Dosimetry, scattering theory, and Monte Carlo simulation

Gordon McCabe

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Abstract

The purpose of this paper is to provide an introduction to the physics of scattering theory, to define the dosimetric concept of linear energy transfer in terms of scattering theory, and to provide an introduction to the concepts underlying Monte Carlo simulations.

1 Introduction

Whilst the absorbed dose deposited by energetic particles (‘radiation’) in condensed matter is simply the energy per unit mass delivered to the medium, the equivalent dose is a function of both the energy per unit mass, and the spatial distribution with which that energy is deposited. The greater the spatial concentration of deposited energy, the greater the equivalent dose. The average rate at which a type of radiation locally deposits energy in a medium, per unit distance of track length, is called the linear energy transfer (LET) of that radiation in that medium. Radiation with higher linear energy transfer deposits a greater equivalent dose in a medium.

The LET is closely related to the stopping power of the medium, which is the energy lost by an incoming particle, whether it is deposited locally, or transformed into other radiation, such as Bremsstrahlung photons, or the energy of secondary electrons, (so-called ‘delta-rays’). Linear energy transfer and stopping power generally coincide in the case of heavy charged particles, but the linear energy transfer of beta-radiation (i.e, incoming electrons) does not include the energy transformed into Bremsstrahlung photons or delta-rays.

The first purpose of this paper is to define linear energy transfer in terms of the concepts used in scattering theory, and, in particular, the concepts of quantum scattering theory. An exposition will then be provided of the principles underlying Monte Carlo simulations.

2 Scattering

Scattering theory is the branch of physics which describes the collision processes between particles. These are typically considered to be processes in which an
incoming particle, or beam of such particles, interacts with a target particle, or
collection of particles. After an individual interaction, the energy and momen-
tum of both the incoming particle and the target particle can be altered. A
change of momentum includes both a change in the direction of travel, and, in
the case of particle with non-zero mass, a change in the speed of travel. The
target particle is often considered to be a composite particle, and as such, both
its energy of motion, and its internal energy state, can change as a result of the
collision.

Consider first the scattering of a particle beam in terms of classical physics.
In the case of a beam of particles with non-zero mass, the beam has a flux $F$
declared as

$$F = n_i v_i,$$

where $n_i$ is the number of particles per unit volume in the beam, and $v_i$ is
the average velocity of the particles in the beam. The flux has dimensions
of $\text{Area}^{-1} \text{Time}^{-1}$. It can be equivalently defined as the number of particles
passing through a unit cross-sectional area of the beam, per unit time. The flux
should not be confused with the fluence $\Phi$ of a particle beam, which is the
number of particles passing through a unit cross-sectional area of the beam,
over the time duration considered. Hence, the fluence is the definite integral of
the flux over time, $\Phi = \int_{t_0}^{t} F(\tau) \, d\tau$, and the flux is the time derivative of the
fluence, $F = d\Phi/dt$. The fluence has dimensions of $\text{Area}^{-1}$.

A particle detector placed at an angle $\Omega = (\theta, \phi)$ with respect to the direction
of the incoming beam, will detect particles at the rate (Bohm 1979, p312):

$$N/\Delta t = \sigma(\Omega) N_T n_i v_i = \sigma(\Omega) N_T F.$$

$N_T$ is the number of particles in the target, and the constant of proportionality
$\sigma(\Omega)$ is called the differential cross-section in the direction $\Omega$. The differential
cross-section can clearly be expressed as

$$\sigma(\Omega) = \frac{1}{N_T} \frac{N/\Delta T}{n_i v_i},$$

or, in words,

$$\sigma(\Omega) = \frac{1}{N_T} \frac{\text{Number of particles scattered into } \Omega \text{ per unit time}}{\text{Incident Flux}}.$$

The dimensions of the differential cross-section are $\text{Area} \cdot \text{Solid Angle}^{-1}$.

Integrating the differential cross-section over all possible directions gives the
total scattering cross-section $\sigma$:

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1In the physics literature, the differential cross-section is usually denoted as $d\sigma$, or $d\sigma/d\Omega$. The
expression for $d\sigma$ typically contains a dependence upon both the direction and magnitude
of the outgoing momentum, whilst the expression for $d\sigma/d\Omega$ contains only a dependence upon
direction, and is obtained by integrating over all the outgoing momenta in that direction. We
shall refrain from such mathematically questionable notation in this paper.
\[ \sigma = \int \sigma(\Omega) d\Omega, \]

where \( d\Omega = \sin \theta d\phi \, d\theta \)\(^2\). The dimensions of the total cross-section are simply Area. One can think of the cross-section as effectively the area which the target presents to the incoming beam.

In terms of the quantum mechanics of a scattering process, an incoming particle is represented by a quantum state, or \('\text{wave-function}'\) \( \Psi_i \), the interaction process is represented by a scattering operator \( S \), the final outgoing particle state is represented by another wave-function \( \Psi_f \), and the objective is to calculate the transition probability \( |\langle \Psi_f | S | \Psi_i \rangle|^2 \) between an incoming state and an outgoing state.\(^3\) In many physically relevant situations, the incoming state has a specific energy \( E_i \) and momentum \( k_i \), and each possible outgoing state also has a specific energy \( E_f \) and momentum \( k_f \). An outgoing state with a specific momentum \( k_f \) also has a specific direction \( \Omega \) associated with it.

The square-amplitude \( |\Psi_i|^2 \) of the incoming particle’s wave-function gives the position probability density for the particle. In quantum mechanical terms the incoming flux \( F_{\Psi_i} \) is then the product of the probability density per unit volume, with the velocity of the particle. Equivalently, the quantum mechanical flux is the probability density per unit area, per unit time. Hence, in quantum mechanical terms even an individual particle has a flux associated with it. Given the transition probability \( |\langle \Psi_f | S | \Psi_i \rangle|^2 \), there is also an associated \('\text{transition rate}'\), or transition probability per unit time. In the simplest quantum mechanical terms, cross-sections can be defined as follows (Bohm 1979, p314):

\[ \sigma = \frac{\text{Transition probability}}{\text{Incident probability per unit area}}, \]

or, equivalently,

\[ \sigma = \frac{\text{Transition probability, per unit time}}{\text{Incident probability per unit area, per unit time}}, \]

which itself is equivalent to

\[ \sigma = \frac{\text{Transition rate}}{\text{Incident Flux}}. \]

The quantum mechanical cross-sections used in practice provide an economical way of bundling the transition probabilities between classes of quantum states. For example, the differential cross-section \( \sigma(E, \Omega) \) is proportional to the probability of a transition from \('\text{any}'\) incoming state \( \Psi_i \) of energy \( E \) to \('\text{any}'\) outgoing state \( \Psi_f \) in which the momentum vector \( k_f \) points in the direction of \( \Omega \). As before, integrating a differential cross-section over all possible directions then gives a total scattering cross-section \( \sigma(E) \):

\(^2\)In terms of differential geometry, \( d\Omega \) is the volume form on the 2-sphere, expressible as \( d\Omega = \sin \theta d\phi \wedge d\theta \), where \( \wedge \) is the antisymmetric tensor product.

\(^3\)\( \langle \cdot | \cdot \rangle \) here is the inner product on the space of quantum states.
\[
\sigma(E) = \int \sigma(E, \Omega) d\Omega .
\]

This total cross-section is proportional to the probability of an incoming state of energy \(E\) interacting with the target particle.

Now, an elastic collision is defined to be a collision in which the outgoing particles are the same as the incoming particles, and the total kinetic energy of the particles before the collision is the same as the total kinetic energy of the particles after the collision. Interactions in which this does not occur are called inelastic collisions. For example, an inelastic collision occurs when an incoming particle interacts with an atom, and some of the energy from the incoming particle excites or ionises the atom. Alternatively, the incoming particle can be absorbed by the target, raising the target particle into an excited state, which may then subsequently release various decay products. An example of this is the absorption of an incoming neutron by an atomic nucleus. Hence, there are elastic scattering cross-sections, inelastic scattering cross-sections, and absorption cross-sections, all of which are functions of the energy of the incoming particle(s).

Given the inelastic differential cross-section \(\sigma_\mu(\Omega)\) for an interaction in which the incoming projectile transfers \(\Delta E_\mu\) of energy to a target atom, and the projectile scatters with a momentum \(k_f\) in direction \(\Omega\), the total inelastic cross-section for all interactions in which the projectile transfers \(\Delta E_\mu\) of energy to a target atom is:

\[
\sigma_\mu = \int \sigma_\mu(\Omega) d\Omega \\
= \int_0^{2\pi} d\phi \int_0^\pi \sigma_\mu(\theta, \phi) \sin \theta d\theta .
\]

Given \(N\) target atoms per unit volume in a condensed matter medium, the product \(N \sigma_\mu\) is the probability per unit path-length of the incoming particle track, that the projectile will lose \(\Delta E_\mu\) of energy. Hence, the local energy transfer (linear energy transfer) of the particle is given by the expression:

\[
-\frac{dE}{dx} = N \sum_\mu \Delta E_\mu \sigma_\mu .
\]

To be more precise, this is the quantum mechanical expectation value\(^4\) for the energy loss per unit length:

\[
-\langle \frac{dE}{dx} \rangle = N \sum_\mu \Delta E_\mu \sigma_\mu .
\]

\(^4\)Given the probability \(p_i\) for each possible value \(a_i\) of a quantity \(A\), the expectation value \(\langle A \rangle\) of the quantity is defined to be the probability-weighted sum of those values, \(\langle A \rangle = \sum_i p_i a_i\).
A special case of this equation is Bethe’s formula for the local energy loss, per unit track-length, of a swiftly moving charged particle heavier than an electron. Bethe’s formula applies, for example, to energetic protons, alpha particles, and heavy ions. For swift charged particles heavier than an electron, the inelastic cross-sections are sharply peaked towards the forward direction. If we take the forward direction to correspond to a polar angle of \( \theta = 0 \), such particles scatter into a narrow cone-shaped region circumscribed by a small polar angle \( \Theta \), and all azimuthal angles \( \phi \in [0, 2\pi) \). Bethe’s formula then arises from assuming that the cross-section

\[
\sigma_\mu = \int_0^{2\pi} d\phi \int_0^\pi \sigma_\mu(\theta, \phi) \sin \theta d\theta ,
\]
can be approximated by

\[
\sigma_\mu = \int_0^{2\pi} d\phi \int_0^\Theta \sigma_\mu(\theta, \phi) \sin \theta d\theta .
\]

Assuming the projectile has a non-relativistic speed, Bethe’s formula for linear energy transfer is:

\[
-\frac{dE}{dx} = 4\pi N Z^2 e^4 \frac{\nu^2}{m_e \nu^2} \ln \left( \frac{M \nu^2 \Theta}{I} \right) ,
\]

where \( M \) is the mass of projectile, \( \nu \) is its speed, \( ze \) is its charge, \( m_e \) is the electron mass, \( Z \) is the proton number of the target atoms, \( N \) is the number of target atoms per unit volume, and \( I \) is a parameter, called the ‘mean excitation potential’, characterising only the target atoms. Because the mass \( M \) of the projectile only appears in the natural logarithm, the charge of the incoming projectile has a greater effect upon linear energy transfer than the mass of the incoming projectile.

3 Monte Carlo Simulations

Monte Carlo simulations are computer simulations which use random numbers. Given the inherently probabilistic nature of particle interactions, Monte Carlo simulations can be used to simulate particle tracks, and their local energy deposition in a chosen medium. Monte Carlo simulations can thereby be used to calculate absorbed dose and equivalent dose. The cross-sections obtained from quantum mechanical and quantum field theoretical scattering theory provide the probability distributions used in such Monte Carlo simulations.

A computer can generate random numbers with any specified probability distribution. In other words, a computer can generate numbers with the relative frequencies specified by any probability distribution. The ability of a computer to generate such random numbers is dependent upon the ability of a computer to act as a ‘pseudo-random’ number generator. The computer implements an algorithm which generates random numbers in the interval \((0, 1)\)
with an apparently uniform distribution. The algorithm generates each number from its predecessor according to a deterministic rule, hence the randomness is purely one of appearance. The starting point of the pseudo-random generator is called the ‘seed’, and if one starts successive runs of the program with the same seed, then exactly the same sequence of numbers will be generated, in the same order, in each run. If one wishes to avoid generating the same sequence of numbers on successive runs, then one simply changes the seed of the generator. The important point, however, is that the numbers are, to a specified level of approximation, uniformly distributed in the interval \((0, 1)\).

Given the generation of random numbers with a uniform distribution in \((0, 1)\), random numbers can be generated in any other interval, with any specified distribution. The method of doing so exploits the fact that because the definite integral of any probability distribution \(p(x)\) must equal one,

\[
\int_a^b p(x')dx' = 1 ,
\]

the indefinite integral \(F(x)\), which uses the upper limit of integration as the dependent variable,

\[
F(x) = \int_a^x p(x')dx' ,
\]

must assume values in the interval between 0 and 1, beginning at the value of 0 when \(x = a\), and increasing until it reaches the value of 1 when \(x = b\).

Given a probability distribution \(p(x)\) over a domain \((a, b) \subset \mathbb{R}\), the selection of a random number \(\mu\) between 0 and 1, selects a value \(\zeta \in (a, b)\) such that

\[
F(\zeta) = \int_a^\zeta p(x')dx' = \mu .
\]

When many values in \((a, b)\) are selected by this means, they will approximate the distribution specified by \(p(x)\). The selection of random values according to a specified probability distribution, in this manner, is referred to as ‘sampling from a random distribution.’

In the Monte Carlo simulation of a particle track through a medium, one typically generates random numbers for (i) the distance travelled by the particle before its next collision; (ii) whether the next collision is elastic or inelastic; (iii) the type of inelastic collision in such an event; (iv) the energy transferred in the event of an inelastic collision; and (v) the direction with which the projectile scatters as a consequence of the collision. Let us look at each of these in turn.

To calculate the distance travelled \(l\) by a particle before its next interaction, note first that where \(\sigma_{\text{inelas}}\) denotes the total inelastic scattering cross-section, and \(N\) denotes the number of targets per unit volume, the product \(N\sigma_{\text{inelas}}\) gives the probability per unit path-length of the incoming particle track, that the projectile will undergo some type of inelastic interaction. The reciprocal of this value therefore gives the mean free path \(\lambda_{\text{inelas}}\) for inelastic scattering. In other words, \(\lambda_{\text{inelas}} = 1/N\sigma_{\text{inelas}}\) is the mean distance travelled by a particle.
between inelastic collisions. Similarly, \( \lambda_{elas} = N\sigma_{elas} \) gives the probability per unit path length, that the projectile will undergo some type of elastic interaction, and the reciprocal \( 1/N\sigma_{elas} \) gives the mean free path for elastic scattering. The total mean free path \( \lambda_t \) is then

\[
\lambda_t = \frac{1}{\lambda_{inelas}^{-1} + \lambda_{elas}^{-1}}.
\]

Now, the path-lengths between interactions will have the following inverse-exponential distribution

\[
p(x) = \frac{1}{\lambda_t} \exp\left(-\frac{x}{\lambda_t}\right),
\]

with \( \lambda_t \) as the mean of the distribution. Given a randomly generated number \( \mu_1 \in (0, 1) \), the distance travelled \( l \) by a particle before its next interaction can be randomly generated according to

\[
\mu_1 = \int_0^l \frac{1}{\lambda_t} \exp\left(-\frac{x}{\lambda_t}\right) \, dx.
\]

The indefinite integral of the path-length distribution is

\[
F(x) = \int \frac{1}{\lambda_t} \exp\left(-\frac{x'}{\lambda_t}\right) \, dx' = -\exp\left(-\frac{x}{\lambda_t}\right),
\]

hence

\[
\mu_1 = \int_0^l \frac{1}{\lambda_t} \exp\left(-\frac{x}{\lambda_t}\right) \, dx
\]

\[
= F(l) - F(0)
\]

\[
= -\exp\left(-\frac{l}{\lambda_t}\right) + 1.
\]

Therefore,

\[
1 - \mu_1 = \exp\left(-\frac{l}{\lambda_t}\right),
\]

and

\[
\ln(1 - \mu_1) = -\frac{l}{\lambda_t},
\]

from which it follows that

\[
l = -\lambda_t \ln(1 - \mu_1).
\]

Given that \( \mu_1 \) is uniformly distributed in \((0, 1)\), \( 1 - \mu_1 \) will also be uniformly distributed in \((0, 1)\), hence, for the purposes of generating random numbers, \( \mu_1 \)
can be substituted into this equation in place of $1 - \mu_1$, to obtain the final expression:

$$l = -\lambda t \ln(\mu_1).$$

Given random numbers $\mu_1 \in (0,1)$, one uses this expression to generate the random path lengths between collisions.

To decide whether the next collision is to be elastic or inelastic, one can use the fact that the probability of an inelastic collision $p_{\text{inelas}}$ is specified by

$$p_{\text{inelas}} = \frac{\lambda^{-1}_{\text{inelas}}}{\lambda^{-1}_{\text{inelas}} + \lambda^{-1}_{\text{elas}}}.$$

A random number $\mu_2$ is generated, and if $\mu_2 \leq p_{\text{inelas}}$, then the collision is chosen to be inelastic, otherwise it is chosen to be elastic.

The types of possible inelastic collision then depend upon the type of projectile under consideration. For example, in the case of an incoming gamma-ray photon, there could be a photoelectric interaction, a Compton-effect interaction, or a pair-production interaction. The relative probabilities of the different interaction types depend upon the energy of the incoming particle, and given these relative probabilities, a randomly number $\mu_3 \in (0,1)$ can determine which interaction is selected. Let $\kappa$ denote the linear attenuation coefficient of energy $E$ gamma rays in the medium, let $\tau$ denote the photoelectric attenuation coefficient, and let $\varpi$ denote the Compton attenuation coefficient. If $\mu_3$ is between 0 and $\tau / \kappa$, then photoelectric absorption can be deemed to occur; if $\mu_3$ is between $\tau / \kappa$ and $(\tau + \varpi)/\kappa$, then Compton scattering can be deemed to occur; and if $\mu_3$ is between $(\tau + \varpi)/\kappa$ and 1, then pair production can be deemed to occur (Mackie 1990, p552). The energy lost as a result of the interaction is chosen, once more, by the generation of random numbers, and by the energy loss distributions specific to each type of interaction.

Given the relevant differential cross-section $\sigma(\theta, \phi)$ for the incoming energy $E$, random numbers can be generated which specify the polar angle and azimuthal angle with which the projectile scatters. Assuming the incoming projectile is travelling in the direction $\theta = 0$, the probability $p(\theta)$ of scattering at polar angle $\theta$ is

$$p(\theta) = \frac{\sigma(\theta, \phi) \sin \theta}{\int_0^\pi \sigma(\theta', \phi) \sin \theta' d\theta'}.$$

The integral $\int_0^\pi \sigma(\theta', \phi) \sin \theta' d\theta'$ of the differential cross-section over all polar angles gives a quantity with dimensions of Area · Angle$^{-1}$, proportional to the probability, per unit azimuthal angle, of scattering at any polar angle. The expression $\sigma(\theta, \phi) \sin \theta$ gives a quantity, with the same dimensions, proportional to the probability of scattering, per unit azimuthal angle, at polar angle $\theta$. The ratio of the latter by the former gives the probability $p(\theta)$ of scattering at polar angle $\theta$. Hence, given the selection of a random number $\mu_4 \in (0,1)$, the angle $\theta$ such that
\[
\mu_4 = \int_0^\theta p(\theta') d\theta' \\
= \frac{\int_0^\theta \sigma(\theta', \phi) \sin \theta' d\theta'}{\int_0^\pi \sigma(\theta', \phi) \sin \theta' d\theta'}
\]
is selected. The azimuthal angle \(\phi\) is determined by a uniform distribution over \((0, 2\pi)\), and the selection of another random number \(\mu_5 \in (0, 1)\).

**References**

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