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Non-classical particle transport with angular-dependent path-length distributions. I: Theory

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ABSTRACT

This paper extends a recently introduced theory describing particle transport for random statistically homogeneous systems in which the distribution function $p(s)$ for chord lengths between scattering centers is non-exponential. Here, we relax the previous assumption that $p(s)$ does not depend on the direction of flight $\mathbf{\Omega}$; this leads to a new generalized linear Boltzmann equation that includes angular-dependent cross sections, and to a new generalized diffusion equation that accounts for anisotropic behavior resulting from the statistics of the system.

1. Introduction

The classical theory of linear particle transport defines as $dp = \Sigma_t(\boldsymbol{x}, E)ds$ the incremental probability dp that a particle at point $\boldsymbol{x}$ with energy E will experience an interaction while traveling an incremental distance ds in the background material. Here, the total cross section Σ_t is independent of the direction of flight $\mathbf{\Omega}$, and the path-length s is defined as

$$s = \text{the path-length traveled by the particle since its previous interaction (birth or scattering)}. \quad (1.1)$$

This typically leads to the particle flux decreasing as an exponential function of the path-length (Beer–Lambert law).

However, in an inhomogeneous random medium, particles will travel through different materials with randomly located interfaces. In atmospheric clouds, experimental studies have found evidence of a non-exponential attenuation law (Davis et al., 1996; Marshak et al., 1997; Pfeilsticker, 1999). It has been suggested (Kostinski, 2001) that the locations of the scattering centers (in this case water droplets) are spatially correlated in ways that measurably affect radiative transfer within the cloud (Kostinski and Shaw, 2001; Buldyrev et al., 2001; Shaw et al., 2002; Davis, 2008; Borovoi, 2002; Kostinski, 2002; Davis and Marshak, 2004; Scholl et al., 2006).

An approach to this type of non-classical transport problem was recently introduced (Larsen, 2007), with the assumption that the positions of the scattering centers are correlated but independent of direction $\mathbf{\Omega}$; that is, Σ_t is independent of $\mathbf{\Omega}$ but not $s : \Sigma_t = \Sigma_t(\boldsymbol{x}, E, s)$. A full derivation of this generalized linear Boltzmann equation (GLBE) and its asymptotic diffusion limit can be found in Larsen and Vasques (2011), along with numerical results for an application in 2-D pebble bed reactor (PBR) cores. Existence and uniqueness of solutions, as well as their convergence to the diffusion equation, are rigorously discussed in Frank and Goudon (2010). Furthermore, a similar kinetic equation with path-length as an independent variable has been derived for the periodic Lorentz gas (Golse, 2012).

For specific random systems in which the locations of the scattering centers are correlated and dependent on the direction $\mathbf{\Omega}$, anisotropic particle transport arises (Vasques, 2009; Vasques and Larsen, 2009). This anisotropy is a direct result of the geometry of the random system – for instance, the packing of pebbles close to the boundaries of a pebble bed system leads to particles traveling longer distances in directions parallel to the boundary wall (Vasques, 2013). One may also expect that, due to the "gravitational" arrangement of pebbles in PBR cores, diffusion in the vertical and horizontal directions might differ. This behavior can only be captured if we allow the path-lengths of the particles to depend upon $\mathbf{\Omega}$; that is, $\Sigma_t = \Sigma_t(\boldsymbol{x}, \mathbf{\Omega}, E, s)$. (Implications of angular-dependent cross-sections in anisotropic media have been previously considered in Williams (1978), in connection with charged particle transport in lattice-like structures.)

The goal of this paper is to extend the GLBE formulation in Larsen and Vasques (2011) to include this angular dependence. For simplicity, we do not consider the most general problem here; similarly to Larsen and Vasques (2011), our analysis is based on five primary assumptions:

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i. The physical system is infinite and statistically homogeneous.
ii. Particle transport is monoenergetic. (However, the inclusion of energy- or frequency-dependence is straightforward.)
iii. Particle transport is driven by a known interior isotropic source $Q(\boldsymbol{x})$ satisfying $Q \to 0$ as $|\boldsymbol{x}| \to \infty$ (and the particle flux $\to 0$ as $|\boldsymbol{x}| \to \infty$).
iv. The ensemble averaged total cross section $\Sigma_t(\boldsymbol{\Omega}, s)$, defined as

$$\Sigma_t(\boldsymbol{\Omega}, s)ds = \text{the probability(ensemble-averaged over all physical realizations)that a particle, scattered or born at any point } \boldsymbol{x} \text{ and traveling in the direction } \boldsymbol{\Omega}, \text{ will experience a collision between } \boldsymbol{x} + s\boldsymbol{\Omega} \text{ and } \boldsymbol{x} + (s + ds)\boldsymbol{\Omega},$$

is known. (In the next part of this 2-part paper we discuss how $\Sigma_t(\boldsymbol{\Omega}, s)$ might be numerically derived from hypothesized correlations between the scattering centers.)
v. The distribution function $P(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')$ for scattering from $\boldsymbol{\Omega}'$ to $\boldsymbol{\Omega}$ is independent of s. (The correlation in the scattering center positions affects the probability of collision, but not the scattering properties when scattering events occur.)

For problems in general random media, $\Sigma_t(\boldsymbol{\Omega}, s)$ depends also on $\boldsymbol{x}$. In this paper the statistics are assumed to be homogeneous, in which case the dependence on $\boldsymbol{x}$ is dropped. (In the derivation of the GLBE in Larsen and Vasques (2011), the statistics was assumed to be independent of $\boldsymbol{x}$ and $\boldsymbol{\Omega}$.)

A summary of the remainder of the paper follows. In Section 2 we present definitions and formally derive the new GLBE. In Section 3 we derive (i) the conditional distribution function $q(\boldsymbol{\Omega}, s)$ for the distance s to collision in a given direction $\boldsymbol{\Omega}$ in terms of the total cross section $\Sigma_t(\boldsymbol{\Omega}, s)$; and (ii) the equilibrium path-length spectrum in a given direction. In Section 4 we reformulate the new GLBE in terms of integral equations in which s is absent. In Section 5 we derive the asymptotic diffusion limit of the new GLBE, presenting 3 physically relevant special cases; and in Section 6 we show that if $\Sigma_t(\boldsymbol{\Omega}, s)$ is independent of both $(\boldsymbol{\Omega}, s)$, the theory introduced here reduces to the classical theory. We conclude with a discussion in Section 7.

2. Derivation of the new GLBE

Using the notation $\boldsymbol{x} = (x, y, z) =$ position and $\boldsymbol{\Omega} = (\Omega_x, \Omega_y, \Omega_z) =$ direction of flight (with $|\boldsymbol{\Omega}| = 1$), and using Eq. (1.1) for s, we define:

$$n(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds = \text{the number of particles in } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s), \tag{2.1a}$$

$$v = \frac{ds}{dt} = \text{the particle speed}, \tag{2.1b}$$

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = vn(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \text{the angular flux}, \tag{2.1c}$$

$$\Sigma_t(\boldsymbol{\Omega}, s)ds = \text{the probability that a particle that has traveled a distance s in the direction } \boldsymbol{\Omega} \text{ since its previous interaction (birth or scattering) will experience its next interaction while traveling a further distance } ds, \tag{2.1d}$$

$$c = \text{the probability that when a particle experiences a collision, it will scatter (notice that } c \text{ is independent of } s \text{ and } \boldsymbol{\Omega}), \tag{2.1e}$$

$$P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})d\Omega = \text{the probability that when a particle with direction of flight } \boldsymbol{\Omega}' \text{ scatters, its outgoing direction of flight will lie in } d\Omega \text{ about } \boldsymbol{\Omega}\ (P \text{ is independent of } s), \tag{2.1f}$$

$$Q(\boldsymbol{x})dV = \text{the rate at which source particles are isotropically emitted by an internal source } Q(\boldsymbol{x}) \text{ in } dV \text{ about } \boldsymbol{x}. \tag{2.1g}$$

Classic manipulations directly lead to:

$$\begin{aligned}\frac{\partial}{\partial s}\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds &= \frac{1}{v}\frac{\partial}{\partial t}vn(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds \\ &= \frac{\partial}{\partial t}n(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds \\ &= \text{the rate of change of the number of particles in } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s),\end{aligned} \tag{2.2a}$$

$$|\boldsymbol{\Omega} \cdot \mathbf{n}|\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)dS\, d\Omega\, ds = \text{the rate at which particles in } d\Omega\, ds \text{ about } (\boldsymbol{\Omega}, s) \text{ flow through an incremental surface area } dS \text{ with unit normal vector } \mathbf{n}, \tag{2.2b}$$

$$\boldsymbol{\Omega} \cdot \nabla\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds = \text{the net rate at which particles in } d\Omega\, ds \text{ about } (\boldsymbol{\Omega}, s) \text{ flow (leak) out of } dV \text{ about } \boldsymbol{x}, \tag{2.2c}$$

$$\begin{aligned}\Sigma_t(\boldsymbol{\Omega}, s)\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds &= \Sigma_t(\boldsymbol{\Omega}, s)\frac{ds}{dt}n(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds \\ &= \frac{1}{dt}[\Sigma_t(\boldsymbol{\Omega}, s)ds][n(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds] \\ &= \text{the rate at which particles in } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s) \text{ experience collisions}.\end{aligned} \tag{2.2d}$$

The treatment of the inscattering and source terms requires extra care. From Eq. (2.2d),

$$\left[\int_0^\infty \Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'\right]dV\, d\Omega' = \text{the rate at which particles in } dV\, d\Omega' \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}') \text{ experience collisions}.$$

Multiplying this expression by $cP(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')d\Omega$, we obtain:

$$cP(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')\left[\int_0^\infty \Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'\right]dV\, d\Omega'\, d\Omega = \text{the rate at which particles in } dV\, d\Omega' \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}') \text{ scatter into } dV\, d\Omega \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}).$$

Integrating this expression over $\boldsymbol{\Omega}' \in 4\pi$, we get:

$$\left[c\int_{4\pi}\int_0^\infty P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})\Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'\, d\Omega'\right]dV\, d\Omega = \text{the rate at which particles scatter into } dV\, d\Omega \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}).$$

Finally, when particles emerge from a scattering event their value of s is "reset" to $s = 0$. Therefore, the path-length spectrum of particles that emerge from scattering events is the delta function $\delta(s)$. Multiplying the previous expression by $\delta(s)ds$, we obtain:

$$\left[\delta(s)c\int_{4\pi}\int_0^\infty P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})\Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'\, d\Omega'\right]dV\, d\Omega\, ds = \text{the rate at which particles scatter into } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s). \tag{2.2e}$$

Also,

$$\delta(s)\frac{Q(\boldsymbol{x})}{4\pi}dV\, d\Omega\, ds = \text{the rate at which source particles are emitted into } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s). \tag{2.2f}$$