Nuclear Instruments and Methods in Physics Research B 330 (2014) 99–102

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

# Lewis theory for energy straggling in thin layers

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ARTICLE INFO

*Article history:*
Received 22 February 2014
Received in revised form 28 March 2014
Accepted 1 April 2014
Available online 4 May 2014

*Keywords:*
Energy-loss straggling
Lewis moments
Moment-preserving approximations
Moment-equivalence

ABSTRACT

A Lewis-moments theory for energy straggling is developed that underpins the observed numerical accuracy of moment-preserving approximations for computing charged particle energy-loss distributions in thin layers. Specifically, we prove that for a certain class of straggling models, if an approximate straggling model has identical collisional energy-loss moments as the exact or analog model through a fixed order *N*, then the corresponding energy-moments of the energy-loss distributions are identical to order *N*.


## 1. Introduction

Consider an infinite medium in which charged particles undergo scattering collisions resulting in angular deflections but no energy losses. Let the differential scattering cross section be given by $\Sigma_s^{(A)}(\vec{\Omega}'\cdot\vec{\Omega})$ with $\vec{\Omega}'$ and $\vec{\Omega}$ being pre- and post-collision unit direction vectors and where the label *A* denotes a specific configuration of this problem. The Legendre moments of this cross section are defined by $\Sigma_{s,n}^{(A)} = \int_{4\pi}\Sigma_s^{(A)}(\vec{\Omega}\cdot\vec{\Omega}')P_n(\vec{\Omega}\cdot\vec{\Omega}')d^2\Omega$, where $P_n(\mu)$, $-1\leqslant\mu\leqslant 1$, are the Legendre polynomials. The cross section or its associated moments and the charged particle source completely characterize this problem. Consider now a second configuration, labeled *B*, that is characterized by the same source but a different differential scattering cross section $\Sigma_s^{(B)}(\vec{\Omega}'\cdot\vec{\Omega})$ and hence different Legendre moments $\Sigma_{s,n}^{(B)}$. In general, the particle angular distributions or angular fluxes for the two problems, $\psi_{A,B}(\vec{r},\vec{\Omega})$, will be different. However, if the cross sections are related such that $\Sigma_{s,n}^{(B)} = \Sigma_{s,n}^{(A)}, n = 1,2,\ldots N$, for some fixed order $N$, and $\Sigma_{s,n}^{(B)} \neq \Sigma_{s,n}^{(A)}, \quad n \geqslant N+1$, then a classic result due to Lewis [1] states that space-angle moments of the two angular fluxes defined by $M_{j,k,l}^{m_x,m_y,m_z} = \int_V\int_{|\vec{\Omega}|=1} x^j y^k z^l \Omega_x^{m_x}\Omega_y^{m_y}\Omega_z^{m_z}\psi_{A,B}(\vec{r},\vec{\Omega})d^2\Omega dV$ and commonly referred to as Lewis-moments, are identical through any order satisfying $j+k+l+m_x+m_y+m_z = N$, where $(\Omega_x,\Omega_y,\Omega_z)$ are the direction cosines with respect to the Cartesian axes $(x,y,z)$.

The significance of this observation is that if $\Sigma_s^{(A)}(\vec{\Omega}'\cdot\vec{\Omega})$ is the true or exact differential cross section for scattering of the charged particle by a target nucleus, also referred to as the analog differential cross section, and $\Sigma_s^{(B)}(\vec{\Omega}'\cdot\vec{\Omega})$ is an approximation to it, Lewis' result points to a sharp link between accuracy of the approximate model, as measured by linear functionals (moments) of the angular flux, and number of Legendre moments of the differential cross section that are exactly reproduced in the approximate model. It has been shown that preserving higher order Lewis-moments can significantly improve the computational efficiency and accuracy of the widely used condensed history Monte Carlo method for charged particle transport [2] by enabling large step sizes to be used [2,3]. However, in recent years Lewis theory has also facilitated the development of approximate but accurate transport models that are characterized by longer mean free paths and less peaked differential cross sections than the corresponding analog quantities and hence can be efficiently simulated using single event Monte Carlo [4–7]. A common theme of the latter methods is the regularization of the near-singular collision integrals describing elastic interactions using various moment-preserving strategies.

Recent numerical work has provided strong evidence for the existence of a Lewis-type theory underpinning moment preserving approximations for energy straggling [7–9]. Specifically, it has been noted that approximate transport models for energy straggling that are explicitly constructed to preserve a finite number of energy-loss moments of the exact differential cross section yield more accurate dose distributions and energy spectra than do those that fail to capture these moments. Moreover, the accuracy can be systematically increased by preserving greater numbers of

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http://dx.doi.org/10.1016/j.nimb.2014.04.001
0168-583X/

moments and very accurate results can be realized with surprisingly few moments [7]. The intriguing possibility naturally arises of the existence of a sharp link between number of energy-loss moments preserved and linear functionals of the energy flux or spectrum. In this paper we demonstrate the existence of a Lewis-type theory for a class of straggling models which include the established Landau and Vavilov theories as well as higher order approximations.

## 2. Energy straggling equation

The equation that is commonly used to describe energy loss of a beam of charged particles traversing a target medium is a reduced transport equation that can be expressed as:

$$\frac{\partial\psi(s,E)}{\partial s} = \int_0^{E_0} dE'\Sigma_e(E'\to E)\psi(s,E') - \Sigma_e(E)\psi(s,E), \quad 0<s<T, \tag{1}$$

with initial condition:

$$\psi(0,E) = \delta(E_0 - E). \tag{2}$$

In Eq. (1), $s$ is the path length variable, $E$ is the particle energy and $\psi(s,E)$ is the flux or energy spectrum which gives the distribution of particle energies as a function of $s$. The incident particle energy at $s=0$ is $E_0$ and the target thickness, or step size in condensed history implementations, corresponds to a total path length of $T$. Also $\Sigma_e(E'\to E)$ is the differential energy transfer cross section, and $\Sigma_e(E) = \int_0^{E_0}\Sigma_e(E\to E')dE'$ the total cross section, for collisions between the primary particle and an electron in the target medium. Defining the energy-loss variable as $Q = E - E'$, the energy-loss differential cross section can alternatively be expressed as $\Sigma_e(E,Q)dQ = \Sigma_e(E\to E')dE'$. Energy-loss moments are then defined by:

$$Q_n(E) = \int_0^{E_0} Q^n\Sigma_e(E,Q)dQ, \quad n = 1,2\ldots, \tag{3}$$

where in practice the lower limit of energy loss may be given by the average excitation-ionization potential and the upper limit by the maximum value determined by kinematics [11]. Physically, $Q_1(E)$ is the mean energy loss per path length traveled and defines the stopping power of the medium, and $Q_2(E)$ is the mean-square energy loss per path length, also known as the straggling coefficient. For sufficiently thick targets or for low energies, energy spectra and dose depend predominantly on these two moments, while the higher moments assume increasing importance for thin targets and at high energies.

The straight ahead transport equation given in Eq. (1) accurately describes energy-loss straggling when angular deflection can be neglected, such as in the penetration of heavy charged particles in thin layers. The model is also used in condensed history Monte Carlo methods where the angular and energy distributions are separately computed over fixed but short track segments or steps [2,10] from multiple scattering and ionization/excitation distributions that are obtained from approximate solutions of reduced transport equations. In particular, the Landau [12] and Vavilov [13] straggling distributions are obtained from semi-analytic solutions of Eq. (1) subject to the assumption that the energy transfers in the medium are small enough that the mean free path of the particle may be held constant at its initial value. For later reference, we note that under these conditions, the energy loss moments $Q_n$ also become independent of energy.

Energy-loss moments play a key role in the development of approximate models and solutions for the straggling distribution. Central to the construction of the Landau/Vavilov straggling distributions is that the lower energy-loss moments, the first two in particular, are accurately captured but the higher moments are approximated. This idea has been generalized in more recent approaches that allow increasingly higher order moments to be captured and the accuracy systematically improved to a desired level [7–9]. Experience with these methods [9,7] shows that the accuracy of approximate energy straggling models is strongly correlated with the number of energy loss moments $\{Q_n, n = 1,2\ldots\}$ that are exactly preserved by these models. Moreover, numerical results show that approximations which are moment-preserving are capable of yielding greater accuracy than non-preserving approaches, for both differential (spectra) and integrated (dose) quantities. With reference to Lewis theory for angular moments [1], these observations are suggestive of the existence of an underlying Lewis-type theory that ties the accuracy of linear functionals of the flux or energy spectrum to the preservation of energy-loss moments. We demonstrate in the next section that such a link indeed exists for a widely used class of energy straggling models.

## 3. Lewis-type theory for energy straggling

We define energy-moments of the flux or spectrum by:

$$I_n(s) = \int_0^{E_0} dEE^n\psi(s,E), \quad n = 1,2,\ldots \tag{4}$$

We refer to these moments as the energy-flux moments. It follows that $I_0(s)$ is the total number of particles that have traveled a path length $s, I_1(s)/I_0(s)$ is the average energy of the particles at $s, I_2(s)/I_0(s)$ the mean-square energy at $s$, and so on. Our goal is to show that under certain conditions there exists a direct relationship between these energy-flux moments and the energy-loss moments.

Let $\{Q_n(E), n = 1,2,\ldots\}$ be energy-loss moments of the analog differential cross section, as defined by Eq. (3), and let $\{I_n, n = 1,2,\ldots\}$ be the energy moments of the corresponding analog transport problem flux, as defined by Eq. (4). Likewise, let $\{\widehat{Q}_n(E), n = 1,2,\ldots\}$ be energy-loss moments of an approximate differential cross section and $\{\widehat{I}_n, n = 1,2,\ldots\}$ the energy moments of the corresponding approximate transport problem flux.

We begin by developing equations that are satisfied by the energy-flux moments. Multiplying Eq. (1) by $E^n$, integrating over all energies, and manipulating the terms we get:

$$\begin{aligned}\frac{dI_n(s)}{ds} &= \int_0^{E_0} dEE^n\int_0^{E_0} dE'\Sigma_e(E'\to E)\psi(s,E') - \int_0^{E_0} dEE^n\Sigma_e(E)\psi(s,E)\\ &= \int_0^{E_0} dE'\psi(s,E')\int_0^{E_0} dEE^n\Sigma_e(E'\to E) - \int_0^{E_0} dEE^n\Sigma_e(E)\psi(s,E)\\ &= \int_0^{E_0} dE\psi(s,E)\int_0^{E_0} dE'E'^n\Sigma_e(E\to E') - \int_0^{E_0} dEE^n\Sigma_e(E)\psi(s,E),\end{aligned} \tag{5}$$

where in the last step the $E$ and $E'$ variables have been interchanged. Next, the total cross section $\Sigma_e(E)$ is expressed in terms of the differential cross section as:

$$\Sigma_e(E) = \int_0^{E_0} dE'\Sigma_e(E\to E'). \tag{6}$$

Substituting Eq. (6) in Eq. (5) and combining the inscatter and outscatter terms then yields:

$$\frac{dI_n(s)}{ds} = -\int_0^{E_0} dE\psi(s,E)\int_0^{E_0} dE'\left(E^n - E'^n\right)\Sigma_e(E\to E'). \tag{7}$$

Note that for $n = 0$ the right hand side of Eq. (7) vanishes which indicates that $I_0(s)$ must be a constant and equal to its value at $s = 0$, i.e., $I_0(s) = I_0(0)$. Eqs. (2) and (4) then yield $I_0(0) = 1$ and hence $I_0(s) = 1, s \geqslant 0$. This is just an expression of conservation of particles since particles are assumed not to be absorbed. Proceeding, it is convenient to rewrite the integral over $E'$ in terms of the energy transfer variable $Q = E - E'$. To this end, $E'^n$ is first expressed as a binomial expansion:

$$E'^n = (E - Q)^n = \sum_{m=0}^{n}(-1)^m \binom{n}{m} Q^m E^{n-m}, \tag{8}$$

and this result is then used to write:

$$E^n - E'^n = -\sum_{m=1}^{n}(-1)^m \binom{n}{m} Q^m E^{n-m}. \tag{9}$$

Substituting Eq. (9) in Eq. (7) and also introducing the energy transfer cross section $\Sigma_e(E,Q)$, the equation for the energy-flux moments becomes:

$$\frac{dI_n(s)}{ds} = \sum_{m=1}^{n}(-1)^m \binom{n}{m} \int_0^{E_0} dEE^{n-m}\psi(s,E) \int_0^{E_0} dQQ^m \Sigma_e(E,Q), \tag{10}$$

or, more compactly,

$$\frac{dI_n(s)}{ds} = \sum_{m=1}^{n} c_{nm} \int_0^{E_0} dEE^{n-m} Q_m(E)\psi(s,E), \quad n = 1,2\ldots, \tag{11}$$

where

$$c_{nm} = (-1)^m \binom{n}{m}, \tag{12}$$

and we have introduced the energy-loss moments $Q_m(E)$ defined previously in Eq. (3). Assuming these coefficients are continuous functions for $0 \leqslant E \leqslant E_0$, then according to the first mean value theorem for integrals there exists an $E^* \in (0, E_0)$ such that:

$$\int_0^{E_0} dEE^{n-m} Q_m(E)\psi(s,E) = Q_m(E^*) \int_0^{E_0} dEE^{n-m}\psi(s,E). \tag{13}$$

Using this result in Eq. (11) gives:

$$\frac{dI_n(s)}{ds} = \sum_{m=1}^{n} c_{nm} Q_m(E^*) I_{n-m}(s), \quad I_n(0) = E_0^n, \quad n = 1,2\ldots, \tag{14}$$

Considering now the approximate transport problem and repeating the above procedure using hatted variables to denote the moments characterizing this problem, we obtain:

$$\frac{d\widehat{I}_n(s)}{ds} = \sum_{m=1}^{n} c_{nm} \int_0^{E_0} dEE^{n-m} \widehat{Q}_m(E)\widehat{\psi}(s,E), \quad n = 1,2\ldots, \tag{15}$$

where the approximate energy-loss moments, $\widehat{Q}_m(E)$, are defined by:

$$\widehat{Q}_n(E) = \int_0^{E_0} dQQ^n \widehat{\Sigma}_e(E,Q) \quad n = 1,2,\ldots, \tag{16}$$

and $\hat{\Sigma}_e(E,Q)$ is the differential cross section for this approximate model. Applying the first mean value theorem for integrals to Eq. (16) for some energy $E^+ \in (0,E_0)$ we obtain the analog of Eq. (14) for the energy-flux moments of the approximate transport problem:

$$\frac{d\widehat{I}_n(s)}{ds} = \sum_{m=1}^{n} c_{nm} \widehat{Q}_m(E^+)\widehat{I}_{n-m}(s); \quad \widehat{I}_n(0) = E_0^n, \quad n = 1,2\ldots \tag{17}$$

Although Eqs. (14) and (17) are closed equations for the energy-flux moments, the specific energies $E^*$ and $E^+$ are unknown so that it is not possible to relate the respective flux moments for the two problems. In order to establish a relationship, we now introduce the following two constraints:

1. The second problem represents a moment-preserving approximation to the analog problem. That is, the two problems have identical energy-loss moments up to some fixed order:
$$\widehat{Q}_n(E) = Q_n(E), \quad n = 1,2,\ldots N. \tag{18}$$
Note, this condition does not require the differential energy transfer cross sections to be identical so that the energy-loss moments for $n > N$ will in general differ for the two problems.
2. We restrict considerations to thin targets where the mean energy loss is small so that the moments $\{Q_n(E), n = 1\ldots N\}$ are weak functions of energy. In particular, they are assumed not to differ from their corresponding values at $E = E_0$, so that $E^*$ and $E^+$ can be equated to $E_0$ to obtain:
$$\widehat{Q}_n(E^+) = Q_n(E^*) = Q_n(E_0), \quad n = 1,2,\ldots N. \tag{19}$$

Under these conditions, substituting Eq. (19) in Eq. (17) and Eq. (14), then subtracting Eq. (17) from Eq. (14) yields;

$$\frac{d\Delta_n(s)}{ds} = \sum_{m=1}^{n} c_{nm} Q_m(E_0)\Delta_{n-m}(s), \quad \Delta_n(0) = 0, \quad n = 1,2\ldots N, \tag{20}$$

where we have defined the residual:

$$\Delta_n(s) = I_n(s) - \widehat{I}_n(s). \tag{21}$$

Clearly, the unique solution of Eq. (20) is given by:

$$\Delta_n(s) = 0, \quad n = 1,2\ldots N, \quad 0 \leqslant s \leqslant T, \tag{22}$$

which then yields the desired relationship between the analog and approximate energy-flux moments:

$$\widehat{I}_n(s) = I_n(s), \quad n = 0,1,\ldots N, \quad 0 \leqslant s \leqslant T. \tag{23}$$

This sharp result can be encapsulated by the following

**Theorem** (*Moment-Equivalence Theorem for Energy Straggling*). *Let $\psi(s,E)$ be the energy distribution corresponding to an analog energy-straggling problem defined by Eq. (1). Let $\widehat{\psi}(s,E)$ be an approximate energy distribution obtained under the assumption that the mean energy-loss over the path length $0 \leqslant s \leqslant T$ is negligible compared to the incident particle energy $E_0$. If the collisional energy-loss moments, defined by Eq. (3), for the approximate and analog problems satisfy:*

$$\widehat{Q}_n(E) = Q_n(E) \equiv Q_n(E_0), \quad n = 1,2,\ldots N, \quad 0 \leqslant E \leqslant E_0, \tag{24}$$

*for some fixed but finite N, then $\widehat{\psi}(s,E)$ is an $N^{th}$-order moment-preserving approximation to $\psi(s,E)$, in the sense that:3*

$$\int_0^{E_0} E^n \left[\psi(s,E) - \widehat{\psi}(s,E)\right] dE = 0, \quad n = 1,2,\ldots N, \quad 0 \leqslant s \leqslant T. \tag{25}$$

In particular, the straggling theories of Landau and Vavilov satisfy the conditions of this theorem. However, it is readily shown that the moment-equivalence theory also holds when the energy-loss moments can be approximated by linear functions of energy over the energy loss range in the thin layer, such as $Q_n(E) = Q_n(E_0) - Q_n'(E_0)(E_0 - E)$. That is, the result holds under conditions that are somewhat more general than in the Landau-Vavilov straggling theories. Finally, it is worth noting that the energy-flux moment-equivalence is spatially local, that is, it holds at every value of $s$, unlike Lewis-theory for scattering which is a global moment-equivalence theory.

## 4. Conclusions

We have shown that moment-preserving energy straggling models in thin layers are underpinned by a Lewis-type moment-equivalence theory. Using an appropriate transport equation for the energy distribution, and under conditions of well-established straggling theories, we have derived the sharp result that if an approximate straggling model has $N$ identical collisional energy-loss moments as the exact model, then the first $N$ energy-moments of the spectrum will be identical for the approximate and exact models.

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