gamma'-\beta^2\right]
\end{aligned}$$

The Vavilov parameters are simply related to the Landau parameter by $\lambda_L=\lambda_v/\kappa-\ln\kappa$. It can be shown that as $\kappa\to 0$, the distribution of the variable λ_L approaches that of Landau. For $\kappa\leq 0.01$ the two distributions are already practically identical. Contrary to what many textbooks report, the Vavilov distribution *does not* approximate the Landau distribution for small κ, but rather the distribution of λ_L defined above tends to the distribution of the true λ from the Landau density function. Thus the routine `GVAVIV` samples the variable λ_L rather than λ_v. For $\kappa\geq 10$ the Vavilov distribution tends to a Gaussian distribution (see next section).

4 GAUSSIAN THEORY

Various conflicting forms have been proposed for Gaussian straggling functions, but most of these appear to have little theoretical or experimental basis. However, it has been shown [3] that for $\kappa\geq 10$ the Vavilov distribution can be replaced by a Gaussian of the form:

$$f(\epsilon,\delta s)\approx\frac{1}{\xi\sqrt{\frac{2\pi}{\kappa}\left(1-\beta^2/2\right)}}\exp\left[\frac{(\epsilon-\bar{\epsilon})^2}{2}\frac{\kappa}{\xi^2(1-\beta^2/2)}\right]$$

thus implying

$$\begin{aligned}
\text{mean} &= \bar{\epsilon}\\
\sigma^2 &= \frac{\xi^2}{\kappa}(1-\beta^2/2)=\xi E_{\max}(1-\beta^2/2)
\end{aligned}$$

5 URBÁN MODEL

The method for computing restricted energy losses with δ-ray production above given threshold energy in `GEANT` is a Monte Carlo method that can be used for thin layers. It is fast and it can be used for any thickness of a medium. Approaching the limit of the validity of Landau's theory, the loss distribution approaches smoothly the Landau form as shown in Figure 2.

It is assumed that the atoms have only two energy levels with binding energy E_1 and E_2. The particle–atom interaction will then be an excitation with energy loss E_1 or E_2, or an ionisation with an energy loss distributed according to a function $g(E)\sim 1/E^2$:

$$g(E)=\frac{(E_{\max}+I)I}{E_{\max}}\frac{1}{E^2} \tag{1}$$

The macroscopic cross-section for excitations ($i=1,2$) is

$$\Sigma_i=C\frac{f_i}{E_i}\frac{\ln(2m\beta^2\gamma^2/E_i)-\beta^2}{\ln(2m\beta^2\gamma^2/I)-\beta^2}(1-r) \tag{2}$$

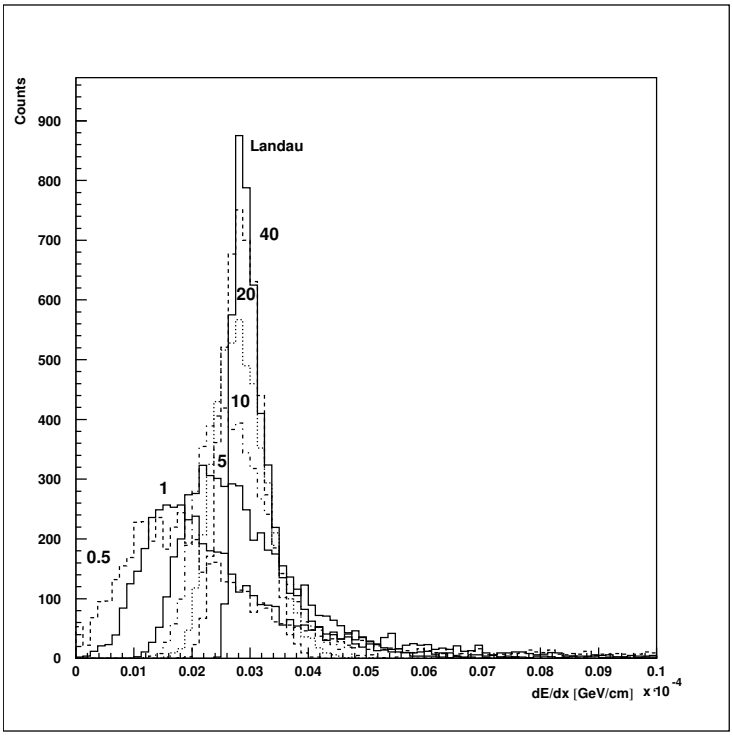

Fig. 2: Energy loss distribution for a 3 GeV electron in Argon as given by standard GEANT. The width of the layers is given in centimeters.

and the macroscopic cross-section for ionisation is

$$\Sigma_3 = C\frac{E_{\max}}{I(E_{\max}+I)\ln(\frac{E_{\max}+I}{I})}\,r \tag{3}$$

$E_{\max}$ is the GEANT cut for δ-production, or the maximum energy transfer minus mean ionisation energy, if it is smaller than this cut-off value. The following notation is used:

r, C	parameters of the model
E_i	atomic energy levels
I	mean ionisation energy
f_i	oscillator strengths

The model has the parameters f_i, E_i, C and r $(0 \leq r \leq 1)$. The oscillator strengths f_i and the atomic level energies E_i should satisfy the constraints

$$f_1 + f_2 = 1 \tag{4}$$

$$f_1 \ln E_1 + f_2 \ln E_2 = \ln I \tag{5}$$

The parameter C can be defined with the help of the mean energy loss dE/dx in the following way: The numbers of collisions (n_i, i = 1,2 for the excitation and 3 for the ionisation) follow the Poisson distribution with a mean number $\langle n_i \rangle$. In a step Δx the mean number of collisions is

$$\langle n_i \rangle = \Sigma_i \Delta x \tag{6}$$

The mean energy loss dE/dx in a step is the sum of the excitation and ionisation contributions

$$\frac{dE}{dx}\Delta x = \left[\Sigma_1 E_1 + \Sigma_2 E_2 + \Sigma_3 \int_I^{E_{\max}+I} E\; g(E)\; dE\right]\Delta x \tag{7}$$

From this, using the equations (2), (3), (4) and (5), one can define the parameter C

$$C = \frac{dE}{dx} \tag{8}$$

The following values have been chosen in GEANT for the other parameters:

$$\begin{aligned} f_2 &= \begin{cases} 0 & \text{if } Z \leq 2 \\ 2/Z & \text{if } Z > 2 \end{cases} & \Rightarrow \quad & f_1 = 1 - f_2 \\ E_2 &= 10Z^2\text{eV} & \Rightarrow \quad & E_1 = \left(\frac{I}{E_2^{f_2}}\right)^{\frac{1}{f_1}} \\ r &= 0.4 \end{aligned}$$

With these values the atomic level E_2 corresponds approximately the K-shell energy of the atoms and Zf_2 the number of K-shell electrons. r is the only variable which can be tuned freely. It determines the relative contribution of ionisation and excitation to the energy loss.

The energy loss is computed with the assumption that the step length (or the relative energy loss) is small, and—in consequence—the cross-section can be considered constant along the path length. The energy loss due to the excitation is

$$\Delta E_e = n_1 E_1 + n_2 E_2 \tag{9}$$

where n_1 and n_2 are sampled from Poisson distribution as discussed above. The loss due to the ionisation can be generated from the distribution $g(E)$ by the inverse transformation method:

$$\begin{aligned} u = F(E) &= \int_I^E g(x)dx \\ E = F^{-1}(u) &= \frac{I}{1 - u\frac{E_{\max}}{E_{\max}+I}} \end{aligned} \tag{10}$$

$$\tag{11}$$

where u is a uniform random number between $F(I) = 0$ and $F(E_{\max} + I) = 1$. The contribution from the ionisations will be

$$\Delta E_i = \sum_{j=1}^{n_3} \frac{I}{1 - u_j \frac{E_{\max}}{E_{\max}+I}} \tag{12}$$

where n_3 is the number of ionisation (sampled from Poisson distribution). The energy loss in a step will then be $\Delta E = \Delta E_e + \Delta E_i$.

5.1 Fast simulation for $n_3 \geq 16$

If the number of ionisation n_3 is bigger than 16, a faster sampling method can be used. The possible energy loss interval is divided in two parts: one in which the number of collisions is large and the sampling can be done from a Gaussian distribution and the other in which the energy loss is sampled for each collision. Let us call the former interval $[I, \alpha I]$ the interval A, and the latter $[\alpha I, E_{\max}]$ the interval B. α lies between 1 and $E_{\max}/I$. A collision with a loss in the interval A happens with the probability

$$P(\alpha) = \int_I^{\alpha I} g(E)\, dE = \frac{(E_{\max} + I)(\alpha - 1)}{E_{\max}\alpha} \tag{13}$$

The mean energy loss and the standard deviation for this type of collision are

$$\langle \Delta E(\alpha) \rangle = \frac{1}{P(\alpha)} \int_I^{\alpha I} E\, g(E)\, dE = \frac{I\alpha \ln \alpha}{\alpha - 1} \tag{14}$$

and

$$\sigma^2(\alpha) = \frac{1}{P(\alpha)} \int_I^{\alpha I} E^2 \, g(E) \, dE = I^2 \alpha \left(1 - \frac{\alpha \ln^2 \alpha}{(\alpha - 1)^2} \right) \tag{15}$$

If the collision number is high , we assume that the number of the type A collisions can be calculated from a Gaussian distribution with the following mean value and standard deviation:

$$\begin{aligned} \langle n_A \rangle &= n_3 P(\alpha) & (16) \\ \sigma_A^2 &= n_3 P(\alpha)(1 - P(\alpha)) & (17) \end{aligned}$$

It is further assumed that the energy loss in these collisions has a Gaussian distribution with

$$\begin{aligned} \langle \Delta E_A \rangle &= n_A \langle \Delta E(\alpha) \rangle & (18) \\ \sigma_{E,A}^2 &= n_A \sigma^2(\alpha) & (19) \end{aligned}$$

The energy loss of these collision can then be sampled from the Gaussian distribution.

The collisions where the energy loss is in the interval B are sampled directly from

$$\Delta E_B = \sum_{i=1}^{n_3 - n_A} \frac{\alpha I}{1 - u_i \frac{E_{\max} + I - \alpha I}{E_{\max} + I}} \tag{20}$$

The total energy loss is the sum of these two types of collisions:

$$\Delta E = \Delta E_A + \Delta E_B \tag{21}$$

The approximation of equations (16), (17), (18) and (19) can be used under the following conditions:

$$\begin{aligned} \langle n_A \rangle - c \, \sigma_A &\geq 0 & (22) \\ \langle n_A \rangle + c \, \sigma_A &\leq n_3 & (23) \\ \langle \Delta E_A \rangle - c \, \sigma_{E,A} &\geq 0 & (24) \end{aligned}$$

where $c \geq 4$. From the equations (13), (16) and (18) and from the conditions (22) and (23) the following limits can be derived:

$$\alpha_{\min} = \frac{(n_3 + c^2)(E_{\max} + I)}{n_3(E_{\max} + I) + c^2 I} \leq \alpha \leq \alpha_{\max} = \frac{(n_3 + c^2)(E_{\max} + I)}{c^2(E_{\max} + I) + n_3 I} \tag{25}$$

This conditions gives a lower limit to number of the ionisations n_3 for which the fast sampling can be done:

$$n_3 \geq c^2 \tag{26}$$

As in the conditions (22), (23) and (24) the value of c is as minimum 4, one gets $n_3 \geq 16$. In order to speed the simulation, the maximum value is used for α.

The number of collisions with energy loss in the interval B (the number of interactions which has to be simulated directly) increases slowly with the total number of collisions n_3. The maximum number of these collisions can be estimated as

$$n_{B,max} = n_3 - n_{A,min} \approx n_3(\langle n_A \rangle - \sigma_A) \tag{27}$$

From the previous expressions for $\langle n_A \rangle$ and σ_A one can derive the condition

$$n_B \leq n_{B,max} = \frac{2 n_3 c^2}{n_3 + c^2} \tag{28}$$

The following values are obtained with $c = 4$:

n_3	$n_{B,max}$	n_3	$n_{B,max}$
16	16	200	29.63
20	17.78	500	31.01
50	24.24	1000	31.50
100	27.59	∞	32.00

5.2 Special sampling for lower part of the spectrum

If the step length is very small (≤ 5 mm in gases, $\leq$ 2-3 μm in solids) the model gives 0 energy loss for some events. To avoid this, the probability of 0 energy loss is computed

$$P(\Delta E = 0) = e^{-(\langle n_1 \rangle + \langle n_2 \rangle + \langle n_3 \rangle)} \tag{29}$$

If the probability is bigger than 0.01 a special sampling is done, taking into account the fact that in these cases the projectile interacts only with the outer electrons of the atom. An energy level $E_0 = 10$ eV is chosen to correspond to the outer electrons. The mean number of collisions can be calculated from

$$\langle n \rangle = \frac{1}{E_0} \frac{dE}{dx} \Delta x \tag{30}$$

The number of collisions n is sampled from Poisson distribution. In the case of the thin layers, all the collisions are considered as ionisations and the energy loss is computed as

$$\Delta E = \sum_{i=1}^{n} \frac{E_0}{1 - \frac{E_{\max}}{E_{\max}+E_0} u_i} \tag{31}$$

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