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THE FOKKER–PLANCK OPERATOR AS AN ASYMPTOTIC LIMIT

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It is shown that the Fokker–Planck operator describing a highly peaked scattering process in the linear transport equation is a formal asymptotic limit of the exact integral operator. It is also shown that such peaking is a necessary, but not sufficient, condition for the Fokker–Planck operator to be a legitimate description of such scattering. In particular, the widely used Henyey–Greenstein scattering kernel does not possess a Fokker–Planck limit.

1. Introduction

In this paper we deal with a certain aspect of particle flow through a prescribed background medium. Such flow is described by a linear kinetic, or transport, equation that is simply a particle balance in phase space. The description of particle scattering interactions with the background medium is a linear integral operator in this equation, and the kernel of this operator describes the probability of scattering from an initial (before scattering) particle energy and direction to a final (after scattering) energy and direction. In certain applications, in particular charged particle transport, this kernel is very peaked about both a zero energy transfer and a zero direction change. However, in such applications the number of scattering collisions is generally very large. That is, the average distance a particle travels between scattering events (the scattering mean free path) is very small. Thus we have the physical picture of a very large number of scattering events occurring per unit path length, with any single event affecting the particle phase space coordinates only slightly. The slight effect of a single scattering can loosely be characterized as an $O(\varepsilon \ll 1)$ effect, and the small scattering mean free path can similarly be characterized as an $O(\Delta \ll 1)$ distance. Thus in an $O(1)$ distance in the medium, one can possibly observe a significant change in the energy and direction of the particle, depending upon the relationship between ε and Δ.

To solve such a scattering transport problem numerically using deterministic methods is very difficult since the mesh size in such a calculation must be on the same scale as the mean free path, which in this case is very small. This implies an unrealistically fine degree of numerical resolution. Likewise, a Monte–Carlo simulation is very time consuming since a very large number of scattering interactions must be followed for each particle before its demise by either absorption or leakage out of the system. To circumvent these difficulties, it has been suggested to replace the integral scattering operator in the transport equation with a differential Fokker–Planck operator. The effect of this replacement is that the dominant (large) in and out scattering terms cancel, thus effectively increasing the mean free path. The classic contributions in this regard are summarized by Chandrasekhar[2] and Rosenbluth,[9] and more recent papers specifically within the context of linear particle transport are also available.[5–7]

All of these works give a heuristic derivation of the Fokker–Planck operator, which can be described quite easily. The integral scattering operator L in the transport equation is the difference between out and in scattering, and has the generic form

$$Lf(x) = \int_a^b dx'[K(x,\, x')f(x) - K(x',\, x)f(x')]\,, \quad a \le x \le b\,, \tag{1}$$

where the kernel K is presumed to be peaked about $x = x'$. One first rewrites this kernel $K(x',\, x)$ as $G(x',\, x' - x)$ to obtain

$$Lf(x) = \int_a^b dx'[G(x,\, x - x')f(x) - G(x',\, x' - x)f(x')]\,. \tag{2}$$

Because of the assumed peaking of G about $x = x'$, it is reasonable to expand all x' dependences in the second term on the right-hand side of Eq. (2) in a Taylor series about $x' = x$, and in lowest order drop all terms past the first derivative. Equation (2) then becomes

$$\begin{aligned} Lf(x) = \int_a^b dx' \Big\{ & G(x,\, x - x')f(x) - G(x,\, x' - x)f(x) \\ & - \frac{\partial}{\partial y}[(x' - x)G(y,\, x' - x)f(y)]_{y=x} \Big\}\,. \end{aligned} \tag{3}$$

In the two terms in Eq. (3) that arose from this expansion, we change integration variables from x' to x'' according to $x' - x = x - x''$. Of course, this changes the limits of integration, but this is ignored since this heuristic development assumes that as long as the range of integration over x'' encompasses the point x, the assumed peaking in the kernel makes the limits of integration irrelevant. Upon making this change of variables, it is evident that the two nonderivative terms (the dominant scattering terms) cancel, and we are left with

$$Lf(x) = -\frac{\partial}{\partial y}\left[f(y) \int dx''(x - x'')G(y,\, x - x'')\right]_{y=x} \tag{4}$$

This can be written as

$$Lf(x) = -\frac{\partial}{\partial x}[A(x)f(x)], \tag{5}$$

where

$$A(x) = \int d\xi \xi G(x, \xi) = \int dx'(x - x')K(x, x'). \tag{6}$$

Again, the ranges of integration in Eqs. (4) and (6) are irrelevant, but the range of integration over x' in Eq. (6) is naturally chosen as $a \leq x' \leq b$, the range of integration involved in the original integral operator. We see that the linear integral operator in Eq. (1) has been converted to a linear differential operator in Eq. (5), and in particle transport theory (where x will be both energy and direction) this differential operator is referred to as the Fokker–Planck operator. If one retains quadratic terms in the Taylor series expansion, the Fokker–Planck operator contains an additional second derivative term.

In this paper we wish to show that this heuristic derivation of the Fokker–Planck operator can be formalized and regarded as an asymptotic limit of the integral scattering operator. In addition to defining the Fokker–Planck operator in a mathematically formal way, this treatment gives much better insight into the validity of this differential operator as a replacement for the exact integral operator. This treatment also shows that the smallness parameters ε and δ, which describe the peaking of the scattering kernel in energy (ε) and direction (δ), must be related to each other and to the smallness parameter Δ, which describes the small scattering mean free path, in order to obtain a meaningful Fokker–Planck operator. Finally, and perhaps most significantly, the asymptotic treatment shows in a clear manner that a peaked scattering kernel is a necessary but not sufficient condition for the Fokker–Planck operator to be an asymptotically consistent approximation to the integral operator as all the smallness parameters ε, δ, and Δ vanish. This last point has not been discussed in the earlier heuristic treatments. In this regard, one of the most widely used scattering kernels to describe peaked scattering in the angular variable is the so-called Henyey–Greenstein kernel.[4] This kernel is simple in the sense that it contains a single parameter g, the so-called asymmetry factor, that, when varied from $g = 0$ to $g = 1$, gives a smooth transition from isotropic scattering to completely forward scattering. In spite of the fact that the Henyey–Greenstein kernel is a valid representation of a Dirac delta-function in the forward direction as g approaches unity, it does not allow the integral scattering operator to be replaced by the Fokker–Planck operator as $g \to 1$ ($\delta \to 0$). Thus the use of the Fokker–Planck description of scattering is not valid for the Henyey–Greenstein scattering kernel, no matter how close the asymmetry factor g is to unity.

2. The Transport Equation

We define $f(\mathbf{r}, E, \mathbf{\Omega}, t)$ to be a density of particles in phase space. That is, the number of particles dn at time t in a six-dimensional differential volume $d\mathbf{r}dEd\mathbf{\Omega}$

is given by

$$dn = f(\mathbf{r}, E, \mathbf{\Omega}, t) d\mathbf{r} dE d\mathbf{\Omega} . \tag{7}$$

Here $\mathbf{r}$ and E represent the spatial and particle energy variables, respectively, and $\mathbf{\Omega}$ is a unit vector in the flight direction of the particle. As particles flow through a background medium, the interactions allowed are absorption and scattering collisions. Between these collisions, the particles are assumed to stream in straight lines with no energy change. We define the absorption cross section $\sigma_a(\mathbf{r}, E, t)$ such that in traveling a distance ds, a particle has a probability of absorption p_a, given by the Markovian statement

$$p_a = \sigma_a(\mathbf{r}, E, t) ds . \tag{8}$$

In a similar way we define the scattering cross section $\sigma_s(\mathbf{r}, E, t)$ such that in traveling a distance ds, a particle has a probability of scattering p_s given by

$$p_s = \sigma_s(\mathbf{r}, E, t) ds . \tag{9}$$

We note that we have not indicated an $\mathbf{\Omega}$ (direction) dependence for σ_a and σ_s. This implies that we are restricting our attention to an isotropic medium, i.e., a medium with no preferred direction. All of the considerations in this paper can be generalized to an anisotropic medium, but to keep the discussion simple we do not treat this more general case. Further, in most applications of linear particle transport theory, the background can be regarded as isotropic. In an absorption collision, the particle is lost. In a scattering collision, the particle survives with a new energy and a new flight direction. To quantify this, we define the scattering kernel $\sigma_s(\mathbf{r}, E', E, \mathbf{\Omega}' \cdot \mathbf{\Omega}, t)$ such that in traveling a distance ds, the probability $p_{s's}$ of a particle, with energy E' and direction $\mathbf{\Omega}'$ before the collision, scattering to an energy E in an energy increment dE, and to a direction $\mathbf{\Omega}$ in a solid angle increment $d\mathbf{\Omega}$ after the collision, is given by

$$p_{s's} = \sigma_s(\mathbf{r}, E', E, \mathbf{\Omega}' \cdot \mathbf{\Omega}, t) ds dE d\mathbf{\Omega} . \tag{10}$$

We note that we have taken this kernel to depend only upon the single angular variable $\mathbf{\Omega}' \cdot \mathbf{\Omega}$, the cosine of the scattering angle, rather than upon $\mathbf{\Omega}'$ and $\mathbf{\Omega}$ separately. This is a consequence of our assumption that the background medium is isotropic. Since in a scattering event the particle must possess some final energy and angle we have the relationship, omitting the $\mathbf{r}$ and t dependences for notational simplicity (a convention we will adopt throughout this paper),

$$\sigma_s(E') = \int_0^\infty dE \int_{4\pi} d\mathbf{\Omega} \sigma_s(E', E, \mathbf{\Omega}' \cdot \mathbf{\Omega}) . \tag{11}$$

By performing the integration over the unit sphere in Eq. (11) in a standard spherical coordinate system, and aligning the z-axis along $\mathbf{\Omega}'$, Eq. (11) can be rewritten as

$$\sigma_s(E') = 2\pi \int_0^\infty dE \int_{-1}^{1} d\xi \sigma_s(E', E, \xi) . \tag{12}$$

Here $\xi = \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}$ is the cosine of the polar angle, and the 2π factor arises from the integration over the azimuthal angle.

In terms of the interaction coefficients just defined, the flow of particles through the background medium is described by the linear transport equation. This equation is simply a statement of particle conservation in phase space, and is given by[1,3]

$$\begin{aligned}\frac{1}{v}\frac{\partial\psi(E,\,\Omega)}{\partial t} &+ \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(E,\,\boldsymbol{\Omega}) + \sigma(E)\psi(E,\,\boldsymbol{\Omega}) \\ &= \int_0^\infty dE' \int_{4\pi} d\boldsymbol{\Omega}'\sigma_s(E',\,E,\,\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\psi(E',\,\boldsymbol{\Omega}') + Q(E,\,\boldsymbol{\Omega})\,. \qquad (13)\end{aligned}$$

Here $\psi(E,\,\boldsymbol{\Omega})$ is defined by

$$\psi(E,\,\boldsymbol{\Omega}) = vf(E,\,\boldsymbol{\Omega})\,, \qquad (14)$$

where v is the particle speed, $\sigma(E)$ is the total cross-section given by

$$\sigma(E) = \sigma_a(E) + \sigma_s(E)\,, \qquad (15)$$

and $Q(E,\,\boldsymbol{\Omega})$ represents any source of particles. Appropriate initial and boundary conditions apply to Eq. (13), but these will not concern us here.

For our purposes, it is convenient to represent the integral term in Eq. (13), the so-called in-scattering term, as a sum over its surface harmonic components. To this end, we expand the scattering kernel in Legendre polynomials according to

$$\sigma_s(E',\,E,\,\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}) = \sum_{k=0}^{\infty}\left(\frac{2k+1}{4\pi}\right)\sigma_{sk}(E',\,E)P_k(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\,. \qquad (16)$$

The orthogonality of the Legendre polynomials allows us to write the expansion coefficients as

$$\sigma_{sk}(E',\,E) = 2\pi\int_{-1}^{1} d\xi P_k(\xi)\sigma_s(E',\,E,\,\xi)\,. \qquad (17)$$

Further, we expand the solution $\psi(E,\,\boldsymbol{\Omega})$ in surface harmonics according to

$$\psi(E,\,\boldsymbol{\Omega}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(\frac{2n+1}{4\pi}\right)a_{nm}\psi_{nm}(E)Y_{nm}(\boldsymbol{\Omega})\,. \qquad (18)$$

If we follow the definition of the surface harmonics used by Przybylski and Ligou,[7] we have

$$a_{nm} = \frac{(n-|m|)!}{(n+|m|)!}\,, \qquad (19)$$

with the surface harmonics, known to be complete on the unit sphere, given by

$$Y_{nm}(\boldsymbol{\Omega}) = P_n^m(\mu)e^{im\phi}\,, \qquad (20)$$

where

$$P_n^m(\mu) = (1-\mu^2)^{m/2}\frac{d^m P_n(\mu)}{d\mu^m}, \quad m \geq 0, \tag{21}$$

$$P_n^{-m}(\mu) = P_n^m(\mu). \tag{22}$$

Here $\mu = \cos\theta$, where θ is a polar angle, and ϕ is the corresponding azimuthal angle. The surface harmonics are orthogonal according to

$$\int_{4\pi} d\mathbf{\Omega} Y_{nm}(\mathbf{\Omega})Y_{kl}^*(\mathbf{\Omega}) = \left(\frac{4\pi}{2n+1}\right)\left(\frac{1}{a_{nm}}\right)\delta_{nk}\delta_{ml}, \tag{23}$$

where the $*$ indicates complex conjugate. Using this orthogonality condition, the expansion coefficients in Eq. (18) are given by

$$\psi_{nm}(E) = \int_{4\pi} d\mathbf{\Omega}\, Y_{nm}^*(\mathbf{\Omega})\psi(E, \mathbf{\Omega}). \tag{24}$$

A property of the surface harmonics is that they satisfy the partial differential equation given by

$$\left[\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} + \left(\frac{1}{1-\mu^2}\right)\frac{\partial^2}{\partial\phi^2} + n(n+1)\right]Y_{nm}(\mathbf{\Omega}) = 0. \tag{25}$$

We shall use this identity in our Fokker–Planck development in the next section.

Let us define I to be the integrand of the energy integral in the in-scattering term in Eq. (13). That is

$$I = \int_{4\pi} d\mathbf{\Omega}'\sigma_s(E', E, \mathbf{\Omega}'\cdot\mathbf{\Omega})\psi(E', \mathbf{\Omega}'). \tag{26}$$

Using Eq. (16) and (18) in Eq. (26) gives

$$I = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(\frac{2k+1}{4\pi}\right)\left(\frac{2n+1}{4\pi}\right)a_{nm}\sigma_{sk}(E', E)\psi_{nm}(E')$$
$$\cdot\int_{4\pi} d\mathbf{\Omega}' P_k(\mathbf{\Omega}'\cdot\mathbf{\Omega})Y_{nm}(\mathbf{\Omega}'). \tag{27}$$

To simplify this, we consider the integral

$$J = \int_{4\pi} d\mathbf{\Omega}' P_k(\mathbf{\Omega}'\cdot\mathbf{\Omega})Y_{nm}(\mathbf{\Omega}'). \tag{28}$$

If we use the addition formula for the Legendre polynomials, namely

$$P_k(\mathbf{\Omega}'\cdot\mathbf{\Omega}) = \sum_{l=-k}^{k} a_{kl}Y_{kl}(\mathbf{\Omega})Y_{kl}^*(\mathbf{\Omega}'), \tag{29}$$

then Eq. (28) becomes, using the orthogonality condition given by Eq. (23),

$$J = \left(\frac{4\pi}{2n+1}\right) Y_{nm}(\mathbf{\Omega})\delta_{nk}\,. \tag{30}$$

Using this result in Eq. (27) yields

$$I = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{2n+1}{4\pi}\right) a_{nm}\sigma_{sn}(E',\, E) Y_{nm}(\mathbf{\Omega})\,, \tag{31}$$

and then, inserting this into the transport equation given by Eq. (13), we find

$$\frac{1}{v}\frac{\partial\psi(E,\,\mathbf{\Omega})}{\partial t} + \mathbf{\Omega}\cdot\nabla\psi(E,\mathbf{\Omega}) + \sigma(E)\psi(E,\mathbf{\Omega})$$
$$= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{2n+1}{4\pi}\right) a_{nm} Y_{nm}(\mathbf{\Omega}) \int_0^{\infty} dE'\sigma_{sn}(E',\, E)\psi_{nm}(E') + Q(E,\,\mathbf{\Omega})\,. \tag{32}$$

Our final algebraic manipulation is to use Eq. (15) for σ and Eq. (17) for σ_{sn} in Eq. (32) to obtain

$$\frac{1}{v}\frac{\partial\psi(E,\,\mathbf{\Omega})}{\partial t} + \mathbf{\Omega}\cdot\nabla\psi(\dot{E},\,\mathbf{\Omega}) + [\sigma_a(E) + \sigma_s(E)]\psi(E,\,\mathbf{\Omega})$$
$$= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(\frac{2n+1}{2}\right) a_{nm} Y_{nm}(\mathbf{\Omega})$$
$$\cdot \int_0^{\infty} dE'\psi_{nm}(E') \int_{-1}^{1} d\xi P_n(\xi)\sigma_s(E',\, E,\, \xi) + Q(E,\,\mathbf{\Omega})\,. \tag{33}$$

It is Eq. (33), fully equivalent to the fundamental transport equation given by Eq. (13), that forms the starting point of our Fokker–Planck development. As we shall see, at the end of this development we shall be able to eliminate the double sum over the surface harmonic components, and once again write the in-scattering term as an operator, in this case the Fokker–Planck operator, acting on $\psi(E,\,\mathbf{\Omega})$.

3. The Fokker–Planck Development

We begin by assuming that the unit of distance is chosen such that the characteristic size of the system in which the particles transport is $O(1)$. In such a length unit, we take the scattering mean free path to be small, and since this mean free path is the reciprocal of the scattering cross-section, we have $\sigma_s(E) \gg 1$. Accordingly, we scale $\sigma_s(E)$ as

$$\sigma_s(E) = \frac{\hat{\sigma}_s(E)}{\Delta}\,, \tag{34}$$

where $\hat{\sigma}_s = O(1)$ and $\Delta \ll 1$. We apply this same scaling to the scattering kernel $\sigma_s(E',\, E,\, \xi)$, and additionally introduce the fast variables

$$x = \frac{E'-E}{\varepsilon}\,, \quad \varepsilon \ll 1\,, \tag{35}$$

$$y = \frac{1-\xi}{\delta}\,, \quad \delta \ll 1\,. \tag{36}$$

Thus we scale the scattering kernel as

$$\sigma_s(E', E, \xi) = \frac{1}{\Delta}\hat{\sigma}_s\left(E', \frac{E'-E}{\varepsilon}, \frac{1-\xi}{\delta}\right) = \frac{1}{\Delta}\hat{\sigma}_s(E', x, y), \tag{37}$$

where $\hat{\sigma}_s(E', x, y)$ is $O(1)$ and the derivatives of this kernel with respect to both x and y are assumed to be $O(1)$ as $\varepsilon, \delta \to 0$. Physically, the smallness parameter δ is a measure of the peaking of the scattering kernel in angle, and can be roughly thought of as the deviation from unity of the cosine of a characteristic scattering angle. Likewise, the smallness parameter ε is a measure of the peaking of the scattering kernel in energy, and can be thought of as a characteristic value of the fractional energy change due to a single scattering. That is, these scalings imply that the scattering cross-section is large, and that the scattering kernel is very peaked about $\xi = 1$ and $E = E'$. Inserting the scalings given by Eqs. (34) and (37) into Eq. (33), we then have the scaled transport equation

$$\begin{aligned}
&\frac{1}{v}\frac{\partial\psi(E, \mathbf{\Omega})}{\partial t} + \mathbf{\Omega}\cdot\nabla\psi(E, \mathbf{\Omega}) + \left[\sigma_a(E) + \frac{\hat{\sigma}_s(E)}{\Delta}\right]\psi(E, \mathbf{\Omega}) \\
&\quad = \frac{1}{\Delta}\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(\frac{2n+1}{2}\right)a_{nm}Y_{nm}(\mathbf{\Omega}) \\
&\quad\quad \cdot \int_0^{\infty} dE'\psi_{nm}(E')\int_{-1}^{1} d\xi P_n(\xi)\hat{\sigma}_s\left(E', \frac{E'-E}{\varepsilon}, \frac{1-\xi}{\delta}\right) + Q(E, \mathbf{\Omega}).
\end{aligned} \tag{38}$$

We see the asymptotic limit of Eq. (38) as the three smallness parameters ε, δ and Δ approach zero.

To this end, we consider the term K, defined to be

$$K = \frac{2\pi}{\Delta}\int_0^{\infty} dE'\int_{-1}^{1} d\xi P_n(\xi)\hat{\sigma}_s\left(E', \frac{E'-E}{\varepsilon}, \frac{1-\xi}{\delta}\right)\psi_{nm}(E'). \tag{39}$$

We change integration variables in Eq. (39) from E', ξ to x, y according to Eqs. (35) and (36) to obtain

$$K = \frac{2\pi\varepsilon\delta}{\Delta}\int_{-E/\varepsilon}^{\infty} dx\int_0^{2/\delta} dy P_n(1-\delta y)\hat{\sigma}_s(E+\varepsilon x, x, y)\psi_{nm}(E+\varepsilon x). \tag{40}$$

We now Taylor expand the integrand in Eq. (40) about $\varepsilon = \delta = 0$. We carry linear terms in δ and quadratic terms in ε. We will discuss the reason for this asymmetry in the two expansions at the end of our development. We then find, indicating the errors in the neglected terms in the Taylor expansions,

$$\begin{aligned}
K = &\frac{2\pi\varepsilon\delta}{\Delta}\int_{-E/\varepsilon}^{\infty} dx\int_0^{2/\delta} dy[P_n(1) - \delta y P_n'(1) + O(\delta^2)] \\
&\cdot\left[1 + \varepsilon x\frac{\partial}{\partial E} + \frac{\varepsilon^2 x^2}{2}\frac{\partial^2}{\partial E^2} + O(\varepsilon^3)\right][\hat{\sigma}_s(E, x, y)\psi_{nm}(E)].
\end{aligned} \tag{41}$$

To proceed, we assume that we can replace the lower limit of integration over E' by $-\infty$, and that the error we make in doing this is $O(\varepsilon^3)$ or smaller. This is certainly legitimate if the scattering kernel falls off exponentially in energy from its peak at $x = 0$. However, if the kernel falls off algebraically at too weak a rate, this replacement may increase the error in the Fokker–Planck treatment over the $O(\varepsilon^3)$ error indicated in Eq. (41). We note that even if the kernel falls off exponentially in energy from its peak, this integration limit replacement does introduce an error, but this error is exponentially small. It is this exponential error that makes the present development an asymptotic, rather than a convergent, procedure. At this point, we also neglect the cross terms between angle and energy in Eq. (41). That is, we neglect the yx and yx^2 terms in the integrand of Eq. (41). It is not necessary to neglect these terms to obtain a clean result, but the standard Fokker–Planck operator does not have the contributions that arise from these terms.

In view of the above discussion, we then rewrite Eq. (41), using

$$P_n(1) = 1\,, \quad P_n'(1) = \frac{n(n+1)}{2}\,, \tag{42}$$

as

$$\begin{aligned} K = {} & \frac{2\pi\varepsilon\delta}{\Delta}\int_{-\infty}^{\infty} dx \int_0^{2/\delta} dy[1 + O(\delta^2 + \varepsilon\delta + \varepsilon^3)]\hat{\sigma}_s(E,\, x,\, y)\psi_{nm}(E) \\ & - \frac{n(n+1)\pi\varepsilon\delta^2}{\Delta}\int_{-\infty}^{\infty} dx \int_0^{2/\delta} dy y\hat{\sigma}_s(E,\, x,\, y)\psi_{nm}(E) \\ & + \frac{2\pi\varepsilon^2\delta}{\Delta}\frac{\partial}{\partial E}\int_{-\infty}^{\infty} dx \int_0^{2/\delta} dy x\hat{\sigma}_s(E,\, x,\, y)\psi_{nm}(E) \\ & + \frac{\pi\varepsilon^3\delta}{\Delta}\frac{\partial^2}{\partial E^2}\int_{-\infty}^{\infty} dx \int_0^{2/\delta} dy x^2\hat{\sigma}_s(E,\, x,\, y)\psi_{nm}(E)\,. \end{aligned} \tag{43}$$

We now change integration variables in all four double integrals in Eq. (43) from x, y to E', ξ according to

$$x = \frac{E - E'}{\varepsilon}\,, \tag{44}$$

$$y = \frac{1-\xi}{\delta}\,. \tag{45}$$

We note that Eq. (45) is identical to Eq. (36), but Eq. (44) is not identical to Eq. (35) (the E and E' are interchanged). This gives

$$\begin{aligned} K = {} & \frac{2\pi}{\Delta}\int_{-\infty}^{\infty} dE' \int_{-1}^{1} d\xi[1 + O(\delta^2 + \varepsilon\delta + \varepsilon^3)]\hat{\sigma}_s\left(E,\, \frac{E-E'}{\varepsilon},\, \frac{1-\xi}{\delta}\right)\psi_{nm}(E) \\ & - \frac{n(n+1)\pi}{\Delta}\int_{-\infty}^{\infty} dE' \int_{-1}^{1} d\xi(1-\xi)\hat{\sigma}_s\left(E,\, \frac{E-E'}{\varepsilon},\, \frac{1-\xi}{\delta}\right)\psi_{nm}(E) \end{aligned}$$

$$+\frac{2\pi}{\Delta}\frac{\partial}{\partial E}\int_{-\infty}^{\infty}dE'\int_{-1}^{1}d\xi(E-E')\hat{\sigma}_s\left(E,\,\frac{E-E'}{\varepsilon},\,\frac{1-\xi}{\delta}\right)\psi_{nm}(E)$$
$$+\frac{\pi}{\Delta}\frac{\partial^2}{\partial E^2}\int_{-\infty}^{\infty}dE'\int_{-1}^{1}d\xi(E-E')^2\hat{\sigma}_s\left(E,\,\frac{E-E'}{\varepsilon},\,\frac{1-\xi}{\delta}\right)\psi_{nm}(E)\,. \tag{46}$$

We use

$$\frac{1}{\Delta}\hat{\sigma}_s\left(E,\,\frac{E-E'}{\varepsilon},\,\frac{1-\xi}{\delta}\right)=\sigma_s(E,\,E',\,\xi) \tag{47}$$

in Eq. (46), and note that the bottom limit of integration on the E' integral can be replaced by zero since the scattering kernel vanishes for negative E' (the probability of scattering to a negative energy is zero). We then have

$$K=\sigma_s(E)\psi_{nm}(E)-n(n+1)T(E)\psi_{nm}(E)+\frac{\partial}{\partial E}[S(E)\psi_{nm}(E)]$$
$$+\frac{\partial^2}{\partial E^2}[R(E)\psi_{nm}(E)]+O\left(\frac{\delta^2+\varepsilon\delta+\varepsilon^3}{\Delta}\right), \tag{48}$$

where we have defined

$$T(E)=\pi\int_0^{\infty}dE'\int_{-1}^{1}d\xi(1-\xi)\sigma_s(E,\,E',\,\xi)=O\left(\frac{\delta}{\Delta}\right), \tag{49}$$
$$S(E)=2\pi\int_0^{\infty}dE'\int_{-1}^{1}d\xi(E-E')\sigma_s(E,\,E',\,\xi)=O\left(\frac{\varepsilon}{\Delta}\right), \tag{50}$$
$$R(E)=2\pi\int_0^{\infty}dE'\int_{-1}^{1}d\xi(E-E')^2\sigma_s(E,\,E',\,\xi)=O\left(\frac{\varepsilon^2}{\Delta}\right). \tag{51}$$

The order assigned to the terms in Eqs. (49) through (51) seemingly follows from the fact that since x and y are $O(1)$ variables, then according to Eqs. (44) and (45) $(1-\xi)$ is $O(\delta)$, $(E-E')$ is $O(\varepsilon)$, and $(E-E')^2$ is $O(\varepsilon^2)$, with $\sigma_s(E,\,E',\,\xi)$ being $O(1/\Delta)$. However, these ordering are in the integrand, and the assumption we have made in writing Eqs. (49) through (51) is that the integrations do not change the ordering. The same holds true for taking the $O(\delta^2+\varepsilon\delta+\varepsilon^3)$ out from under the integrals in going from Eq. (46) to Eq. (48). It is not obvious that the integrations do not change the ordering since $\sigma_s(E,\,E',\,\xi)$ contains the smallness parameters ε and δ. The situation again depends upon the rate of fall off of the scattering kernel from its peaks in energy and angle. For exponential fall off, Eqs. (48) through (51) are corrected ordered, but for algebraic fall off the order of one or more of these terms may be larger than indicated. This observation again places a restriction on the scattering kernel for the Fokker–Planck differential operator to be an asymptotic limit of the exact integral operator. In the next section, we shall show that the Henyey–Greenstein kernel falls off too slowly from its peak for Eq. (48) to be valid. In particular, the error term in this equation denoted as $O(\delta^2/\Delta)$ is essentially $O(\delta/\Delta)$ for the Henyey–Greenstein kernel. Thus the neglected term is of the same order as the term retained, thereby invalidating the Fokker–Planck description in this case.

With the above caution in mind concerning the validity of the expression for K, we proceed to complete our development. Recalling the definition of K according to Eq. (40), substitution of Eq. (48) into the scaled transport equation given by Eq. (38) yields, also making use of Eq. (34) for $\hat{\sigma}_s(E)$,

$$\begin{aligned}
&\frac{1}{v}\frac{\partial\psi(E,\,\mathbf{\Omega})}{\partial t} + \mathbf{\Omega}\cdot\nabla\psi(E,\,\mathbf{\Omega}) + [\sigma_a(E)+\sigma_s(E)]\psi(E,\,\mathbf{\Omega}) \\
&\quad = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(\frac{2n+1}{4\pi}\right)a_{nm}Y_{nm}(\mathbf{\Omega})\Bigg\{\sigma_s(E)\psi_{nm}(E) \\
&\quad - n(n+1)T(E)\psi_{nm}(E) + \frac{\partial}{\partial E}[S(E)\psi_{nm}(E)] \\
&\quad + \frac{\partial^2}{\partial E^2}[R(E)\psi_{nm}(E)]\Bigg\} + Q(E,\,\mathbf{\Omega}) + O\left(\frac{\delta^2+\varepsilon\delta+\varepsilon^3}{\Delta}\right).
\end{aligned} \tag{52}$$

The $n(n+1)$ factor in Eq. (52) can be eliminated by making use of the equation satisfied by the $Y_{nm}(\mathbf{\Omega})$, namely Eq. (25), and then we can sum over the surface harmonics according to Eq. (18) to obtain our final result. This is given by

$$\begin{aligned}
&\frac{1}{v}\frac{\partial\psi(E,\,\mathbf{\Omega})}{\partial t} + \mathbf{\Omega}\cdot\nabla\psi(E,\,\mathbf{\Omega}) + \sigma_a(E)\psi(E,\,\mathbf{\Omega}) \\
&\quad = T(E)\left[\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} + \left(\frac{1}{1-\mu^2}\right)\frac{\partial^2}{\partial\phi^2}\right]\psi(E,\,\mathbf{\Omega}) \\
&\quad + \frac{\partial}{\partial E}[S(E)\psi(E,\,\mathbf{\Omega})] + \frac{\partial^2}{\partial E^2}[R(E)\psi(E,\,\mathbf{\Omega})] \\
&\quad + Q(E,\,\mathbf{\Omega}) + O\left(\frac{\delta^2+\varepsilon\delta+\varepsilon^3}{\Delta}\right).
\end{aligned} \tag{53}$$

We note that the dominant scattering term, $\sigma_s(E)\psi(E,\,\mathbf{\Omega})$, has canceled out in this equation.

Equation (53) is the conventional Fokker–Planck equation for linear particle transport in an isotropic medium. As we noted during the course of its derivation, a necessary but not sufficient condition for Eq. (53) to be an asymptotic limit of Eq. (13) is that the scattering kernel be peaked in both energy and angle.· The additional sufficient condition is that this peaking be either exponential or strongly algebraic. Assuming that the scattering kernel is such that Eq. (53) is a valid asymptotic limit, it is clear, from the order of the T, S and R terms as given by Eqs. (49) through (51), that the smallness parameters ε, δ and Δ must tend to zero in a correlated way. That is, we must have $O(\delta) = O(\Delta)$ in order to obtain a meaningful (finite and nonzero) angular term in Eq. (53), and we must have $O(\varepsilon) = O(\Delta)$ to obtain a meaningful energy term in Eq. (53). The physical meaning of this is that as the peaking in the scattering kernel increases (ε, $\delta \to 0$), the magnitude of the scattering cross-section must increase ($\Delta \to 0$) in just such a corresponding way that the momentum transfer remains bounded and nonzero. Only in this case does Eq. (53) have any meaning.

Finally, we note that since $R = O(\delta^2/\Delta)$ and $S = O(\delta/\Delta)$, one could in an asymptotically consistent manner always set R to zero and still maintain the leading order behavior in energy transfer. In applications, this is often done, but not always. The reason for retaining R, even though it is a higher order term, is that the R term in Eq. (53) describes entirely different physics than does the S term. The S term, the so-called stopping power term, is convective in nature, whereas the R term is diffusive. In certain applications the diffusion of particles in the energy variable, although small, can be an important effect. To see any such diffusive behavior, the R term in the Fokker–Planck operator must be retained. We also note that the T term in Eq. (53) describes diffusion in angle, and for aesthetic reasons it seems reasonable for the Fokker–Planck operator to describe diffusion in both energy and angle. The reason that no convective term in angle appears in Eq. (53) is that we have restricted our attention to an isotropic background medium. Upon scattering in such a medium, it is equally likely for a particle to be scattered to the left or to the right, and thus the mean scattering angle is zero. The lowest order nonzero measure of the scattering is then the mean square of the scattering angle. Since for small θ we have

$$1 - \cos\theta = \frac{\theta^2}{2}, \tag{54}$$

it is clear that for an isotropic medium the appropriate smallness parameter describing the peaking of the scattering in angle is some function of $1 - \langle\cos\theta\rangle$ according to

$$\delta = F(1 - \langle\cos\theta\rangle), \tag{55}$$

where $F(0) = 0$. Here $\langle\cos\theta\rangle$ is a characteristic value of the cosine of the scattering angle, and the precise form of the function $F(z)$ depends upon the details of the scattering kernel. For the Henyey–Greenstein kernel considered in the next section, we have

$$F(z) = z^2. \tag{56}$$

4. The Henyey–Greenstein Kernel

We begin with the generating function for the Legendre polynomials given by[8]

$$\frac{1}{(1 - 2g\xi + g^2)^{1/2}} = \sum_{n=0}^{\infty} g^n P_n(\xi). \tag{57}$$

Differentiating Eq. (57) with respect to g and multiplying the result by $2g$ gives

$$\frac{2g(\xi - g)}{(1 - 2g\xi + g^2)^{3/2}} = \sum_{n=0}^{\infty} 2ng^n P_n(\xi). \tag{58}$$

If we define the function $f(\xi)$ to be one half of the sum of Eqs. (57) and (58), we then have

$$f(\xi) = \frac{1-g^2}{2(1-2g\xi+g^2)^{3/2}} = \sum_{n=0}^{\infty}\left(\frac{2n+1}{2}\right)g^n P_n(\xi)\,. \tag{59}$$

The Henyey–Greenstein scattering kernel[4] is defined to be

$$\sigma_s(E', E, \mathbf{\Omega}'\cdot\mathbf{\Omega}) = \frac{\sigma_s(E')}{2\pi} f(\mathbf{\Omega}'\cdot\mathbf{\Omega})\delta(E'-E)\,, \tag{60}$$

where $\sigma_s(E')$ is the scattering cross-section and the Dirac delta-function expresses the fact that this kernel describes coherent (no energy exchange) scattering. The essence of this scattering kernel is the angular distribution $f(\xi)$, and for our purposes there is no need to consider the other factors on the right-hand side of Eq. (60).

We first note that as the asymmetry factor g approaches unity, $f(\xi)$ indeed describes completely forward peaked scattering. That is, as $g \to 1$, $f(\xi)$ is a valid representation of a Dirac delta-function at $\xi = 1$, i.e.,

$$\int_{-1}^{1} d\xi f(\xi) = 1\,, \tag{61}$$

$$\lim_{g\to 1} f(\xi) = 0\,, \quad \xi \neq 1\,. \tag{62}$$

If we define f_n as the nth Legendre moment of $f(\xi)$, Eq. (59) immediately establishes the result

$$f_n = \int_{-1}^{1} d\xi P_n(\xi) f(\xi) = g^n\,. \tag{63}$$

To write Eq. (59) in terms of a scaled variable, we define

$$\delta = (1-g)^2\,, \quad y = \frac{1-\xi}{\delta}\,. \tag{64}$$

Then Eq. (58) can be written as

$$f(\xi) = \hat{f}(y) = \frac{2-\sqrt{\delta}}{2\delta[1+2(1-\sqrt{\delta})y]^{3/2}}\,, \tag{65}$$

and as $g \to 1$ $(\delta \to 0)$, we find the simple result

$$\hat{f}(y) \xrightarrow[\delta\to 0]{} \frac{1}{\delta(1+2y)^{3/2}}\,. \tag{66}$$

According to Eq. (64), for the Henyey–Greenstein scattering kernel the smallness parameter δ expressing the peaking of the scattering in angle is the square of the deviation of the scattering cosine from unity.

Now, we can represent the Legendre moment of the kernel, f_n, according to

$$f_n = \sum_{i=0}^{n} f_{in}\,, \tag{67}$$

with

$$f_{in} = \frac{(-1)^i}{n!} P_n^{(i)}(1) \int_{-1}^{1} d\xi (1-\xi)^i f(\xi)\,, \tag{68}$$

where $P_n^{(i)}(1)$ is the ith derivative of $P_n(z)$ at $z = 1$. In the Fokker–Planck treatment of the last section, the presumption was

$$f_{in} = O(\delta^i)\,, \tag{69}$$

and accordingly Eq. (67) was replaced, in the limit $\delta \to 0$, with

$$f_n = f_{0n} + f_{1n} + O(\delta^2)\,. \tag{70}$$

From Eqs. (42), (63), (64) and (68) we immediately deduce that

$$f_{0n} = P_n(1) \int_{-1}^{1} d\xi f(\xi) = 1\,, \tag{71}$$

$$f_{1n} = -P_n'(1) \int_{-1}^{1} d\xi (1-\xi) f(\xi) = -\frac{n(n+1)}{2}(1-g) = O(\sqrt{\delta})\,. \tag{72}$$

We see that $f_{1n} = O(\sqrt{\delta})$, not $O(\delta)$ as presumed in Eq. (69). This per se is no problem, as long as f_{2n}, the first neglected term, is higher order in δ. We can easily compute this term. We have

$$f_{2n} = \frac{1}{2} P_n''(1) \int_{-1}^{1} d\xi (1-\xi)^2 f(\xi)\,. \tag{73}$$

$P_n''(1)$ is easily found by using the differential equation satisfied by the Legendre polynomials, namely[8]

$$\frac{d}{d\xi}(1-\xi^2)\frac{dP_n(\xi)}{d\xi} + n(n+1)P_n(\xi) = 0\,. \tag{74}$$

Differentiating Eq. (74) with respect to ξ and setting $\xi = 1$ gives

$$P_n''(1) = \frac{(n-1)(n)(n+1)(n+2)}{8}\,. \tag{75}$$

To compute the integral in Eq. (73), we express $(1-\xi)^2$ in terms of Legendre polynomials according to

$$(1-\xi)^2 = \frac{4}{3}P_0(\xi) - 2P_1(\xi) + \frac{2}{3}P_2(\xi)\,. \tag{76}$$

Making use of Eqs. (63) and (75), we then find that Eq. (73) becomes

$$f_{2n} = \frac{(n-1)n(n+1)(n+2)(2-g)(1-g)}{24} = O(\sqrt{\delta})\,. \tag{77}$$

We see that f_{2n} is the same order as f_{1n}, namely $O(\sqrt{\delta})$. Thus as $\delta \to 0$, the neglect of f_{2n} in computing f_n is not justified. In fact, one can easily show that all of the higher order terms in Eq. (67) are of the same order, namely

$$f_{in} = O(\sqrt{\delta})\,, \quad i \geq 1\,. \tag{78}$$

To demonstrate this, we consider the integral

$$I_i = \int_{-1}^{1} d\xi (1-\xi)^i f(\xi)\,. \tag{79}$$

We change integration variables in Eq. (79) according to Eq. (64). Then Eq. (66) shows, as $\delta \to 0$, that we have

$$I_i = \delta^i \int_0^{2/\delta} dy \frac{y^i}{(1+2y)^{3/2}}\,. \tag{80}$$

For $i \geq 1$, the δ behavior of this integral comes from the upper limit of integration, and hence

$$I_i = O\left[\delta^i \int^{1/\delta} dy y^{(i-3/2)}\right] = O(\sqrt{\delta})\,, \quad i \geq 1\,. \tag{81}$$

Thus for the Henyey–Greenstein kernel, all of the terms neglected in passing from Eq. (67) to Eq. (70), namely those terms erroneously indicated by $O(\delta^2)$ in Eq. (70), are in fact the same order as f_{1n}, and this is $O(\sqrt{\delta})$. This state of affairs obviously invalidates their neglect, and we thus conclude that the Fokker–Planck treatment of the last section does not apply to the Henyey–Greenstein scattering kernel; the algebraic falloff of this kernel from its peak at $y = 0$ ($\xi = 1$) is simply too weak. It can be seen from Eq. (66) that this weak falloff rate is $y^{-3/2}$.

In summary, then, the Henyey–Greenstein scattering kernel given by Eq. (60) does not possess the Fokker–Planck differential scattering operator as an asymptotic limit of the exact integral scattering operator. This is the case in spite of the fact that the Henyey–Greenstein kernel is a valid representation of a Dirac delta-function in angle as $g \to 1$ ($\delta \to 0$), as shown by Eqs. (61) and (62). Of course, the Henyey–Greenstein kernel we have analyzed here is simply an example, albeit a common representation of peaked scattering, of a class of scattering kernels that does not possess a Fokker–Planck asymptotic limit. Thus in applications, it is essential to verify that the scattering kernel of interest is peaked sufficiently strongly in both energy and angle to legitimately use the differential Fokker–Planck scattering operator in the limit as both ε (the energy smallness parameter) and δ (the angular smallness parameter) become vanishingly small.

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