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Generalized linear Boltzmann equation, describing non-classical particle transport, and related asymptotic solutions for small mean free paths

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ABSTRACT

In classical kinetic models a particle free path distribution is exponential, but this is more likely to be an exception than a rule. In this paper we derive a generalized linear Boltzmann equation (GLBE) for a general free path distribution in the framework of Alt's model. In the case that the free path distribution has at least first and second finite moments we construct an asymptotic solution to the initial value problem for the GLBE for small mean free paths. In the special case of the one-speed transport problem the asymptotic solution results in a diffusion approximation to the GLBE.

1. Introduction

Classical neutron transport or transport of thermal energy by photons is described by the linear Boltzmann kinetic (or transport) equation (LBE) [1–3]

$$\partial_t \psi + \boldsymbol{v} \cdot \nabla \psi = \int_{\mathbb{V}} K(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{v}') v' \sigma_s(\boldsymbol{r}, \boldsymbol{v}') \psi(\boldsymbol{r}, t, \boldsymbol{v}')\, \mathrm{d}\boldsymbol{v}' - v\sigma(\boldsymbol{r}, \boldsymbol{v})\psi + F(\boldsymbol{r}, t, \boldsymbol{v}), \tag{1.1}$$

where $\psi(\boldsymbol{r}, t, \boldsymbol{v})$ is the phase space density, $\boldsymbol{r}$ is the spatial variable, t is the time variable, $\boldsymbol{v}$ is a velocity vector, $v = |\boldsymbol{v}|$, σ and σ_s are the extinction and scattering coefficients (or total and scattering cross sections), respectively, K is the scattering (or transition) kernel and F is the source term. If scattering and sources are absent, i. e., $\sigma_s = 0$ and $F = 0$, and a medium is homogeneous, i. e., $\sigma = \text{const}$, the solution of Eq. (1.1) is given by

$$\xi(\boldsymbol{r}, t, \boldsymbol{v}) = \mathrm{e}^{-\sigma l} \xi(\boldsymbol{r} - \boldsymbol{\Omega} l, t_0, \boldsymbol{v}),$$

where $l = v(t - t_0)$ is a free path passed by a particle, and $\boldsymbol{\Omega} = v/\boldsymbol{v}$ is the direction of motion. This means that the distribution of free paths, i. e., distances between two consecutive collisions, is exponential (exponential extinction law), or, equivalently, collision events form the Poisson process [4]. This is a very restrictive assumption, and, therefore, in many cases it is violated [5–10]. In particular, a power-like extinction law may be observed.

Kinetic models, based on the LBE, are also widely used for description of various transport processes in biology [11–20]. The common assumption in these models is also the exponential distribution of free paths, but this is more likely to be an exception than a rule. Indeed, the exponential distribution of free paths is applicable mainly to transport in rarefied media,

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when obstacles are spatially uncorrelated. However, many biological media are dense and obstacles cannot be considered as spatially uncorrelated. Therefore, the assumption of the exponential distribution may fail. Distributions of free paths may also be non-exponential by different reasons. Examples of non-exponential distributions of free paths in animal movements are given in Refs. [21–23].

A special case of biological motion is intracellular transport of cargos (organelles, vesicles, etc.) through a network of microtubules and actin filaments (cytoskeleton) [24]. In the course of cargo movement active motion along cytoskeleton driven by molecular motors alternates with passive diffusion in the cytoplasm. Cytoskeleton is not static but highly dynamic, and a kinetic-like framework seems to be a natural way for mean-field description of cargo transport. To the best of the author's knowledge all kinetic-like models of intracellular cargo transport assume exponential distribution of free paths [17,18,25–27]. However, cellular cytoplasm is overcrowded and obstacles cannot be considered as spatially uncorrelated. Therefore, the assumption of the exponential distribution is also questionable, see, e. g., Ref. [28].

In this paper we derive a generalized linear Boltzmann equation (GLBE) for a general free path distribution in the framework of Alt's model [29]. In the special case of the exponential free path distribution the GLBE becomes the LBE. To the best of the author's knowledge no Boltzmann-like equation for a general free path distribution was derived in the framework of Alt's model. In Ref. [29] a partial integro-differential kinetic equation and its diffusion approximation (Patlak–Keller–Segel equation) were derived under the assumption that the free path distribution was asymptotically exponential. A model similar to Alt's one in the framework of the position jump model of the continuous-time random walks (CTRWs) was proposed in Ref. [30], see also Ref. [31]. A similar equation, including acceleration of the particles due to external forces but without absorption and sources, was obtained in the framework of the velocity jump model of the CTRWs in Refs. [32,33].

Even the LBE is in most cases very difficult to solve. This is all the more valid for the GLBE. Therefore, approximations to the GLBE would be more convenient for use. One of the most useful approximations to the LBE is the diffusion one, see, e. g., Refs. [34,35]. In this paper in the case that the free path distribution has at least first and second finite moments we construct an asymptotic solution to the initial value problem for the GLBE for small mean free paths like in Ref. [34], where an asymptotic solution was constructed for the LBE, see also Ref. [35]. The asymptotic solution results in a diffusion approximation in the special case of the one-speed GLBE. In the steady state this diffusion approximation coincides with that obtained in Ref. [36] and differs from the diffusion approximation in Ref. [37] by small terms of the second order.

The paper is organized as follows. Section 2 describes the model of non-classical particle transport. In Section 3 we derive the GLBE, which describes transport with an arbitrary free path distribution. In Section 4 we construct an asymptotic solution of the equation for small mean free paths. In Section 5 the diffusion approximation to the one-speed GLBE, as a particular case of the asymptotic solution, is obtained. Section 6 contains concluding remarks.

2. Non-classical particle transport: a model

The model generalizes that of classical linear transport [1,3], where the extinction and scattering coefficients (or total and scattering cross sections) do not depend on a free path travelled by a particle. In the non-classical transport the coefficients depend on the free path length. In this case the phase space density of particles (or individuals) takes the form $\xi(\boldsymbol{r}, t, \boldsymbol{v}, l)$, where $\boldsymbol{r}$ is the spatial variable, t is the time variable, $\boldsymbol{v}$ is a velocity vector, l is the free path length of the particle. We consider transport in d-dimensional space, therefore $\boldsymbol{r} \in \mathbb{R}^d$ and $\boldsymbol{v} \in \mathbb{V} \subset \mathbb{R}^d$. The phase space density obeys, see Ref. [29], the equation

$$\partial_t \xi + v\partial_l \xi + \boldsymbol{v} \cdot \nabla \xi + v\sigma \xi = 0, \tag{2.1}$$

where ∇ means the gradient with respect to $\boldsymbol{r}$, $\sigma \equiv \sigma(\boldsymbol{r}, \boldsymbol{v}, l)$ is the extinction coefficient (or total cross section), $v = |\boldsymbol{v}|$. This equation describes noninteracting particles moving at the point $\boldsymbol{r}$ with the velocity $\boldsymbol{v}$ so that they stop free runs (scatter or disappear) with the rate $v\sigma$. We do not consider here particle acceleration due to external forces, taking it into account is straightforward.

Eq. (2.1) is supplemented by the condition, which describes the density of particles beginning a free run,

$$\xi|_{l=0} \equiv \eta(\boldsymbol{r}, t, \boldsymbol{v}) = \mathcal{K}\left[\int_0^\infty \sigma_s(\boldsymbol{r}, \boldsymbol{v}, l')\, \xi(\boldsymbol{r}, t, \boldsymbol{v}, l')\, \mathrm{d}l'\right] + \frac{1}{v} F(\boldsymbol{r}, t, \boldsymbol{v}) \tag{2.2}$$

where

$$\mathcal{K} f(\boldsymbol{r}, t, \boldsymbol{v}) \stackrel{\text{def}}{=} \int_{\mathbb{V}} K(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{v}') f(\boldsymbol{r}, t, \boldsymbol{v}')\, \mathrm{d}\boldsymbol{v}' \tag{2.3}$$

is the scattering (or transition) operator, $K(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{v}') \equiv K(\boldsymbol{r}, \boldsymbol{v}' \to \boldsymbol{v})$ is the scattering (or transition) kernel such that

$$K \geq 0 \quad \text{and} \quad \int_{\mathbb{V}} K(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{v}')\, \mathrm{d}\boldsymbol{v} = 1$$

(i. e., $K(\boldsymbol{r}, \cdot, \boldsymbol{v}')$ is a probability density function), $\sigma_s \equiv \sigma_s(\boldsymbol{r}, \boldsymbol{v}, l)$ is the scattering coefficient (or scattering cross section), $\sigma_s \leq \sigma$, F is the source term. The condition (2.2) is a straightforward modification of the corresponding condition given in Ref. [29]. This condition means that particles beginning a free run arise as a result of scattering (changing direction and/or