On the accuracy of the Fokker–Planck and Fermi pencil beam equations for charged particle transport

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Electron beam dose calculations are often based on pencil beam formulas such as the Fermi–Eyges formula. The Fermi–Eyges formula gives an exact solution of the Fermi equation. The Fermi equation can be derived from a more fundamental mathematical model, the linear Boltzmann equation, in two steps. First, the linear Boltzmann equation is approximated by the Fokker–Planck equation. Second, the Fokker–Planck equation is approximated by the Fermi equation. In this paper, we study these approximations. We use a simplified model problem, but choose parameter values closely resembling those relevant in electron beam therapy. Our main conclusions are: (1) The inaccuracy of the Fokker–Planck approximation is primarily due to neglect of large-angle scattering. (2) When computing an approximate solution to the Fokker–Planck equation by Monte Carlo simulation of a transport process, one should let the polar scattering angle be deterministic. (3) At shallow depths, the discrepancy between the linear Boltzmann and Fokker–Planck equations is far more important than that between the Fokker–Planck and Fermi equations. The first of these conclusions is certainly not new, but we state and justify it more rigorously than in previous work. © 1996 American Association of Physicists in Medicine.

Key words: electron beam, pencil beam, Fermi–Eyges theory, Fokker–Planck approximation

1. INTRODUCTION

The main computational algorithms currently in clinical use for electron dose calculations are the pencil beam algorithms.^{1–9} These algorithms are based on approximate closed-form descriptions of steady pencil beams. A pencil beam is a particle beam that enters an object through a single point on the boundary, with all particles moving in a single direction, as illustrated in Fig. 1. Approximate closed-form descriptions of pencil beams can be obtained by fitting computational or laboratory data, or they can be derived mathematically.^{10–14} Combinations of these approaches are also possible. For example, approximate pencil beam formulas derived mathematically may suggest efficient ways of accurately fitting experimental data.

The earliest pencil beam formula was proposed by Fermi.¹⁰ Starting from a microscopic model of monoenergetic particle transport, he derived, in a nonrigorous way, a partial differential equation resembling the Fokker–Planck equation. For the Fermi equation, the boundary value problem describing a pencil beam normally incident on a homogeneous, scattering, nonabsorbing object filling a half-space can be solved in closed form. This is described in Ref. 11, with possible energy loss modeled in the form of a depth-dependent scattering power. (No such closed-form solution is known for the Fokker–Planck equation itself.) Various modifications of the resulting formula have been proposed. Often they involve parameters that are used to improve agreement with laboratory data. An example is Ref. 12, where it is proposed to describe electron beams by a sum of three different expressions that have the same form as the

Fermi–Eyges formula, but contain weights and other free parameters to be determined experimentally.

The Fermi equation can be viewed as the leading term in a certain asymptotic expansion of the Fokker–Planck equation.^{13,14} The Fokker–Planck equation in turn can be viewed as the leading term in an asymptotic expansion of the linear Boltzmann equation.^{15,16} In the present paper, we study these two approximations. We use a simplified model problem, monoenergetic linear particle transport through a homogeneous, anisotropically scattering, nonabsorbing medium occupying a half-space. In our numerical experiments, we use the screened Rutherford differential scattering cross section, with parameter values reminiscent of the transport of electrons at about 10 MeV through about a centimeter of water. 10 MeV is a typical energy level in electron beam cancer therapy, and electron transport through soft human tissue resembles electron transport through water.

Screened Rutherford scattering is the simplest realistic model of the scattering of electrons by nuclei surrounded (“screened”) by electron clouds. It is derived without taking relativistic effects into account, and is therefore not a realistic model of the transport of electrons at about 10 MeV. At such energies, the screened Mott cross section would be more appropriate. However, the Mott and Rutherford cross sections differ only by a positive factor that depends continuously on the angle of deflection, and equals 1 at zero deflection; see Ref. 17, p. 211. We will show that such a factor is not important in the context of this paper; see Lemmas 1 and 7 of the Appendix. This is why we have chosen to use the

FIG. 1. Pencil beam.

FIG. 2. Definitions of ϑ_0 and φ_0 .

simpler Rutherford cross section for our numerical experiments.

The problems that arise in radiotherapy planning are significantly more complicated than our model problem in several other ways as well. In particular, real electron transport is not monoenergetic, and of course a patient's body is not a homogeneous half-space. Nevertheless we hope that the understanding gained by studying this simple model problem may contribute to a better understanding of realistic problems.

Our main conclusions, supported by both analysis and computational evidence, are as follows.

- (1) The inaccuracy of the Fokker–Planck approximation is primarily due to neglect of large-angle scattering.
- (2) When computing an approximate solution to the Fokker–Planck equation by Monte Carlo simulation of a transport process, one should let the polar scattering angle be deterministic.
- (3) At shallow depths, the discrepancy between the linear Boltzmann and Fokker–Planck equations is far more important (on the order of 20% in our computational experiments) than that between the Fokker–Planck and Fermi equations (on the order of 1%).

The first of these conclusions is not new; see for instance Refs. 18 and 19. However, we state it in a way that is more mathematically precise than previous formulations.

II. MAIN RESULTS

The monoenergetic, time independent linear Boltzmann equation is

$$\omega \cdot \nabla_{\mathbf{x}} f(\mathbf{x}, \omega) = Qf(\mathbf{x}, \omega),$$

with

$$Qf(\mathbf{x}, \omega) = \frac{1}{\bar{\lambda}} \left(\frac{1}{2\pi} \int_{S^2} p(\omega \cdot \omega') f(\mathbf{x}, \omega') d\omega' - f(\mathbf{x}, \omega) \right).$$

The independent variables are the particle position $\mathbf{x}$ and the particle direction $\omega \in S^2$; here S^2 denotes the set of unit vectors in three-dimensional space. The dependent variable is the phase space number density f . The constant $\bar{\lambda}$ is the mean free path. The function p is the probability density function of the cosine μ_0 of the polar deflection angle ϑ_0 in a single collision; see Fig. 2. In electron transport, the scattering is typically strongly forward-peaked, i.e., $p(\mu)$ is peaked near $\mu=1$. We focus on screened Rutherford scattering, i.e.,

$$p(\mu) = \frac{2\eta(\eta+1)}{(1+2\eta-\mu)^2}, \quad (1)$$

where $\eta > 0$ is a typically small constant called the screening parameter.²⁰ Screened Rutherford scattering is one of the simplest models of elastic scattering of electrons from nuclei taking into account the screening of the nuclei by atomic electrons. It is obtained from the Schrödinger equation in the first Born approximation, using an exponential factor in the potential to model the screening effect; see e.g. Ref. 21, Sec. 3.1.5. An approximate formula for the screening parameter can be found in the same reference:

$$\eta = C \frac{Z^{2/3}}{(mv)^2}, \quad (2)$$

where Z denotes the atomic number of the nucleus, mv is the (relativistic) momentum of the electron that is being scattered, and C is a constant. In terms of the Planck constant $\hbar$ and the Bohr radius a_H , $C = \hbar^2/4a_H^2$.

As mentioned in the introduction, the screened Rutherford cross section is derived without taking into account relativistic

istic effects, which are important at the energies used in electron beam therapy. For the screened Mott cross section, which does take into account relativistic effects,

$$p(\mu) = R(\mu) \frac{C(\eta)}{(1 + 2\eta - \mu)^2}, \quad (3)$$

where R is a continuous, positive, bounded function of μ with $R(1)=1$, and $C(\eta)>0$ is determined by the condition $\int_{-1}^1 p(\mu) d\mu = 1$; see Ref. 17, p. 211.

The expected value of μ_0 will play an important role in this paper. It is given by the formula

$$\bar{\mu}_0 = \int_{-1}^1 \mu p(\mu) d\mu.$$

Forward peakedness of the scattering means $\bar{\mu}_0 \approx 1$. For screened Rutherford scattering, a straightforward calculation shows

$$\bar{\mu}_0 = 1 - 2\eta \ln\left(\frac{1}{\eta}\right) + O(\eta). \quad (4)$$

Equation (2) implies that η tends to zero as the energy tends to infinity, so the scattering is highly forward peaked for large energies. It is not hard to show that the factor $R(\mu)$ in Eq. (3) does not essentially alter Eq. (4), and in particular $1 - \bar{\mu}_0$ will still be $O(\eta \ln(1/\eta))$; see Lemma 1 of the Appendix.

The limit

$$\bar{\lambda} \rightarrow 0, \quad \bar{\mu}_0 \rightarrow 1,$$

with

$$\bar{\lambda}_{tr} = \frac{\bar{\lambda}}{1 - \bar{\mu}_0} > 0$$

fixed, is called the Fokker–Planck limit.¹⁵ The constant $\bar{\lambda}_{tr}$ is called the “transport mean free path.” It equals $2/T$, where T is the “linear scattering power.”²² In the Fokker–Planck limit, collisions become infinitely frequent ($\bar{\lambda} \rightarrow 0$), while the expected effect of a single collision becomes infinitesimal ($\bar{\mu}_0 \rightarrow 1$). Often, but not always,

$$Qf(\mathbf{x}, \omega) \rightarrow \frac{1}{2\bar{\lambda}_{tr}} \Delta_{\omega} f(\mathbf{x}, \omega)$$

in this limit. Here Δ_{ω} denotes the Laplace operator on the unit sphere. Using the notation

$$\omega = (\omega_1, \sqrt{1 - \omega_1^2} \cos \varphi, \sqrt{1 - \omega_1^2} \sin \varphi),$$

with $\varphi \in [0, 2\pi]$, Δ_{ω} is given by

$$\Delta_{\omega} = \frac{\partial}{\partial \omega_1} (1 - \omega_1^2)^2 \frac{\partial}{\partial \omega_1} + \frac{1}{(1 - \omega_1^2)^2} \frac{\partial^2}{\partial \varphi^2}.$$

The equation

$$\omega \cdot \nabla_{\mathbf{x}} f(\mathbf{x}, \omega) = \frac{1}{2\bar{\lambda}_{tr}} \Delta_{\omega} f(\mathbf{x}, \omega)$$

is called the Fokker–Planck equation.

To understand the Fokker–Planck limit, we take the following point of view. Let $g = g(\omega)$ be a function defined on the unit sphere, and ask whether Qg converges to $\Delta_{\omega} g / (2\bar{\lambda}_{tr})$. For a rigorous statement and proof of the answer, see the Appendix. We state it in a nonrigorous, intuitive form here:

$$Qg(\omega) \rightarrow \frac{1}{2\bar{\lambda}_{tr}} \Delta_{\omega} g(\omega) \quad \text{for all } g$$

if and only if $\frac{\text{var}(\mu_0)}{1 - \bar{\mu}_0} \rightarrow 0,$

and to leading order, the discrepancy between Qg and $1/(2\bar{\lambda}_{tr})\Delta_{\omega} g$ is proportional to $\text{var}(\mu_0)/(1 - \bar{\mu}_0)$. Here $\text{var}(\mu_0)$ denotes the variance of μ_0 . Notice that $\text{var}(\mu_0)$ is a measure of the frequency of large-angle scattering, or more precisely, of exceptional (large- and small-angle) scattering. We conclude that exceptional scattering is the main cause of the discrepancy between the linear Boltzmann and Fokker–Planck equations.

We now consider specific examples of families of probability densities p . In all of these examples, we consider the limit $\bar{\lambda} \rightarrow 0$, $\bar{\mu}_0 \rightarrow 1$, with $\bar{\lambda}/(1 - \bar{\mu}_0)$ fixed. The question whether or not the Fokker–Planck equation is obtained in the limit is then decided by the behavior of $\text{var}(\mu_0)/(1 - \bar{\mu}_0)$.

Example 1: Henyey–Greenstein scattering.²³

$$p(\mu) = \frac{1}{2} \frac{1 - \bar{\mu}_0^2}{(1 - 2\bar{\mu}_0\mu + \bar{\mu}_0^2)^{3/2}}.$$

We obtain

$$\begin{aligned} \frac{\text{var}(\mu_0)}{1 - \bar{\mu}_0} &= \frac{1}{1 - \bar{\mu}_0} \int_{-1}^1 (1 - \mu)^2 p(\mu) d\mu - (1 - \bar{\mu}_0) \\ &= \frac{\bar{\mu}_0 + 1}{3}. \end{aligned}$$

As $\bar{\mu}_0 \rightarrow 1$, we obtain $\text{var}(\mu_0)/(1 - \bar{\mu}_0) \rightarrow 2/3$, so the Fokker–Planck equation is not a valid approximation to the linear Boltzmann equation with Henyey–Greenstein scattering. This fact was first observed by Pomraning.¹⁵

Example 2: Screened Rutherford scattering:

$$p(\mu) = \frac{2\eta(\eta + 1)}{(1 + 2\eta - \mu)^2}.$$

A straightforward computation shows

$$\frac{\text{var}(\mu_0)}{1 - \bar{\mu}_0} = \frac{2}{\ln(1/(1 - \bar{\mu}_0))} + o\left(\frac{1}{\ln(1/(1 - \bar{\mu}_0))}\right).$$

Therefore, $\text{var}(\mu_0)/(1 - \bar{\mu}_0)$ tends to zero, but quite slowly. As will be seen later from our computational results, in the problems of interest in radiation oncology, $\bar{\lambda}$ is not small enough and $\bar{\mu}_0$ not close enough to 1 for the Fokker–Planck approximation to be accurate.

Screened Rutherford scattering lies on the border of the domain of validity of the Fokker–Planck approximation in the following sense. For $\alpha > 0$, define

$$p_\alpha(\mu) = \frac{C(\alpha, \eta)}{(1 + 2\eta - \mu)^\alpha},$$

where $C(\alpha, \eta) > 0$ is chosen such that $\int_{-1}^1 p_\alpha(\mu) d\mu = 1$. Then it is not hard to verify that $\text{var}(\mu_0)/(1 - \bar{\mu}_0) \rightarrow 0$ as $\bar{\mu}_0 \rightarrow 1$ if and only if $\alpha \geq 2$.

Example 3: Screened Mott scattering:

$$p(\mu) = R(\mu) \frac{C(\eta)}{(1 + 2\eta - \mu)^2},$$

where $R(\mu) > 0$, and $C(\eta)$ is chosen such that $\int_{-1}^1 p(\mu) d\mu = 1$. If R is a continuous function with $R(1) = 1$, then

$$\frac{\text{var}(\mu_0)}{1 - \bar{\mu}_0} = O\left(\frac{1}{\ln(1/(1 - \bar{\mu}_0))}\right)$$

as $\eta \rightarrow 0$; see Lemma 7 of the Appendix.

Example 4: Scattering with a deterministic scattering cosine:

$$p(\mu) = \delta(\mu - \bar{\mu}_0),$$

where δ denotes the Dirac δ function. This means $\mu_0 = \bar{\mu}_0$ with probability 1. (Notice that the scattering is still random, since the azimuthal scattering angle φ_0 is random.) We have

$$\frac{\text{var}(\mu_0)}{1 - \bar{\mu}_0} = 0.$$

Thus for $p(\mu) = \delta(\mu - \bar{\mu}_0)$, $\text{var}(\mu_0)/(1 - \bar{\mu}_0)$ takes its smallest possible value, namely 0.

One way of computing approximate solutions of the Fokker–Planck equation is to compute, by direct Monte Carlo simulation, solutions to a linear Boltzmann equation with $\bar{\lambda}$ small, $\bar{\mu}_0$ close to 1, and $\bar{\lambda}/(1 - \bar{\mu}_0)$ equal to the desired value of $\lambda_{\text{tr}} > 0$. There are two approximation errors in such a procedure. The first is a “truncation error,” due to the fact that what is being simulated is not the limit as $\bar{\lambda} \rightarrow 0$ and $\bar{\mu}_0 \rightarrow 1$ with $\bar{\lambda}/(1 - \bar{\mu}_0) = \bar{\lambda}_{\text{tr}}$, but rather one particular transport problem with a value of $\bar{\lambda}$ close to 0 but not equal to 0, a value of $\bar{\mu}_0$ close to 1 but not equal to 1, and $\bar{\lambda}/(1 - \bar{\mu}_0) = \bar{\lambda}_{\text{tr}}$. The second is a statistical error, due to the fact that the number of simulated particle trajectories is finite. The value of $\bar{\mu}_0$ does not of course determine p , and the freedom in the choice of p can be used to minimize the first of the two errors. Our discussion, and in particular example 4, suggests: When computing an approximate solution to the Fokker–Planck equation by Monte Carlo simulation of a transport process, we should use $p(\mu) = \delta(\mu - \bar{\mu}_0)$.

The corresponding transport process seems artificial, but the convergence, as $\bar{\mu}_0 \rightarrow 0$, to the Fokker–Planck process is faster for this family of probability densities than for any other family.

For illustration, Table I shows the value of $\text{var}(\mu_0)/(1 - \bar{\mu}_0)$ for various values of $1 - \bar{\mu}_0$, and for the choices of p of examples 1, 2, and 4.

We next briefly review the Fermi–Eyges formula; see Refs. 13 and 14 for a much more detailed discussion. Consider a pencil beam entering the half space $x_1 > 0$ through the

TABLE I. $\text{var}(\mu_0)/(1 - \bar{\mu}_0)$, the quantity that measures large-angle scattering and determines the accuracy of the Fokker–Planck approximation to leading order, for various values of $1 - \bar{\mu}_0$ and three differential scattering cross sections.

$1 - \bar{\mu}_0$	$\delta(\mu_0 - \bar{\mu}_0)$	scr. Rutherford	Henyey–Greenstein
10^{-3}	0	0.23	0.67
10^{-4}	0	0.18	0.67
10^{-5}	0	0.14	0.67
10^{-6}	0	0.12	0.67
10^{-7}	0	0.11	0.67

point $\mathbf{x} = (0, 0, 0)$ with all particles moving in the direction of the positive x_1 axis. The following boundary value problem for the time independent Fokker–Planck equation describes such a beam:

$$\omega \cdot \nabla_{\mathbf{x}} f = \frac{1}{2\lambda_{\text{tr}}} \Delta_{\omega} f \quad (5)$$

for $x_1 > 0$, $\omega \in S^2$, and

$$f(0, x_2, x_3, \omega) = \frac{q}{v} \delta(x_2) \delta(x_3) \delta(\omega - (1, 0, 0)), \quad (6)$$

for $-\infty < x_2, x_3 < \infty$, $\omega \in S^2$ with $\omega_1 > 0$. In Eq. (6), q denotes the number of particles entering the half-space in unit time. Fermi’s approximate solution to this problem is¹⁰

$$f(\mathbf{x}, \omega) \approx f^F(\mathbf{x}, \omega) = \frac{3q\bar{\lambda}_{\text{tr}}^2}{\pi^2 x_1^4 v} \exp\left[-2\bar{\lambda}_{\text{tr}} \left(\frac{\omega_2^2 + \omega_3^2}{x_1} - 3 \frac{x_2 \omega_2 + x_3 \omega_3}{x_1^2} + 3 \frac{x_2^2 + x_3^2}{x_1^3}\right)\right] \quad (7)$$

if $\omega_1 > 0$, and $f^F(\mathbf{x}, \omega) = 0$ if $\omega_1 \leq 0$. We note that for fixed x_1 , ω_2 , and ω_3 , f^F is a Gaussian in x_2 and x_3 , and for fixed x_1 , x_2 , and x_3 , it is a Gaussian in ω_2 and ω_3 .

If we allow ω_2 and ω_3 to range from $-\infty$ to ∞ and integrate in Eq. (7), we obtain Fermi’s approximate formula for the scalar density:

$$F(\mathbf{x}) = \int_{S^2} f(\mathbf{x}, \omega) d\omega \approx F^F(\mathbf{x}) = \frac{3q\bar{\lambda}_{\text{tr}}}{2\pi x_1^3 v} \exp\left[-\frac{3\bar{\lambda}_{\text{tr}}}{2} \left(\frac{x_2^2 + x_3^2}{x_1^3}\right)\right]. \quad (8)$$

For fixed x_1 , this is a Gaussian in x_2 and x_3 .

We will now report on computational comparisons between the linear Boltzmann equation with screened Rutherford scattering, and the Fokker–Planck and Fermi equations. For brevity, we write “Boltzmann equation” instead of “linear Boltzmann equation with screened Rutherford scattering” from now on. In our figures, we always use the following symbols to denote approximate solutions of the Fermi, Fokker–Planck, and Boltzmann equations:

- Fermi,
- + Fokker–Planck,
- * Boltzmann.

Our test problem is a pencil beam incident on a homogeneous slab $0 < x_1 < L$. The particles enter the slab at $\mathbf{x}=(0,0,0)$ in the direction $\omega=(1,0,0)$. We consider the non-dimensionalized scalar density,

$$\phi(r) = \frac{v}{q} L^2 F(L, Lr \cos \beta, Lr \sin \beta) \quad (0 \leq \beta \leq 2\pi).$$

Equation (8) yields

$$\phi(r) \approx \phi^F(r) = \frac{3}{2\pi} \frac{\bar{\lambda}_{tr}}{L} \exp\left[-\frac{3}{2} \frac{\bar{\lambda}_{tr}}{L} r^2\right]. \quad (9)$$

Monte Carlo simulations do not directly yield point values of ϕ , but can be used to approximate local averages of the form

$$\frac{2\pi \int_{r-\Delta r/2}^{r+\Delta r/2} \phi(\rho) \rho d\rho}{\pi[(r+\Delta r/2)^2 - (r-\Delta r/2)^2]}. \quad (10)$$

All of our plots show such averages, taken over the cells of a uniform grid along the r axis. We denote the cell centers by

$$r_j = (j - 1/2)\Delta r, \quad j = 1, 2, \dots \quad (11)$$

(These will only be used for graphically displaying the results of our computations.)

The scalar flux ϕ obtained from the Boltzmann equation depends on the dimensionless parameters $\bar{\lambda}/L$ and $\bar{\lambda}_{tr}/L$. The approximations ϕ^{FP} and ϕ^F to the scalar flux obtained from the Fokker–Planck and Fermi equations depend on $\bar{\lambda}_{tr}/L$ only.

For electrons at 10 MeV passing through water, $\bar{\lambda}_{tr} = 2/T \approx 28.5$ cm; see Ref. 6, p. 134, Table I. Mean free paths of electrons passing through water can be computed from Ref. 24. The elastic collision cross section for electron–hydrogen interactions is approximately 13 000 barns, and that for electron–oxygen interactions is approximately 210 000 barns; see Ref. 24, pp. 3 and 32. Therefore the total cross section for elastic collisions of electrons in water is approximately $2 \times 13\,000 + 210\,000$ barns = 236 000 barns. Denoting Avogadro's number by N_A , the number of elastic collisions per centimeter is approximately

$$\frac{1}{\text{cm}^3} \times \frac{N_A}{g} \times \frac{1}{18} \text{ elastic collision cross section in cm}^2 \\ \times 1 \text{ cm} \approx 8000.$$

The numbers that we have just cited motivate our choice of parameters:

$$\frac{\bar{\lambda}}{L} = \frac{1}{11\,000}, \quad \frac{\bar{\lambda}_{tr}}{L} = 20,$$

corresponding to a depth on the order of a centimeter.

To approximate solutions of the Fokker–Planck equation, we perform direct Monte Carlo simulations of transport processes with $p(\mu) = \delta(\mu - \bar{\mu}_0)$. (See the discussion of example 4.) In this context, the value of $\bar{\lambda}/L$ is to be thought of

FIG. 3. Exit profile of pencil beam penetrating slab, computed using the Fermi ('○') and Fokker–Planck ('+') equations. Beam profiles (left column), percentage discrepancies between Fermi and Fokker–Planck results (middle column), and estimated standard deviations in the Fokker–Planck results as percentages of those results (right column). Different rows correspond to different degrees of accuracy in the Fokker–Planck computation.

as a *computational* parameter, not a *physical* one. The Fokker–Planck solution is obtained in the limit $\bar{\lambda}/L \rightarrow 0$.

The computing resources at our disposal are insufficient for accurate direct Monte Carlo simulations with $\bar{\lambda}/L = 1/11\,000$. To compute approximate solutions to the Boltzmann equation, we therefore use a relatively small number of particle trajectories only. The results contain a substantial level of statistical noise. However, the discrepancy between the Fokker–Planck and Boltzmann solutions is significantly above the noise level.

Figure 3 compares the Fermi and Fokker–Planck approximations. The Fokker–Planck results were obtained from Monte Carlo simulations of transport processes with $p(\mu) = \delta(\mu - \bar{\mu}_0)$. The different rows in Fig. 3 correspond to different values of $\bar{\lambda}/L$ used in these simulations. The top row corresponds to $\bar{\lambda}/L = 1/100$, the middle one to $\bar{\lambda}/L = 1/200$, and the bottom one to $\bar{\lambda}/L = 1/400$. For each value of $\bar{\lambda}/L$, 10^7 particle trajectories were simulated to obtain the Fokker–Planck results. The plots in the left column show local averages of ϕ^{FP} and ϕ^F as a function of the distance r from the central axis of the beam. For precise specification of the quantities plotted, see formulas (10) and (11). Notice that there are no visible differences between the three plots in the left column of Fig. 3. We are therefore confident that the profiles labeled with the symbol '+' in these plots very closely approximate the Fokker–Planck limit. [For additional confirmation, we have repeated our experiments with $p(\mu) = C \exp(\alpha\mu)$, where $\alpha > 0$ and $C > 0$ are determined by the conditions $\int_{-1}^1 p(\mu) d\mu = 1$ and $\int_{-1}^1 \mu p(\mu) d\mu = \bar{\mu}_0$. The results are very close to those with $p(\mu) = \delta(\mu - \bar{\mu}_0)$.] The plots in the middle column show percentage discrepancies between the Fermi and Fokker–Planck results, and the ones in the right column show Monte Carlo estimates of the stan-

TABLE II. Profile of scalar density of a pencil beam, as a function of the distance r from the beam center, based on the Fermi and Fokker–Planck equations.

r	Fermi	Fokker–Planck	discrepancy
0.0224	9.27	9.38	–1.2%
0.0671	8.23	8.29	–0.71%
0.112	6.49	6.50	–0.094%
0.157	4.54	4.54	0.12%
0.201	2.83	2.87	–1.5%
0.246	1.56	1.66	–5.8%
0.291	0.765	0.884	–14%
0.335	0.333	0.444	–25%
0.380	0.129	0.212	–39%
0.425	0.0442	0.0994	–56%
0.470	0.0135	0.0453	–70%
0.514	0.00364	0.0209	–83%

standard deviations in the Fokker–Planck results, as percentages of those results.

Table II displays the numbers used to generate the left and middle plots of the last row of Fig. 3. The first column of the table gives the cell centers r_j , i.e., the r coordinates of the points displayed in Fig. 3. The second column gives the Fermi results. It is not obtained by pointwise evaluation of formula (7), but by computing local averages of the form (10) of formula (7). The third column shows the Fokker–Planck results, the fourth the percentage discrepancies between the Fermi and Fokker–Planck results. The entries in the first three columns of the table have been rounded to three significant digits. The percentage discrepancies have been rounded to two significant digits. The percentage discrepancy is negative when the Fermi result is smaller than the Fokker–Planck result. Our results show that the Fermi solution deviates from the Fokker–Planck solution by only about 1% in the beam center, although the discrepancy becomes substantial near the edge of the beam.

Figure 4 compares the Fokker–Planck and Boltzmann approximations. Different rows in Fig. 4 correspond to different initial seeds used for the random number generator when computing the Boltzmann results. The Fokker–Planck results in Fig. 4 are identical to those of the bottom row of Fig. 3. The Boltzmann results were obtained by simulating 100 000 trajectories with screened Rutherford scattering, using $\bar{\lambda}/L = 1/11\,000$ and $\bar{\lambda}_{tr}/L = 20$. As in Fig. 3, the plots in the left column show local averages of ϕ and ϕ^{FP} as functions of the distance r from the central axis of the beam; see formulas (10) and (11). The middle column shows percentage discrepancies between the Fokker–Planck and Boltzmann results, and the right one Monte Carlo estimates of the standard deviations in the Boltzmann results, as percentages of those results.

It may come as a surprise that the Boltzmann profiles are narrower than the Fokker–Planck profiles as a result of a relatively large amount of large-angle scattering. However, for a fixed value of $\bar{\mu}_0$, the larger the number of exceptional deflections with relatively large values of $1 - \mu_0$, the smaller must be the average value of $1 - \mu_0$ in the other, nonexceptional collisions. That is, for a given value of $\bar{\mu}_0$, if large-

FIG. 4. Exit profile of pencil beam penetrating slab, computed using the Fokker–Planck equation ('+''), and the linear Boltzmann equation with screened Rutherford scattering ('*'). Beam profiles (left column), percentage discrepancies between Fokker–Planck and Boltzmann results (middle column), and estimated standard deviations in the Boltzmann results as percentages of those results (right column). Different rows correspond to different initial seeds in the Monte Carlo simulation.

angle scattering is frequent, so is small-angle scattering. A scattering law with a large amount of large-angle scattering typically leads to beams with a narrow core, surrounded by a smaller number of erratic particles with flight trajectories at large angles with the central axis of the beam. This is illustrated by Figs. 1, 5, and 6. Each of the three plots in these figures shows 200 simulated particle trajectories, with $\bar{\lambda}/L = 1/100$, $\bar{\lambda}_{tr}/L = 50$. The plot in Fig. 1 was obtained using

FIG. 5. Particle trajectories with screened Rutherford scattering.

FIG. 6. Particle trajectories with Henyey-Greenstein scattering.

$p(\mu) = \delta(\mu - \bar{\mu}_0)$, the one in Fig. 5 using screened Rutherford scattering, and the one in Fig. 6 using Henyey-Greenstein scattering.

Table III displays the numbers used to generate the left and middle plots of the first row of Fig. 4. The first column of the table gives the cell centers r_j . The second column gives the Fokker-Planck results, the third the Boltzmann results, the fourth the percentage discrepancies between the Fokker-Planck and Boltzmann results. The entries in the first three columns of the table have been rounded to three significant digits. The percentage discrepancies have been rounded to two significant digits. The percentage discrepancy is negative when the Fokker-Planck result is smaller than the Boltzmann result.

In spite of the statistical noise in our Monte Carlo results, we can say with confidence that in the beam center, the dis-

TABLE III. Profile of scalar density of a pencil beam, as a function of the distance r from the beam center, based on the Fokker-Planck and linear Boltzmann equations.

r	Fokker-Planck	Boltzmann	discrepancy
0.0224	9.38	13.1	-28%
0.0671	8.29	10.6	-22%
0.112	6.50	7.41	-12%
0.157	4.54	4.46	1.8%
0.201	2.87	2.38	21%
0.246	1.66	1.17	42%
0.291	0.884	0.556	59%
0.335	0.444	0.271	64%
0.380	0.212	0.146	45%
0.425	0.0994	0.0758	31%
0.470	0.0453	0.0438	3.4%
0.514	0.0209	0.0289	-28%

crepancy between the linear Boltzmann and Fokker-Planck pencil beam profiles is on the order of 20% to 30%, while that between the Fokker-Planck and Fermi profiles is only on the order of 1%. Near the edge of the beam, both discrepancies are substantial in a relative sense, but small in an absolute sense. In summary, we arrive at our third main conclusion: At shallow depths, the discrepancy between the linear Boltzmann and Fokker-Planck equations is far more significant than that between the Fokker-Planck and Fermi equations.

III. DISCUSSION AND SOME OPEN QUESTIONS

It is widely known that the Fokker-Planck equation is an accurate description of linear, monoenergetic particle transport with frequent, highly forward-peaked scattering if and only if large-angle scattering is sufficiently insignificant. However, it does not appear to be widely known that the latter condition can be stated simply as $\text{var}(\mu_0)/(1-\bar{\mu}_0) \ll 1$.

The condition $\text{var}(\mu_0)/(1-\bar{\mu}_0) \ll 1$ means that the standard deviation of $1-\mu_0$ should be much smaller than $\sqrt{1-\bar{\mu}_0}$. Therefore collisions in which $1-\mu_0$ is significant in comparison with $\sqrt{1-\bar{\mu}_0}$ might be called "large-angle" collisions. For instance, if $\bar{\mu}_0 = 0.999995$, then $\sqrt{1-\bar{\mu}_0} \approx 2 \times 10^{-3}$, so a collision in which $1-\mu_0$ is a significant fraction of 10^{-3} should be considered a "large-angle" collision. Since $1-\mu_0 = 10^{-3}$ corresponds to a polar angle of deflection $\vartheta_0 \approx 2.5^\circ$, and $1-\mu_0 = 10^{-4}$ corresponds to $\vartheta_0 \approx 0.8^\circ$, "large-angle" collisions do not necessarily result in large deflections in an absolute sense.

The observation that $\text{var}(\mu_0)/(1-\bar{\mu}_0)$ measures closeness to the Fokker-Planck limit may also be useful in the construction of Boltzmann-Fokker-Planck splitting methods.^{18,19} Such methods are based on writing the Boltzmann collision operator as a sum of two collision operators. The first can accurately be approximated by the Fokker-Planck operator. The second is less singular than the original collision operator, in the sense that the scattering is less forward peaked, and the mean free path is larger.

Our conclusion that screened Rutherford scattering lies on the border of the range of validity of the Fokker-Planck approximation is similar to the result of Ref. 26. The latter result applies to a different and more difficult problem than ours, since it concerns a nonlinear Boltzmann transport equation.

Our numerical results demonstrate that at shallow depths, the Fokker-Planck and Fermi solutions agree reasonably well for monoenergetic pencil beam problems, but they do not quantitatively agree with the Boltzmann solution for screened Rutherford scattering. This casts doubt on the accuracy of the Fokker-Planck and Fermi approximations for pencil beam problems with realistic scattering kernels. We have noted that such doubts, and possible remedies, have been discussed previously in the literature.^{12,18,19} The theorem of the Appendix, together with the results in Table I, give a precise mathematical reason for these concerns. They demonstrate that the neglect of large-angle scattering leads to significant quantitative errors.

We note that the discrepancy between the Fokker–Planck and Fermi approximations becomes much more significant at greater depths; compare Figs. 8–10 of Ref. 27. The reason is that the assumption of approximate monodirectionality underlying the Fermi approximation becomes increasingly inaccurate with increasing depth.

The results in this paper apply only to monoenergetic pencil beams. Broad, energy-dependent beams are used in radiation therapy. It is likely that the extra physical aspects of such problems will influence the accuracy of the corresponding approximations (the Fokker–Planck equation with continuous slowing down, or the Fermi equation with depth-dependent scattering power) in ways that are not discussed in this paper. We plan to investigate these questions in future work.

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APPENDIX: MATHEMATICAL ANALYSIS OF THE FOKKER–PLANCK LIMIT

We begin by listing some standard mathematical notation and definitions used later in this appendix.

$L^2(-1,1)$ = set of all real-valued functions $f=f(x)$ ($-1 < x < 1$) with

$$\int_{-1}^1 |f(x)|^2 dx < \infty,$$

and for $f \in L^2(-1,1)$,

$$\|f\|_{L^2(-1,1)} = \sqrt{\int_{-1}^1 |f(x)|^2 dx}.$$

Similarly, $L^2(S^2)$ = set of all complex-valued functions $f=f(\omega)$ ($\omega \in S^2$) with

$$\int_{S^2} |f(\omega)|^2 d\omega < \infty,$$

and for $f \in L^2(S^2)$,

$$\|f\|_{L^2(S^2)} = \sqrt{\int_{S^2} |f(\omega)|^2 d\omega}.$$

A sequence of functions $f_n \in L^2$ ($n=1,2,3,\dots$) is said to converge in L^2 with limit $f \in L^2$ if

$$\lim_{n \rightarrow \infty} \|f - f_n\|_{L^2} = 0.$$

This is also called strong convergence. The sequence is said to converge weakly in L^2 with limit $f \in L^2$ if

$$\lim_{n \rightarrow \infty} \int f_n g = \int f g$$

for all $g \in L^2$. Strong convergence implies weak convergence, but the converse is not true. Since convergence of a series means convergence of the partial sums, this also defines strong and weak convergence of series in L^2 .

We next present a derivation of the Fokker–Planck equation from the linear Boltzmann equation. We let $g \in L^2(S^2)$, assume $\Delta_\omega g \in L^2(S^2)$, and analyze whether

$$Qg \rightarrow \frac{1}{2\lambda_{tr}} \Delta_\omega g \quad \text{weakly in } L^2(S^2) \quad (A1)$$

in the Fokker–Planck limit. We use spherical harmonics expansions of Qg and $\Delta_\omega g$. This is an idea that we learned from Ref. 15. Our analysis is less general than that in Ref. 15, since we assume the problem to be monoenergetic, but more complete. In particular, we prove a simple necessary and sufficient condition for (A1).

We begin with a lemma that says that in a certain sense, the screened Rutherford and Mott cross sections behave similarly; compare the lemma with Eq. (4).

Lemma 1: Let

$$R: [-1,1] \rightarrow \mathbb{R}_+$$

be a continuous function with $R(1)=1$. Let p be defined as in Eq. (3). Then

$$\int_{-1}^1 (1-\mu)p(\mu)d\mu = O\left(\eta \ln\left(\frac{1}{\eta}\right)\right) \quad \text{as } \eta \rightarrow 0.$$

Proof: Let A_1 be a constant with $-1 \leq A < 1$ such that $R(\mu) \geq 1/2$ for $\mu \in [A,1]$. As $\eta \rightarrow 0$,

$$\int_{-1}^A \frac{1}{(1+2\eta-\mu)^2} d\mu = O(1)$$

and

$$\int_A^1 \frac{1}{(1+2\eta-\mu)^2} d\mu = O\left(\frac{1}{\eta}\right).$$

Therefore

$$\int_{-1}^1 R(\mu) \frac{1}{(1+2\eta-\mu)^2} d\mu = O\left(\frac{1}{\eta}\right),$$

so

$$C(\eta) = O(\eta).$$

Since

$$\int_{-1}^A \frac{1-\mu}{(1+2\eta-\mu)^2} d\mu = O(1)$$

and

$$\int_A^1 \frac{1-\mu}{(1+2\eta-\mu)^2} d\mu = O\left(\ln \frac{1}{\eta}\right),$$

the assertion follows. ■

Next we review some facts about Legendre polynomials and spherical harmonics; see Ref. 25, Chap. 12. The Legendre polynomials $P_k = P_k(\mu)$, $k=0,1,2,\dots$, form an orthonormal basis of $L^2(-1,1)$, with $\|P_k\|_{L^2(-1,1)} = \sqrt{2/(2k+1)}$. Thus if $p \in L^2(-1,1)$, then

$$p(\mu) = \sum_{k=0}^{\infty} \frac{2k+1}{2} c_k P_k(\mu), \quad (\text{A2})$$

with

$$c_k = \int_{-1}^1 P_k(\mu) p(\mu) d\mu,$$

and the series converges in $L^2(-1,1)$. For all k ,

$$\max_{\mu \in [-1,1]} |P_k(\mu)| = P_k(1) = 1. \quad (\text{A3})$$

Using the recursion relation

$$\frac{d}{d\mu} P_{k+1}(\mu) - \frac{d}{d\mu} P_{k-1}(\mu) = (2k+1)P_k(\mu) \quad (\text{A4})$$

[Ref. 25, p. 647, Eq. (12.23)], estimates on derivatives of arbitrary order of $P_k(\mu)$ can be derived from Eq. (A3). In particular, by induction on k , it is straightforward to verify

$$\max_{-1 \leq \mu \leq 1} \left| \frac{dP_k}{d\mu}(\mu) \right| = \frac{dP_k}{d\mu}(1) = \frac{k(k+1)}{2} \quad (\text{A5})$$

and

$$\max_{-1 \leq \mu \leq 1} |P_k''(\mu)| = P_k''(1) = \frac{(k-1)k(k+1)(k+2)}{8}. \quad (\text{A6})$$

The spherical harmonics $Y_n^m = Y_n^m(\omega)$, $n=0,1,2,\dots$, $m=-n, -n+1, \dots, n-1, n$, form an orthonormal basis of $L^2(S^2)$. Thus if $g \in L^2(S^2)$, then

$$g(\omega) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \left[\int_{S^2} g(\omega') \overline{Y_n^m(\omega')} d\omega' \right] Y_n^m(\omega),$$

and the series converges in $L^2(S^2)$. [In the last equation, $\overline{Y_n^m(\omega')}$ denotes the complex conjugate of $Y_n^m(\omega')$.] Furthermore, the Y_n^m are eigenfunctions of Δ_ω with eigenvalues $-n(n+1)$:

$$\Delta_\omega Y_n^m(\omega) = -n(n+1)Y_n^m(\omega). \quad (\text{A7})$$

The addition theorem for spherical harmonics states that

$$P_n(\omega \cdot \omega') = \frac{4\pi}{2n+1} \sum_{m=-n}^n Y_n^m(\omega) \overline{Y_n^m(\omega')}$$

for $\omega \in S^2$, $\omega' \in S^2$, and $n \geq 0$. The series converges in $L^2(S^2 \times S^2)$.

Since we want to expand Qg into a spherical harmonics series, we first prove that $Qg \in L^2(S^2)$.

Lemma 2: If $g \in L^2(S^2)$, then $Qg \in L^2(S^2)$.

Proof: Since

$$Qg(\omega) = \frac{1}{\lambda} \left(\frac{1}{2\pi} \int_{S^2} p(\omega \cdot \omega') g(\omega') d\omega' - g(\omega) \right),$$

we only have to prove that the function h defined by

$$h(\omega) = \int_{S^2} p(\omega \cdot \omega') g(\omega') d\omega' \quad \text{for } \omega \in S^2$$

is an element of $L^2(S^2)$. But in fact h is bounded, since by the Cauchy-Schwarz inequality,

$$\begin{aligned} |h(\omega)| &\leq \sqrt{\int_{S^2} p(\omega \cdot \omega')^2 d\omega'} \sqrt{\int_{S^2} g(\omega')^2 d\omega'} \\ &= \sqrt{2\pi} \int_{-1}^1 p(\mu)^2 d\mu \|g\|_{L^2(S^2)} \\ &= \sqrt{2\pi} \|p\|_{L^2(-1,1)} \|g\|_{L^2(S^2)}. \end{aligned}$$

■

Next we expand $Qg(\omega)$ into a spherical harmonics series.

Lemma 3: If $g \in L^2(S^2)$, then

$$Qg(\omega) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{c_n-1}{\lambda} \left[\int_{S^2} g(\omega') \overline{Y_n^m(\omega')} d\omega' \right] Y_n^m(\omega),$$

where the c_n are the Legendre coefficients of p . The series converges in $L^2(S^2)$.

Proof: We define

$$\gamma_n^m = \int_{S^2} Qg(\omega') \overline{Y_n^m(\omega')} d\omega'.$$

It suffices to show that

$$\gamma_n^m = \frac{c_n-1}{\lambda} \int_{S^2} g(\omega') \overline{Y_n^m(\omega')} d\omega'. \quad (\text{A8})$$

Using the definition of Q ,

$$\begin{aligned} \gamma_n^m &= \int_{S^2} \frac{1}{\lambda} \left[\frac{1}{2\pi} \int_{S^2} p(\omega' \cdot \omega'') g(\omega'') d\omega'' \right. \\ &\quad \left. - g(\omega') \right] \overline{Y_n^m(\omega')} d\omega'. \end{aligned} \quad (\text{A9})$$

Inserting Eq. (A2) into Eq. (A9), we find

$$\begin{aligned} \gamma_n^m &= \frac{1}{\lambda} \int_{S^2} \left[\int_{S^2} \sum_{k=0}^{\infty} \frac{2k+1}{4\pi} c_k P_k(\omega' \cdot \omega'') g(\omega'') d\omega'' \right. \\ &\quad \left. - g(\omega') \right] \overline{Y_n^m(\omega')} d\omega'. \end{aligned}$$

Using the addition theorem for spherical harmonics,

$$\begin{aligned} \gamma_n^m &= \frac{1}{\lambda} \int_{S^2} \left[\int_{S^2} \sum_{k=0}^{\infty} \sum_{l=-k}^k c_k Y_k^l(\omega') \overline{Y_k^l(\omega'')} g(\omega'') d\omega'' \right. \\ &\quad \left. - g(\omega') \right] \overline{Y_n^m(\omega')} d\omega'. \end{aligned}$$

The assertion now follows immediately from the orthonormality of the spherical harmonics. ■

We also expand $\Delta_\omega g(\omega)$ into a spherical harmonics series.

Lemma 4: Let $g \in L^2(S^2)$ with $\Delta_\omega g \in L^2(S^2)$. Then

$$\Delta_\omega g(\omega) = - \sum_{n=0}^{\infty} \sum_{m=-n}^n n(n+1) \times \left[\int_{S^2} g(\omega') \overline{Y_n^m(\omega')} d\omega' \right] Y_n^m(\omega).$$

The series converges in $L^2(S^2)$.

Proof: Since $\Delta_\omega g \in L^2(S^2)$,

$$\Delta_\omega g(\omega) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \left[\int_{S^2} \Delta_\omega g(\omega') \overline{Y_n^m(\omega')} d\omega' \right] Y_n^m(\omega).$$

Integration by parts gives

$$\int_{S^2} \Delta_\omega g(\omega') \overline{Y_n^m(\omega')} d\omega' = \int_{S^2} g(\omega') \overline{\Delta_\omega Y_n^m(\omega')} d\omega'.$$

Using Eq. (A7), the assertion follows. ■

We now consider the Fokker–Planck limit, i.e., the limit of infinitely frequent collisions ($\bar{\lambda} \rightarrow 0$) of infinitesimal strength ($\bar{\mu}_0 \rightarrow 1$). Since convergence of the spherical harmonics coefficients is equivalent to weak convergence in $L^2(S^2)$, we conclude from Lemmas 3 and 4:

Lemma 5: In the limit $\bar{\lambda} \rightarrow 0$ and $\bar{\mu}_0 \rightarrow 1$ with $\bar{\lambda}_{tr} = \bar{\lambda}/(1-\bar{\mu}_0) > 0$ fixed, we have

$$Qg \rightarrow \frac{1}{2\bar{\lambda}_{tr}} \Delta_\omega g \quad \text{weakly in } L^2(S^2)$$

for all $g \in L^2(S^2)$ with $\Delta_\omega g \in L^2(S^2)$ if and only if

$$\forall n \quad \frac{c_n - 1}{\bar{\lambda}} \rightarrow - \frac{n(n+1)}{2\bar{\lambda}_{tr}}. \quad (\text{A10})$$

We rewrite this condition in simpler form:

Lemma 6: Condition (A10) is equivalent to

$$\frac{(1-\mu_0)^2}{1-\bar{\mu}_0} \rightarrow 0, \quad (\text{A11})$$

where $(1-\mu_0)^2$ denotes the expected value of $(1-\mu_0)^2$.

Proof: We begin with the identity

$$\frac{c_n - 1}{\bar{\lambda}} = \frac{1}{\bar{\lambda}} \left[\int_{-1}^1 P_n(\mu) p(\mu) d\mu - 1 \right].$$

With the change of variable $\nu = (1-\mu)/(1-\bar{\mu}_0)$,

$$\frac{c_n - 1}{\bar{\lambda}} = \frac{1}{\bar{\lambda}} \left[(1-\bar{\mu}_0) \int_0^{2/(1-\bar{\mu}_0)} P_n(1-\nu(1-\bar{\mu}_0)) \times p(1-\nu(1-\bar{\mu}_0)) d\nu - 1 \right]. \quad (\text{A12})$$

We use Taylor's theorem with remainder to expand $P_n(1-\nu(1-\bar{\mu}_0))$:

$$P_n(1-\nu(1-\bar{\mu}_0)) = P_n(1) - P'_n(1)\nu(1-\bar{\mu}_0) + \frac{1}{2}P''_n(1-\theta\nu(1-\bar{\mu}_0))\nu^2(1-\bar{\mu}_0)^2,$$

where $\theta \in (0,1)$ depends on $\nu(1-\bar{\mu}_0)$. Inserting this into Eq. (A12), using

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

then reversing the change of variable, we obtain

$$\frac{c_n - 1}{\bar{\lambda}} = - \frac{1}{2\bar{\lambda}_{tr}} n(n+1) + E_n,$$

with

$$E_n = \frac{1}{2\bar{\lambda}} \int_{-1}^1 P''_n(1-\theta(1-\mu))(1-\mu)^2 p(\mu) d\mu.$$

Because of Eq. (A6), we conclude

$$|E_n| \leq \frac{(n-1)n(n+1)(n+2)}{16\bar{\lambda}_{tr}} \frac{(1-\mu_0)^2}{1-\bar{\mu}_0}.$$

Therefore (A11) implies (A10).

To show that conversely, (A10) implies (A11), we show that the condition in (A10) for $n=2$ is already equivalent to (A11):

$$\begin{aligned} \lim \frac{c_2 - 1}{\bar{\lambda}} &= - \frac{3}{\bar{\lambda}_{tr}} \\ \Leftrightarrow \lim \frac{1}{\bar{\lambda}_{tr}(1-\bar{\mu}_0)} \left[\int_{-1}^1 \left(\frac{3}{2} \mu^2 - \frac{1}{2} \right) p(\mu) d\mu - 1 \right] &= - \frac{3}{\bar{\lambda}_{tr}} \\ \Leftrightarrow \lim \frac{1}{1-\bar{\mu}_0} \int_{-1}^1 ((1-\mu)^2 + 2\mu - 2) p(\mu) d\mu &= -2 \\ \Leftrightarrow \lim \frac{1}{1-\bar{\mu}_0} \int_{-1}^1 (1-\mu)^2 p(\mu) d\mu &= 0 \\ \Leftrightarrow \lim \frac{(1-\mu_0)^2}{1-\bar{\mu}_0} &= 0. \end{aligned}$$

■

Rewriting the condition in yet another slightly different, clarifying form, we obtain:

Theorem: Let $g \in L^2(S^2)$ with $\Delta_\omega g \in L^2(S^2)$, and let $\bar{\lambda} \rightarrow 0$ and $\bar{\mu}_0 \rightarrow 1$ with $\bar{\lambda}_{tr} = \bar{\lambda}/(1-\bar{\mu}_0) > 0$ fixed. Then

$$Qg \rightarrow \frac{1}{2\bar{\lambda}_{tr}} \Delta_\omega g \quad \text{weakly in } L^2(S^2)$$

if and only if

$$\frac{\text{var}(\mu_0)}{1-\bar{\mu}_0} \rightarrow 0. \quad (\text{A13})$$

Proof: Condition (A13) is equivalent to (A11) because

$$\frac{\text{var}(\mu_0)}{1-\bar{\mu}_0} + (1-\bar{\mu}_0) = \frac{(\bar{\mu}_0 - \mu_0)^2}{1-\bar{\mu}_0} + (1-\bar{\mu}_0) = \frac{(1-\mu_0)^2}{1-\bar{\mu}_0}. \quad (\text{A14})$$

■

This theorem gives a necessary and sufficient condition for weak convergence of Qg to $1/(2\bar{\lambda}_{tr})\Delta_\omega g$. However, if

stronger smoothness assumptions are imposed on g , it is not hard to prove that the condition in fact implies strong convergence in $L^2(S^2)$.

Finally we state and prove a lemma that implies that the difference between the Rutherford and Mott cross sections is not of large importance with regard to the question of validity of the Fokker–Planck approximation.

Lemma 7: Under the assumptions of Lemma 1,

$$\frac{\text{var}(\mu_0)}{1 - \bar{\mu}_0} = O\left(\frac{1}{\ln(1/(-\bar{\mu}_0))}\right)$$

as $\eta \rightarrow 0$.

Proof: Obviously

$$\int_{-1}^1 R(\mu) \frac{(1-\mu)^2}{(1+2\eta-\mu)^2} d\mu = O(1).$$

Since $C(\eta) = O(\eta)$ (see the proof of Lemma 1), and using Eq. (A14), we conclude

$$\text{var}(\mu_0) = O(\eta).$$

Combining this with Lemma 1,

$$\frac{\text{var}(\mu_0)}{1 - \bar{\mu}_0} = O\left(\frac{1}{\ln(1/\eta)}\right).$$

Lemma 1 implies that

$$\ln(1/(1 - \bar{\mu}_0)) = O(\ln(1/\eta)),$$

and therefore Lemma 7 is proved. ■

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