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Technical Note

# Spreading of Collimated Particle Beams Within a Generalized Fokker-Planck Diffusion Description

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**Abstract**—*Recently, an expansion of the Boltzmann scattering operator describing the angular spreading of particle beams was given that included the effects of large angle scattering processes, thus generalizing the classical Fokker-Planck equation, valid in the limit of small angle scattering. The present work aims at making an analytical comparison between predictions based on the classical Fokker-Planck equation and those based on a generalized one, which includes a first-order correction term in the expansion of the Boltzmann scattering operator. The analysis is carried out for thin slabs where backscattering effects can be neglected and makes use of a moment approach, which leads to an infinite system of recursively coupled ordinary differential equations. The system is truncated in a consistent manner, and the effects of large angle scattering on the evolution of the moments are determined in explicit analytical form. An approximate similarity solution of the generalized Fokker-Planck equation is also found, and the results of both approaches provide a clear picture of the increased diffusive beam spreading due to large angle scattering. A comparison with previously published Monte Carlo simulation results shows good agreement.*

## I. INTRODUCTION

The scattering and concomitant angular spreading of an initially collimated pencil beam of particles have a wide range of applications—from cosmic rays to electron beams for cancer therapy—and have been studied intensively over many years.[1] The scattering process is most rigorously described using the nonlocal Boltzmann scattering operator, an operator with a differential scattering cross section that depends on the details of the actual scattering process under investigation. Since a general analysis of the beam transport equation (including the general Boltzmann scattering operator) is very difficult, analytically as well as numerically, various simplifications of the modeling of the scattering process have been used. In particular, in situations involving strongly forward peaked scattering, e.g., high-energy electrons or heavy charged particles, the Fokker-Planck approximation of the Boltzmann scattering operator is often used. In this approximation, the scattering is treated as a diffusion process where the angular deflection in each collision is assumed small. However, the Boltzmann operator has also been expanded to account for finite angle scattering effects, giving rise to a generalization of the scattering operator in the Fokker-Planck approximation.[2] The resulting transport equation for the angular spreading of the beam involves an expansion in terms of powers of the conventional scattering operator, with coefficients determined by suitable moments of the scattering cross section. This generalized Fokker-Planck (GFP) equation has been analyzed analytically using several different techniques, e.g., in terms of an expansion in Legendre polynomials, being the eigenfunctions of the Fokker-Planck angular scattering operator[3]; in terms of a coupled system of diffusion equations[4]; and using an approach based on moments of the GFP equation.[3] It is interesting to note that the Fokker-Planck equation and the generalized forms of this equation have recently also found applications in the area of light propagation and scattering in biological tissues and that within this context

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several extensive numerical investigations of the scattering equations have been carried out,[5,6] including situations involving significant backscattering, i.e., optically thick slabs.

In this work, we will present an analytical analysis of the angular spreading within the GFP description using the moment approach,[3] which is applied to the GFP equation, expanded to second order. Moment methods often give rise to closure problems in the sense that different moments are recursively coupled, and some strategy for truncating the recursive system must be adopted. We discuss this point in light of previous attempts[3,4] and derive explicit expressions for the evolution of the most important lower-order moments of the distribution function, which provide a clear picture of the corrections caused by taking large angle scattering into account. The approaches used in Refs. 1 through 4 and 7 are all restricted to describe the initial evolution of the beam spreading, where effects of backscattering can be neglected (i.e., for thin scattering slabs). For thicker slabs, however, the spreading of the beam will eventually involve particles being scattered into the backward direction, and the problem becomes more complicated to solve. Actually, it becomes a problem of the two-way diffusion or backward-forward type, which involves a coupling between forward and backward scattering. The Fokker-Planck two-way diffusion problem was in fact considered analytically already in 1938 by Bethe, Rose, and Wandenburg,[8] where a simple approximate solution for the decrease of the flux through the slab as a function of slab thickness was derived, and the problem was analyzed further in Refs. 9 and 10. In the present analysis we apply Bethe's simple approach to the GFP equation and show that the corresponding variation of flux with slab thickness is predicted to be the same as that for the classical Fokker-Planck equation. In recent works on optical applications,[5,6] extensive numerical simulations have been carried out, comparing results obtained from different scattering models. One important result for the present work is the agreement between the results for the transmitted flux obtained for the Fokker-Planck equation and for the generalized form of this equation given in Ref. 6 even for thick slabs where backscattering plays an important role for the scattering dynamics.

## II. ANALYSIS OF THE GENERALIZED FOKKER-PLANCK EQUATION

The transport of a collimated particle beam through a scattering medium can be described by the Boltzmann equation[1–3]

$$\mu \frac{\partial f}{\partial z} = S[f] \ , \tag{1}$$

where $f(z,\mu)$ is the azimuthally integrated angular particle flux and $\mu = \cos\theta$ is the cosine of the pitch angle (i.e., the projection of the beam velocity unit vector on the axis of propagation, the $z$-axis). The operator $S$ on the right side represents the effect of interactions between the beam and the background particles in the slab, including, e.g., absorption and collisions, and is usually represented by the nonlocal Boltzmann operator.

In the case of high-energy particle beams (consisting of, e.g., energetic electrons, protons, or alpha particles), absorption can often be neglected, and the transport may be modeled as a pure angular scattering process. In the simplest approximation, this scattering process is considered as a series of infinitesimally small angular deflections,[1] and the operator $S$ is proportional to the Lorentz differential operator $\mathcal{L}$:

$$S = \frac{\sigma}{2}\mathcal{L} = \frac{\sigma}{2}\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} \ , \tag{2}$$

where $\sigma$ is the transport or momentum transfer cross section. When this form of the scattering operator is substituted into the Boltzmann equation, one obtains the classical Fokker-Planck equation

$$\mu\frac{\partial f}{\partial z} = \frac{\sigma}{2}\mathcal{L}(f) = \frac{\sigma}{2}\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial f}{\partial\mu} \ , \tag{3}$$

which must be complemented with the initial condition of a unidirectional incident beam, i.e., $f(0,\mu) = \delta(1-\mu)$.

An explicit analytical solution of Eq. (3) is not available, but a convenient approach to obtain important information about the solution is to form the moments $\Phi_n$, defined by[2,7]

$$\Phi_n(z) = \int_{-1}^{1}(1-\mu)^n f(z,\mu)\,d\mu \ . \tag{4}$$

Multiplying the Fokker-Planck equation, Eq. (3), by $(1-\mu)^n$ and integrating over $\mu \in [-1,1]$ yield a set of coupled recursion equations for the different moments $\Phi_n$ given by

$$\frac{d}{dz}(\Phi_n - \Phi_{n+1}) = n^2\Phi_{n-1} - \frac{1}{2}n(n+1)\Phi_n \ , \quad n = 0,1,2\ldots \ , \tag{5}$$

where the scattering cross section $\sigma$ has been absorbed into the propagation variable, i.e., $\sigma z \to z$. In particular, we note that making use of the initial condition, the first three moments are related as

$$\frac{d}{dz}(\Phi_0 - \Phi_1) = 0 \qquad \to \Phi_0 - \Phi_1 = 1 \ , \tag{6a}$$

and

$$\frac{d}{dz}(\Phi_1 - \Phi_2) = \Phi_0 - \Phi_1 \quad \to \Phi_1 - \Phi_2 = z \ . \tag{6b}$$

Furthermore, Eq. (6a) implies that the particle flux $\Gamma$ is conserved throughout the slab and that it is equal to unity (for the considered initial condition); i.e.,

$$\Gamma \equiv \int_{-1}^{1} \mu f(z,\mu)\, d\mu = \Phi_0 - \Phi_1 = 1 \ . \tag{7}$$

Various ways of how to suitably close the infinite system of coupled, ordinary differential equations given by Eq. (5) are discussed in Refs. 1 and 7. One of these closing procedures[3,7] involved neglecting the term proportional to $d\Phi_{n+1}/dz$. This closure prescription is not quite consistent, however. The "smallness" of the higher-order terms is expressed by the lowest power of $z$ in the power expansions of the moments. Thus, when we truncate according to

$$\frac{d}{dz}(\Phi_n - \Phi_{n+1})^2\Phi_{n-1} - \frac{n(n+1)}{2}\Phi_n$$

$$\rightarrow \frac{d}{dz}\Phi_n \approx n^2\Phi_{n-1} - \frac{n(n+1)}{2}\Phi_n \tag{8}$$

and then proceed to solve for the $\Phi_n(z)$, these solutions are not consistent to higher order than $z^n$. Clearly, neglecting the term $d\Phi_{n+1}(z)/dz$ on the left side of Eq. (5), which is actually of order $z^n$, is not consistent with keeping the term proportional to $\Phi_n(z)$ on the right side, which is also of order $z^n$, unless the final result is later expanded to order $z^n$ only.

A more consistent closure procedure can be based on the fact that $\Phi_n(z) \sim A_n z^n$ as $z \rightarrow 0$, so that the leading-order term in the small $z$ expansion of $\Phi_n$ is given by

$$\frac{d\Phi_n}{dz} \approx n^2\Phi_{n-1} + \mathcal{O}(z^n) \ . \tag{9}$$

Making use of this information in Eq. (5), the leading-order contributions to each $\Phi_n$ can be found recursively. As an illustration, we note that going as far as to the third moment, we obtain

$$\Phi_0 \sim 1 \ , \quad \Phi_1 \sim z \ , \quad \Phi_2 \sim 2z^2 \ , \quad \Phi_3 \sim 6z^3 \ , \tag{10}$$

which may iteratively be inserted back into lower-order expansions to finally obtain the following third-order expansion in $z$ for the lowest-order moment $\Phi_0(z)$ (consistent with the corresponding expansion result found in Refs. 1 and 7):

$$\Phi_0(z) = 1 + z + 2z^2 + \frac{20}{3}z^3 + \mathcal{O}(z^4) \ . \tag{11}$$

In order to take large angle scattering effects into account, a more detailed analysis of the Boltzmann operator was performed in Refs. 2 and 3, where it was shown that the collision operator $S$ can be written (at least for certain well-behaved scattering kernels) as a power expansion in the Lorentz differential operator $\mathcal{L}$. Truncated at order $K$, this gives rise to the generalized GFP equation

$$\mu\frac{\partial f}{\partial z} = \sum_{k=1}^{K} \alpha_k^K \mathcal{L}^k[f] \ , \tag{12}$$

where the $\alpha_k^K$ are given by

$$\alpha_k^K = \sum_{l=k}^{K} \frac{(-1)^{l+k}}{l!}\sigma_l c_k^{(l)} \ , \tag{13}$$

where $\sigma_l$ is the $(1-\mu)^l$ moment of the differential scattering cross section and $c_k^{(l)}$ are certain coefficients related to derivatives of the Legendre polynomials,[3] evaluated at $\mu = 1$. Thus, the classical Fokker-Planck equation, Eq. (3), actually corresponds to the GFP equation with $K = 1$.

The following analysis will consider the case $K = 2$ (assuming that higher powers of $\mathcal{L}$ do not contribute significantly to the large angle corrections). The resulting GFP equation becomes

$$\begin{aligned}\mu\frac{\partial f}{\partial z} &= \left(\frac{\sigma_1}{2} + \frac{\sigma_2}{8}\right)\mathcal{L}[f] + \frac{\sigma_2}{16}\mathcal{L}^2[f] \\ &= \left(\frac{\sigma_1}{2} + \frac{\sigma_2}{8}\right)\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial f}{\partial\mu} \\ &\quad + \frac{\sigma_2}{16}\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial^2}{\partial\mu^2}(1-\mu^2)\frac{\partial f}{\partial\mu} \ . \end{aligned} \tag{14}$$

We will once again make use of the moments $\Phi_n$, defined in Eq. (4), but the corresponding system of coupled ordinary differential equations becomes more complicated than the system given by Eq. (5). In particular, at step $n$, the coupling involves not merely moments of order $n-1$, $n$, $n+1$, as previously, but also the moment of order $n-2$. The new system reads

$$\begin{aligned}&\frac{d}{dz}(\Phi_n - \Phi_{n+1}) \\ &\quad = \epsilon n^2(n-1)^2\Phi_{n-2} + n^2[1+\epsilon(1-n^2)]\Phi_{n-1} \\ &\quad\quad - \frac{n(n+1)}{2}\left[1+\epsilon\left(1-\frac{n(n+1)}{2}\right)\right]\Phi_n \ , \end{aligned} \tag{15}$$

where $\sigma_1$ has again been absorbed into the variable $z$ and we have introduced the small parameter $\epsilon = \sigma_2/4\sigma_1$. It is worth noting that for $n = 0,1$ in Eq. (15), all terms proportional to $\epsilon$ vanish, and the first two equations are in fact once again given by Eq. (6). Furthermore, the total particle flux is still a conserved quantity, given by $\Gamma = \Phi_0 - \Phi_1 = 1$.

TABLE I

Comparison Among Coefficients of $\Phi_0$

| | Fokker-Planck | $\epsilon = 0.5 \times 10^{-3}$ | | $\epsilon = 0.5 \times 10^{-2}$ | |
|---|---|---|---|---|---|
| | | GFP-2 | Simulations | GFP-2 | Simulations |
| $a_0$ | 1 | 1 | 1 | 1 | 1 |
| $a_1$ | 1 | 1.002 | 1.002 | 1.020 | 1.020 |
| $a_2$ | 2 | 2.017 | 2.017 | 2.170 | 2.175 |

To close the infinite system in Eq. (15), we observe that the lowest-order terms are not of order $z^n$ but rather of order $z^{n-1}$ due to the extended coupling. Hence, the leading-order terms of the moments $\Phi_n$ can be obtained via the approximate equation

$$\frac{d\Phi_n}{dz} = \epsilon n^2(n-1)^2\Phi_{n-1} + \mathcal{O}(z^n) \ . \tag{16}$$

Using Eq. (16) for closure (and iteratively improving the expansions of the moments analogously to what was described above for the Fokker-Planck equation), the expansion of $\Phi_0$ to second order in $z$ (and first order in $\epsilon$) is found to be

$$\Phi_0(z) = 1 + (1+4\epsilon)z + 2(1+17\epsilon)z^2 \ , \tag{17}$$

which is also consistent with the Fokker-Planck result, Eq. (11), in the limit $\epsilon \to 0$. The corrections due to large angle scattering in Eq. (17) thus tend to increase the spreading rate of the beam, which agrees with physical intuition. Finally, we note that the simple expression for $\Phi_0(z)$ predicted by Eq. (17) is in very good agreement with Monte Carlo simulations[3] carried out for $\epsilon = 0.5 \times 10^{-3}$ and $\epsilon = 0.5 \times 10^{-2}$; see Table I, where a comparison is made among different results for $\Phi_0(z) = a_0 + a_1 z + a_2 z^2$, obtained analytically based on the Fokker-Planck equation, the GFP equation expanded to second order (GFP-2), and numerical simulation results taken from Ref. 3.

## III. AN APPROXIMATE SIMILARITY SOLUTION OF THE GFP EQUATION

Although the moment approach provides important general information about the properties of the solutions of the Fokker-Planck and GFP equations, approximate solutions can also be obtained using the method outlined by Goodman[11] and previously applied to the Fokker-Planck equation.[7] The main idea of this approach is to construct an approximate solution by making a diffusive-like similarity ansatz for the evolution of the profile $f(z,\mu)$ in $\mu$ space as the particle beam traverses the slab. The ansatz has a prescribed (and physically reasonable) dependence on the coordinate $\mu$ but involves parameter functions that depend on the evolution variable $z$. The ansatz function is, however, not unique.[7] The evolution of the parameter functions is determined by suitable moments of the diffusion equation. While the result of such an analysis depends quantitatively, but not qualitatively, on the chosen form of the similarity function, it gives good physical insight into the diffusion dynamics of the angular beam scattering.

In the present analysis we choose the diffusion profile

$$f(z,\mu) = A(z)e^{-(1-\mu)/\Delta(z)} \ , \tag{18}$$

where $\Delta(z)$ is a measure of the (increasing) width of the profile in $\mu$ space and $A(z)$ characterizes the (decaying) amplitude of the distribution at $\mu = 1$. In order to obtain equations determining the evolution of $A(z)$ and $\Delta(z)$, we evaluate the first two moments using the ansatz function. This yields

$$\Phi_0 = A(z)\Delta(z)$$

and

$$\Phi_1 = A(z)\Delta^2(z) \ . \tag{19}$$

Inserting these expressions for $\Phi_0$ and $\Phi_1$ into Eq. (6), while using the approximate leading-order result $\Phi_2 \approx 4\epsilon z$, one obtains

$$\Delta(z) \approx (1+4\epsilon)z$$

and

$$A(z) \approx \frac{1}{(1+4\epsilon)z} + 2 = \frac{1}{\Delta(z)} + 2 \ , \tag{20}$$

which reduces to the corresponding similarity solution for the Fokker-Planck equation[7] when $\epsilon = 0$. The physical implications of this result are the same as that of Eq. (17): Large angle scattering tends to increase the diffusive spreading of the beam.

## IV. TWO-WAY DIFFUSION

The previous analysis was implicitly restricted to the case of thin slabs, where the spreading is comparatively small so that the particle distribution of the beam is confined to the interval $0 \le \mu \le 1$; i.e., no backscattering has been generated. For thick slabs, however, the simple diffusion problem turns into a two-way-diffusion problem where boundary conditions at both $z = 0$ and $z = L$ must be taken into consideration. The appropriate boundary conditions for this problem are a collimated beam incident at $z = 0$ on a slab of thickness $L$ and no particles entering the slab at $z = L$. In mathematical terms this implies

$$f(0,\mu) = \delta(1-\mu) \quad \text{for } 0 \le \mu \le 1$$

and

$$f(L,\mu) = 0 \qquad \text{for } -1 \le \mu \le 0 \ . \tag{21}$$

It should be emphasized that nothing is known a priori about $f(0,\mu)$ for $\mu < 0$ nor about $f(L,z)$ for $\mu > 0$. For this situation, Bethe, Rose, and Wandenburg[8] used a beautifully simple approximation based on the particular so-called diffusion solution to the Fokker-Planck equation, i.e., the solution of the form

$$f(z,\mu) = A(z-\mu) + B \ , \tag{22}$$

where $A$ and $B$ are constants determined by the boundary conditions. The boundary conditions for the two-way-diffusion problem imply

$$\int_0^1 \mu f(0,\mu)\, d\mu = 1$$

and

$$\int_{-1}^0 \mu f(L,\mu)\, d\mu = 0 \ . \tag{23}$$

By inserting the diffusion solution given by Eq. (22) into these two conditions, the parameters $A$ and $B$ can be determined. They are given by

$$A = -\frac{3}{2}\,\frac{1}{1+3L/4}$$

and

$$B = \frac{1+3L/2}{1+3L/4} \ . \tag{24}$$

The total flux, $\Gamma \equiv \Phi_1 - \Phi_0$, inside the slab is still constant, and evaluating this flux using the diffusion solution, one obtains

$$\Gamma \equiv \int_{-1}^{+1} \mu f(L,\mu)\, d\mu = \int_{-1}^{+1} \mu f(0,\mu)\, d\mu$$

$$= \frac{1}{1+3L/4} \ . \tag{25}$$

This result implies that the flux is no longer independent of the slab thickness $L$ but rather decreases with increasing $L$. The physical mechanism behind this is clearly the increasing importance of the backscattering. As long as $L$ is small, this effect can be neglected, and the previous simplified diffusion analysis is valid. The variation of the flux with the slab thickness, predicted by Eq. (25), is in good agreement with more detailed solutions for large values of $L$ (Ref. 9).

It is interesting to consider the same approach for the GFP equation, which can be written explicitly as

$$\mu\,\frac{\partial f}{\partial z} = \frac{1}{2}\,(1+\epsilon)\,\frac{\partial}{\partial \mu}\,(1-\mu^2)\,\frac{\partial f}{\partial \mu}$$

$$+ \frac{\epsilon}{2}\,\frac{\partial}{\partial \mu}\,(1-\mu^2)\,\frac{\partial^2}{\partial \mu^2}\,(1-\mu^2)\,\frac{\partial f}{\partial \mu} \ . \tag{26}$$

Inserting a diffusion form ansatz $f(z,\mu) = A_1\mu + A_2 z + B_1$ into Eq. (26), we find that $A_1 = -A_2 = A$ and $B_1 = B$, where $A$ and $B$ are again given by Eq. (24). The GFP diffusion solution is thus, somewhat surprisingly at first sight, independent of the large angle scattering correction parameter $\epsilon$, even though $\epsilon$ figures in the coefficients of Eq. (26). Hence, Bethe, Rose, and Wandenburg's approach predicts that the decay of the transmitted flux with slab thickness is identical for the Fokker-Planck and GFP equations, which is a physically somewhat counterintuitive result. However, this result is supported by the numerical results in Ref. 6, which indicate small differences in transmitted flux between the Fokker-Planck and GFP equations.

## V. CONCLUSION

An analytical analysis has been given of a GFP equation describing the influence of large angle scattering on the angular spreading of particle pencil beams. This analysis complements recent numerical simulation works by providing explicit analytical results for the properties of the scattering process and relies on two complementary approaches: a moment approach, which leads to an infinite recursively coupled system of ordinary differential equations for angular moments of increasing order, and a similarity approach, which provides an approximate solution of the equation in the form of a self-similar profile describing the diffusive angular spreading of the particle distribution during propagation. These solutions provide a good physical picture of the influence of large angle scattering processes on the evolution of an initially collimated beam. As expected from physical intuition and demonstrated previously, when large angle scattering is taken into account, the spreading of the beam occurs more rapidly than in the case of the classical Fokker-Planck equation, which includes only small angle scattering collisional processes. The analytical predictions are compared with recent results based on Monte Carlo simulations and show good agreement. A short discussion is also made of the effects of backscattering, which turns the problem into a more complicated one (of the two-way-diffusion or backward-forward type). Using a simple approximate approach, originally employed by Bethe, Rose, and Wandenburg[8] in analyzing the corresponding problem for the classical Fokker-Planck equation, it is found that the particle flux through the slab decreases in the same way for the classical and GFP equations, in agreement with recent numerical simulations.[5]

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