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THE NONCLASSICAL BOLTZMANN EQUATION AND DIFFUSION-BASED APPROXIMATIONS TO THE BOLTZMANN EQUATION*

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Abstract. We show that several diffusion-based approximations (classical diffusion or SP_1, SP_2, SP_3) to the linear Boltzmann equation can (for an infinite, homogeneous medium) be represented *exactly* by a nonclassical transport equation. As a consequence, we indicate a method to solve these diffusion-based approximations to the Boltzmann equation via Monte Carlo methods, with only statistical errors—no truncation errors.

Key words. Boltzmann equation, diffusion approximation, nonclassical transport, Monte Carlo

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1. Introduction.

In the classical theory of linear particle transport, the total cross section Σ_t is independent of the path length s (the distance traveled by the particle since its previous interaction), and of the direction of flight $\mathbf{\Omega}$. In this situation, the probability density function for a particle's distance-to-collision is given by a simple exponential,

$$p(s) = \Sigma_t e^{-\Sigma_t s}. \tag{1}$$

However, in certain inhomogeneous random media in which the locations of the scattering centers are spatially correlated, the particle flux will experience a nonexponential attenuation law. A "nonclassical" theory for this type of transport problem was recently introduced [9], with the assumption that the positions of the scattering centers are correlated but independent of direction. In the case of isotropic scattering, the nonclassical linear Boltzmann equation is writen as

$$\begin{aligned}&\frac{\partial \psi}{\partial s}(\mathbf{x},\mathbf{\Omega},s) + \mathbf{\Omega}\cdot\nabla\psi(\mathbf{x},\mathbf{\Omega},s) + \Sigma_t(s)\psi(\mathbf{x},\mathbf{\Omega},s)\\ &\qquad = \frac{\delta(s)}{4\pi}\left[c\int_{4\pi}\int_0^\infty \Sigma_t(s')\psi(\mathbf{x},\mathbf{\Omega}',s')ds'd\Omega' + Q(\mathbf{x})\right].\end{aligned} \tag{2}$$

Here, c is the scattering ratio (probability of scattering), and $Q(\mathbf{x})$ is a source. The path length distribution

$$p(s) = \Sigma_t(s)e^{-\int_0^s \Sigma_t(s')ds'} \tag{3}$$

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does not have to be exponential. If $p(s)$ is exponential, (2) reduces to the classical Boltzmann equation for the classical angular flux

$$\psi(\mathbf{x}, \mathbf{\Omega}) = \int_0^\infty \psi(\mathbf{x}, \mathbf{\Omega}, s) ds. \tag{4}$$

A full derivation of this nonclassical linear Boltzmann equation and its asymptotic diffusion limit can be found in [10], along with numerical results for an application in two-dimensional (2-D) pebble bed reactor (PBR) cores. Existence and uniqueness of solutions, as well as their convergence to the diffusion equation, are rigorously discussed in [2]. The nonclassical theory was extended in [15] to include angularly dependent path-length distributions in order to investigate anisotropic diffusion of neutrons in three-dimensional (3-D) PBR cores [14, 16].

A similar kinetic equation with path length as an independent variable has been rigorously derived for the periodic Lorentz gas in a series of papers by Golse et al. (cf. [6] for a review), and by Marklof and Strömbergsson (cf. [11]). Furthermore, related work has been performed by Grosjean [7]; it considers a generalization of neutron transport that includes arbitrary path-length distributions, and presents a derivation of diffusion solutions for infinite isotropic point and plane source problems.

In this paper we do not (directly) deal with a random medium. Instead, we show that by selecting $\Sigma_t(s)$ properly, (2) can be converted to an integral equation for the scalar flux

$$\phi_0(\mathbf{x}) = \int_{4\pi} \psi(\mathbf{x}, \mathbf{\Omega}) d\Omega, \tag{5}$$

which is *identical* to the integral equation that can be constructed for several diffusion-based approximations to the *classical* Boltzmann transport equation

$$\mathbf{\Omega} \cdot \nabla \psi(\mathbf{x}, \mathbf{\Omega}) + \Sigma_t \psi(\mathbf{x}, \mathbf{\Omega}) = \frac{\Sigma_s}{4\pi} \int_{4\pi} \psi(\mathbf{x}, \mathbf{\Omega}') d\Omega' + \frac{Q(\mathbf{x})}{4\pi}. \tag{6}$$

More specifically, we show that for an infinite homogeneous medium in which

(i) $\Sigma_s < \Sigma_t$,
(ii) $Q(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$,
(iii) $\psi(\mathbf{x}, \mathbf{\Omega}) \to 0$ as $|\mathbf{x}| \to \infty$,

the classical linear Boltzmann equation (6) and several of its diffusion-based approximations can *all* be exactly represented by the nonclassical Boltzmann equation (2) with a correctly chosen $\Sigma_t(s)$. Moreover, the exact definition of $\Sigma_t(s)$ for each method can be determined (semi-)analytically.

To describe the diffusion-based approximations to the transport equation (6), we integrate (6) over $\mathbf{\Omega}$, defining $\phi(\mathbf{x})$ by (5), and

$$\boldsymbol{\phi}_1(\mathbf{x}) = \int \mathbf{\Omega} \psi(\mathbf{x}, \mathbf{\Omega}) d\Omega = \text{current},$$

to obtain the exact *balance equation*

$$\mathbf{\Omega} \cdot \nabla \boldsymbol{\phi}_1(\mathbf{x}) + \Sigma_t \phi_0(\mathbf{x}) = \Sigma_s \phi_0(\mathbf{x}) + Q(\mathbf{x}). \tag{7}$$

Diffusion-based methods invoke a closure relation, which expresses $\boldsymbol{\phi}_1$ in terms of ϕ_0. The classical diffusion approximation invokes *Fick's Law*,

$$\boldsymbol{\phi}_1(\mathbf{x}) = -\frac{1}{3\Sigma_t} \nabla \phi_0(\mathbf{x}), \tag{8}$$

to give (with $\Sigma_t - \Sigma_s = \Sigma_a$)

$$-\frac{1}{3\Sigma_t}\nabla^2\phi_0(\mathbf{x}) + \Sigma_a\phi_0(\mathbf{x}) = Q(\mathbf{x}). \tag{9}$$

The classical diffusion equation has been generalized to the hierarchy of SP_N equations. A recent and complete review on these equations is given in [12]. The SP_N equations were first derived by Gelbard [3, 4, 5] in an ad hoc way. Theoretical justifications were presented later [8, 13].

In the SP_2 approximation, (9) is generalized to

$$-\frac{1}{3\Sigma_t}\nabla^2\left[\phi_0 + \frac{4}{5\Sigma_t}(\Sigma_a\phi_0 - Q)\right] + \Sigma_a\phi_0 = Q. \tag{10}$$

In the SP_3 approximation, (9) is generalized to the system

$$-\frac{1}{3\Sigma_t}\nabla^2(\phi_0 + 2\phi_2) + \Sigma_a\phi_0 = Q, \tag{11a}$$

$$-\frac{9}{35\Sigma_t}\nabla^2\phi_2 + \Sigma_t\phi_2 = \frac{2}{5}(\Sigma_a\phi_0 - Q). \tag{11b}$$

The work in this paper accomplishes the following:

(i) It demonstrates (for an infinite homogeneous medium) that the original Boltzmann equation *and* the abovementioned diffusion-based approximations to this equation are all special cases of the nonclassical Boltzmann equation. This sheds new light on the various diffusion approximations.

(ii) Since the nonclassical Boltzmann equation (2) can be solved by Monte Carlo methods, the results in these notes show how to solve diffusion-based approximations to the Boltzmann equation via Monte Carlo methods, with only statistical errors—no truncation errors. This has not been done before.

(iii) In connection with (ii), if $p(s)ds =$ the probability that a particle will experience a collision between path length s and $s+ds$ (since the previous collision), then the distance-to-collision s can be sampled by inverse transform sampling from the cumulative distribution function

$$\xi = \int_0^s p(s')ds'. \tag{12}$$

In this paper, we show that for all the diffusion-based methods considered, the forms of $p(s)$ are such that (12) can be *explicitly solved* for s in terms of $\xi =$ (computer-generated) random number, uniformly distributed between 0 and 1. This makes the possibility of using Monte Carlo methods to solve these equations much more realistic.

(iv) Finally, this work shows that nonclassical transport processes have been widely used for many years, without explicit awareness of this. It may make it possible to consider other unknown-at-present applications of nonclassical transport for problems in which the assumptions of classical transport are too limiting.

The remainder of this paper is organized as follows. In section 2 we use the previous work on the nonclassical Boltzmann equation to convert (2) to an integral equation for the scalar flux ϕ_0. In section 3, we use the Green's function for the diffusion operator

$$-\nabla^2\phi + \Sigma_t^2\lambda^2\phi$$

to convert (9) into an integral equation for $\phi_0(\mathbf{x})$. By choosing $\Sigma_t(s)$ correctly, the integral equation obtained in section 2 becomes identical to this (diffusion) integral equation. In sections 4 and 5 we show that the SP_2 and SP_3 approximations to the classical Boltzmann equation can, like the standard diffusion approximation treated in section 3, be represented as nonclassical transport equations. We conclude with a discussion in section 6.

2. Integral equation formulation. To simplify the notation, we define the scattering plus inhomogeneous source (the right-hand side of (2)) by

$$\begin{aligned} S(\mathbf{x}) &= c\int_{4\pi}\int_0^\infty \Sigma_t(s')\psi(\mathbf{x},\mathbf{\Omega}',s')ds'd\Omega' + Q(\mathbf{x}) \\ &= c\int_0^\infty \Sigma_t(s')\phi_0(\mathbf{x},s')ds' + Q(\mathbf{x}) \\ &= cf(\mathbf{x}) + Q(\mathbf{x}), \end{aligned} \tag{13a}$$

where

$$\phi_0(\mathbf{x},s) = \int_{4\pi}\psi(\mathbf{x},\mathbf{\Omega},s)d\Omega = \text{nonclassical scalar flux,} \tag{13b}$$

$$f(\mathbf{x}) = \int_0^\infty \Sigma_t(s')\phi_0(\mathbf{x},s')ds' = \text{collision-rate density.} \tag{13c}$$

Then (2) can be written as

$$\frac{\partial\psi}{\partial s}(\mathbf{x},\mathbf{\Omega},s) + \mathbf{\Omega}\cdot\nabla\psi(\mathbf{x},\mathbf{\Omega},s) + \Sigma_t(s)\psi(\mathbf{x},\mathbf{\Omega},s) = \frac{\delta(s)}{4\pi}S(\mathbf{x}) \tag{14}$$

or, equivalently, as

$$\frac{\partial\psi}{\partial s}(\mathbf{x},\mathbf{\Omega},s) + \mathbf{\Omega}\cdot\nabla\psi(\mathbf{x},\mathbf{\Omega},s) + \Sigma_t(s)\psi(\mathbf{x},\mathbf{\Omega},s) = 0, \quad 0 < s, \tag{15a}$$

with the initial condition

$$\psi(\mathbf{x},\mathbf{\Omega},0) = \frac{S(\mathbf{x})}{4\pi}. \tag{15b}$$

Following [10], we use the method of characteristics to calculate the solution of (15):

$$\psi(\mathbf{x},\mathbf{\Omega},s) = \frac{S(\mathbf{x}-s\mathbf{\Omega})}{4\pi}e^{-\int_0^s \Sigma_t(s')ds'}. \tag{16}$$

Operating on this equation by

$$\int_0^\infty \Sigma_t(s)(\,\cdot\,)ds$$

and using (3), we obtain

$$\int_0^\infty \Sigma_t(s)\psi(\mathbf{x},\mathbf{\Omega},s)ds = \frac{1}{4\pi}\int_0^\infty S(\mathbf{x}-s\mathbf{\Omega})p(s)ds.$$

Next, we operate by $\int_{4\pi}(\,\cdot\,)d\Omega$ and use (13c) to get

$$f(\mathbf{x}) = \int_0^\infty \Sigma_t(s)\phi_0(\mathbf{x}, s)ds = \frac{1}{4\pi}\int_0^\infty \int_{4\pi} S(\mathbf{x} - s\mathbf{\Omega})p(s)d\Omega ds.$$

Now we make the change of spatial variables from the 3-D spherical $(\mathbf{\Omega}, s)$ to the 3-D Cartesian $\mathbf{x}'$ defined by

$$\mathbf{x}' = \mathbf{x} - s\mathbf{\Omega}. \tag{17a}$$

Then

$$s = |\mathbf{x}' - \mathbf{x}| = \text{radial variable}, \tag{17b}$$

$$dV' = dx'dy'dz' = s^2 ds d\Omega, \tag{17c}$$

$$ds d\Omega = \frac{dV'}{s^2} = \frac{dV'}{|\mathbf{x}' - \mathbf{x}|^2}, \tag{17d}$$

and we obtain

$$f(\mathbf{x}) = \int\int\int S(\mathbf{x}')\frac{p(|\mathbf{x}' - \mathbf{x}|)}{4\pi|\mathbf{x}' - \mathbf{x}|^2}dV', \tag{18}$$

where $p(|\mathbf{x}' - \mathbf{x}|)$ and $S(\mathbf{x})$ are given by (3) and (13a), respectively.

For classical particle transport (in which Σ_t is independent of s), we have

$$\begin{aligned} f(\mathbf{x}) &= \int\int\int S(\mathbf{x}')\frac{\Sigma_t e^{-\Sigma_t|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x} - \mathbf{x}'|^2}dV' \\ &= \int\int\int [cf(\mathbf{x}') + Q(\mathbf{x}')]\frac{\Sigma_t e^{-\Sigma_t|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x} - \mathbf{x}'|^2}dV', \end{aligned} \tag{19a}$$

which is equivalent to the classical integral equation for the scalar flux. Hence, (12) for sampling s yields

$$\xi = \int_0^s p(s')ds' = \int_0^s \Sigma_t e^{-\Sigma_t s'}ds' = 1 - e^{-\Sigma_t s}, \tag{19b}$$

which we can rewrite as

$$s = -\frac{1}{\Sigma_t}\ln(1 - \xi). \tag{19c}$$

Equations (19) are all standard results, demonstrating that when $\Sigma_t(s) = \Sigma_t =$ constant, the nonclassical Boltzmann equation reduces to the standard Boltzmann equation. Next, we derive similar results for diffusion-based approximations to (6). These results are *not* standard.

3. Classical diffusion. Let us repeat the statements in the introduction on how diffusion is typically derived: Integrating (6) over $\mathbf{\Omega}$, defining $\phi(\mathbf{x})$ by (5), and

$$\boldsymbol{\phi}_\mathbf{1}(\mathbf{x}) = \int \mathbf{\Omega}\psi(\mathbf{x}, \mathbf{\Omega})d\Omega = \text{current},$$

we obtain the exact balance equation

$$\nabla \cdot \boldsymbol{\phi}_\mathbf{1}(\mathbf{x}) + \Sigma_t\phi(\mathbf{x}) = \Sigma_s\phi(\mathbf{x}) + Q(\mathbf{x}). \tag{20}$$

Diffusion-based methods invoke a closure relation, which expresses $\boldsymbol{\phi_1}$ in terms of ϕ. The classical diffusion aproximation invokes *Fick's Law*,

$$\boldsymbol{\phi_1}(\mathbf{x}) = -\frac{1}{3\Sigma_t}\nabla\phi_0(\mathbf{x}), \tag{21}$$

to give

$$-\frac{1}{3\Sigma_t}\nabla^2\phi_0(\mathbf{x}) + \Sigma_t\phi_0(\mathbf{x}) = \Sigma_s\phi_0(\mathbf{x}) + Q(\mathbf{x}), \tag{22}$$

which is the classical diffusion approximation to (6). (Equation (22) is commonly written in the form

$$-\frac{1}{3\Sigma_t}\nabla^2\phi_0(\mathbf{x}) + \Sigma_a\phi_0(\mathbf{x}) = Q(\mathbf{x}) \tag{23}$$

with $\Sigma_a = \Sigma_t - \Sigma_s$.) If we define $S(\mathbf{x}) = \Sigma_s\phi_0(\mathbf{x}) + Q(\mathbf{x})$, we can rewrite (22) as

$$-\nabla^2\phi_0(\mathbf{x}) + \Sigma_t^2\lambda^2\phi_0(\mathbf{x}) = 3\Sigma_t S(\mathbf{x}), \tag{24}$$

where

$$\lambda^2 = 3.$$

The Green's function for the operator on the left-hand side of (24) is

$$G(|\mathbf{x}-\mathbf{x}'|) = \frac{e^{-\sqrt{3}\Sigma_t|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}. \tag{25}$$

Therefore, we can solve (24) for $\phi_0(\mathbf{x})$ by taking

$$\begin{aligned}\phi_0(\mathbf{x}) &= \int\int\int G(|\mathbf{x}-\mathbf{x}'|)3\Sigma_t S(\mathbf{x}')dV' \\ &= \int\int\int \frac{3\Sigma_t e^{-\sqrt{3}\Sigma_t|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}S(\mathbf{x}')dV' \\ &= \int\int\int \frac{3\Sigma_t|\mathbf{x}-\mathbf{x}'|e^{-\sqrt{3}\Sigma_t|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|^2}S(\mathbf{x}')dV'.\end{aligned}$$

Now we multiply by Σ_t to obtain the collision rate density $f = \Sigma_t\phi_0$:

$$\Sigma_t\phi_0 = \int\int\int \frac{3\Sigma_t^2|\mathbf{x}-\mathbf{x}'|e^{-\sqrt{3}\Sigma_t|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|^2}S(\mathbf{x}')dV'.$$

This result agrees with (18) iff

$$p(s) = 3\Sigma_t^2 s e^{-\sqrt{3}\Sigma_t s}. \tag{26}$$

It is easily confirmed that

$$\int_0^\infty 3\Sigma_t^2 s e^{-\sqrt{3}\Sigma_t s}ds = \int_0^\infty \sqrt{3}\Sigma_t s e^{-\sqrt{3}\Sigma_t s}d(\sqrt{3}\Sigma_t s) = 1,$$

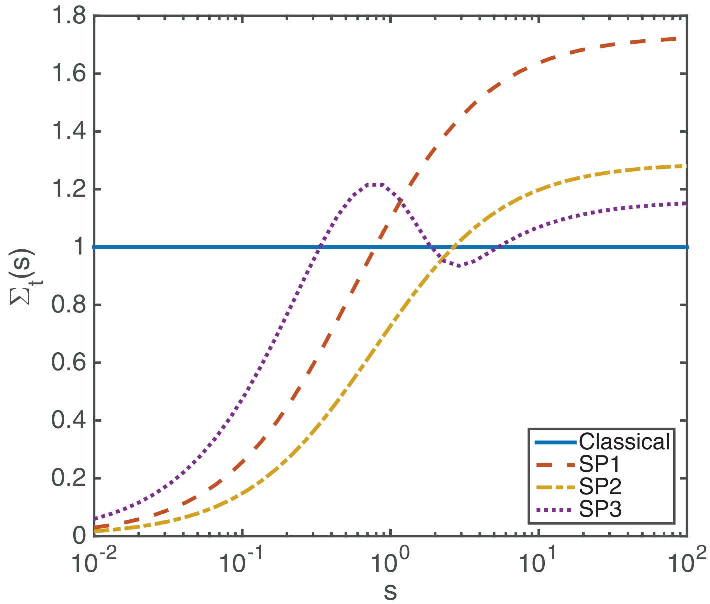

FIG. 1. *Cross section Σ_t as a function of path length s. Comparison of classical transport and diffusion approximations.*

so (26) describes a distribution function. $\Sigma_t(s)$ is given by

$$\Sigma_t(s) = \frac{p(s)}{\int_s^\infty p(s')ds'} = \frac{3\Sigma_t^2 s}{1+\sqrt{3}\Sigma_t s} = \sqrt{3}\Sigma_t \frac{\sqrt{3}\Sigma_t s}{1+\sqrt{3}\Sigma_t s}. \tag{27}$$

Therefore, the nonclassical transport equation reproduces the classical diffusion approximation equation (23) to (2) if $\Sigma_t(s)$ and $p(s)$ are defined by (26) and (27). Both functions are shown in Figures 1 and 2, respectively. This result agrees with the work presented in [1], which uses spherical Fourier transforms to show that $p(s)$ must have the form se^{-s} for diffusion to be an exact transport solution in three dimensions.

We note that the mean distance-to-collision (the mean free path) is

$$\bar{s} = \int_0^\infty sp(s)ds = \int_0^\infty s3\Sigma_t^2 se^{-\sqrt{3}\Sigma_t s}ds = \frac{2}{\sqrt{3}\Sigma_t}. \tag{28}$$

This is greater than $\bar{s} = \Sigma_t^{-1}$ for the original transport equation. Also, s can be sampled by

$$\xi = \int_0^s p(s')ds' = \int_0^s 3\Sigma_t^2 s' e^{-\sqrt{3}\Sigma_t s'}ds' = 1 - (1+\sqrt{3}\Sigma_t s)e^{-\sqrt{3}\Sigma_t s}$$

and thus

$$s = \frac{1}{\sqrt{3}\Sigma_t} f^{-1}(\xi), \tag{29a}$$

where

$$f(z) = (1+z)e^{-z}. \tag{29b}$$

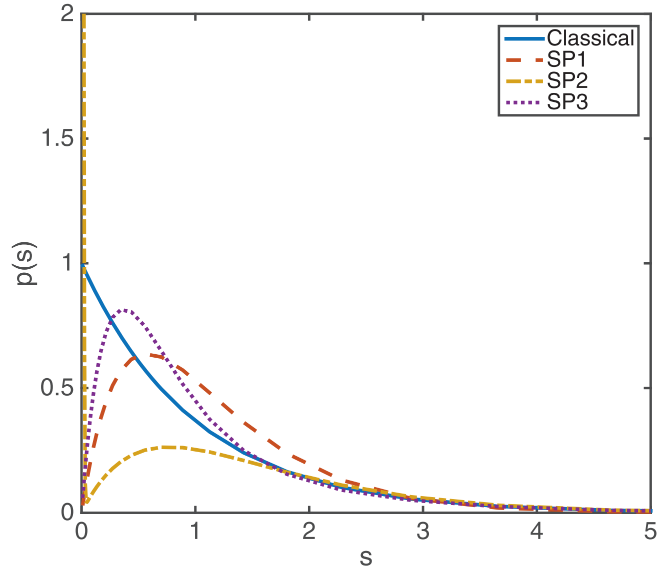

FIG. 2. *Path-length probability density function $p(s)$. Comparison of classical transport and diffusion approximations.*

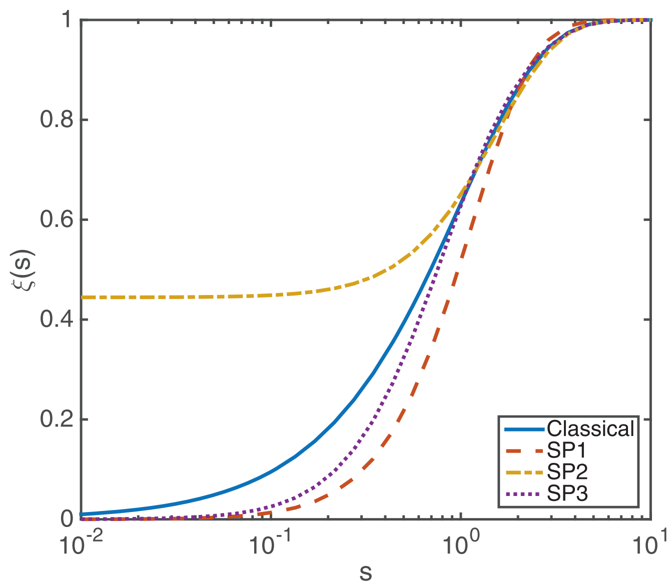

FIG. 3. *Path-length cumulative distribution function $\xi(s)$. Comparison of classical transport and diffusion approximations.*

The function $f(z)$ is monotonic decreasing for $0 < z < \infty$, taking values in $0 < f(z) < 1$. The inverse $f^{-1}(\xi)$ can be precomputed by table, or interpolated, or otherwise computed; we will not consider this here. We show $\xi(s)$ in Figure 3.

4. Simplified P_2 (SP_2). The SP_2 approximation to (6) is

$$-\frac{1}{3\Sigma_t}\nabla^2\left[\phi_0 + \frac{4}{5\Sigma_t}(\Sigma_a\phi_0 - Q)\right] + \Sigma_a\phi_0 = Q. \tag{30}$$

Equivalently,

$$
\begin{aligned}
-\frac{1}{3\Sigma_t}\nabla^2\left(1+\frac{4\Sigma_a}{5\Sigma_t}\right)\phi_0+\Sigma_t\phi_0 &= (\Sigma_s\phi_0+Q)-\frac{4}{15\Sigma_t^2}\nabla^2 Q\\
&= S-\frac{4}{15\Sigma_t^2}\nabla^2[(\Sigma_s\phi_0+Q)-\Sigma_s\phi_0]\\
&= S-\frac{4}{15\Sigma_t^2}\nabla^2 S+\frac{4\Sigma_s}{15\Sigma_t^2}\nabla^2\phi_0,
\end{aligned}
$$

where $S=(\Sigma_s\phi_0+Q)$. Bringing the $\nabla^2\phi_0$ term to the left side, we get

$$
-\nabla^2\left(\frac{1}{3\Sigma_t}+\frac{4\Sigma_a}{15\Sigma_t^2}+\frac{4\Sigma_s}{15\Sigma_t^2}\right)\phi_0+\Sigma_t\phi_0=S-\frac{4}{15\Sigma_t^2}\nabla^2 S
$$

or, since

$$
\frac{1}{3\Sigma_t}+\frac{4}{15}\frac{\Sigma_a+\Sigma_s}{\Sigma_t^2}=\frac{1}{3\Sigma_t}+\frac{4}{15\Sigma_t}=\frac{3}{5\Sigma_t},
$$

we have

$$
-\frac{3}{5\Sigma_t}\nabla^2\phi_0+\Sigma_t\phi_0=S-\frac{4}{15\Sigma_t^2}\nabla^2 S. \tag{31}
$$

Multiplying by $\frac{5\Sigma_t}{3}$, we obtain

$$
\begin{aligned}
-\nabla^2\phi_0+\left(\frac{5}{3}\Sigma_t^2\right)\phi_0 &= \frac{5\Sigma_t}{3}S-\frac{4}{9\Sigma_t}\nabla^2 S\\
&= \frac{5\Sigma_t}{3}S+\frac{4}{9\Sigma_t}\left(-\nabla^2 S+\frac{5}{3}\Sigma_t^2 S-\frac{5}{3}\Sigma_t^2 S\right).
\end{aligned}
$$

Defining

$$
\lambda^2=\frac{5}{3},
$$

we obtain

$$
\begin{aligned}
(-\nabla^2+\Sigma_t^2\lambda^2)\phi_0 &= \left(\frac{5\Sigma_t}{3}-\frac{4}{9\Sigma_t}\frac{5}{3}\Sigma_t^2\right)S+\frac{4}{9\Sigma_t}(-\nabla^2+\Sigma_t^2\lambda^2)S\\
&= \frac{25}{27}\Sigma_t S+\frac{4}{9\Sigma_t}(-\nabla^2+\Sigma_t^2\lambda^2)S.
\end{aligned} \tag{32}
$$

Using the Green's function (25) for $-\nabla^2+\Sigma_t^2\lambda^2$, we get

$$
\phi_0(\mathbf{x})=\frac{25}{27}\Sigma_t\int\int\int GSdV'+\frac{4}{9\Sigma_t}S
$$

or

$$
\Sigma_t\phi_0=\frac{5}{9}(\Sigma_t\lambda)^2\int\int\int GSdV'+\frac{4}{9}S, \tag{33}
$$

where

$$
G(s)=\frac{e^{-\Sigma_t\lambda s}}{4\pi s}. \tag{34}
$$

Now, we use the identity

$$S(\mathbf{x}) = \int_0^\infty S(\mathbf{x}+s\boldsymbol{\Omega})\delta(s)ds = \frac{1}{4\pi}\int_{4\pi}\int \delta(s)S(\mathbf{x}+s\boldsymbol{\Omega})dsd\Omega$$
$$= \int_{4\pi}\int \frac{\delta(|\mathbf{x}-\mathbf{x}'|)}{4\pi}\frac{S(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}dV',$$

(where $\mathbf{x}' = \mathbf{x}+s\boldsymbol{\Omega}$, $|\mathbf{x}-\mathbf{x}'| = s$, $s^2dsd\Omega = dV'$) to obtain, from (31),

$$\Sigma_t\phi_0(\mathbf{x}) = \frac{5}{9}\int\int\int \frac{\Sigma_t^2\lambda^2|\mathbf{x}-\mathbf{x}'|e^{-\Sigma_t\lambda|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|^2}S(\mathbf{x}')dV' + \frac{4}{9}\int\int\int \frac{\delta(|\mathbf{x}-\mathbf{x}'|)}{4\pi|\mathbf{x}-\mathbf{x}'|^2}S(\mathbf{x}')dV'. \tag{35}$$

This implies that for the SP_2 equation,

$$p(s) = \frac{5}{9}\Sigma_t^2\lambda^2 se^{-\Sigma_t\lambda s} + \frac{4}{9}\delta(s), \tag{36a}$$

where

$$\lambda = \sqrt{\frac{5}{3}}. \tag{36b}$$

Thus, with probability $\frac{4}{9}$, a particle that scatters at a point $\mathbf{x}$ undergoes its next "collision" at the same point. Each time a particle experiences a collision (even if it has not moved), it has the probability of being absorbed (with probability Σ_a/Σ_t).

From (27), we have, for $s > 0$,

$$\Sigma_t(s) = \frac{p(s)}{\int_s^\infty p(s')ds'} = \frac{\Lambda^2 se^{-\Lambda s}}{\int_s^\infty \Lambda^2 s'e^{-\Lambda s'}ds'} = \frac{\Lambda^2 s}{1+\Lambda s}, \tag{37}$$

where $\Lambda = \Sigma_t\lambda$. Also, for $s \approx 0$, (26) and (36) give

$$\Sigma_t(s) \approx \frac{4}{9}\delta(s). \tag{38}$$

This agrees with the physical interpretation that

$$\Sigma_t(0)ds = \frac{4}{9} = \text{the probability that a particle at } s = 0 \text{ will experience a collision.}$$

Equations (37) and (38) can be written more compactly as

$$\Sigma_t(s) = \frac{\frac{4}{9}\delta(s) + \Lambda^2 s}{1+\Lambda s}. \tag{39}$$

The mean free path is

$$\bar{s} = \int_0^\infty sp(s)ds = \int_0^\infty s\left[\frac{5}{9}\Lambda^2 se^{-\Lambda s} + \frac{4}{9}\delta(s)\right]ds = \frac{10}{9\Lambda} = \frac{10}{9}\sqrt{\frac{3}{5}}\frac{1}{\Sigma_t} = \sqrt{\frac{20}{27}}\frac{1}{\Sigma_t}. \tag{40}$$

This result is less than the physically correct $\frac{1}{\Sigma_t}$.

Finally, the distance-to-collision can be sampled using

$$\begin{aligned} \xi &= \int_0^s p(s')ds' = \int_0^s \left[\frac{4}{9}\delta(s') + \frac{5}{9}\Lambda^2 s' e^{-\Lambda s'}\right] ds' \\ &= \frac{4}{9} + \frac{5}{9}\left[1 - (1+\Lambda s)e^{-\Lambda s}\right] = 1 - \frac{5}{9} f(\Lambda s), \end{aligned} \tag{41a}$$

where

$$f(z) = (1+z)e^{-z} \tag{41b}$$

was introduced earlier (in equation (29b)). Thus, for $0 \le \xi \le \frac{4}{9}$, $s = 0$. For $\xi > \frac{4}{9}$, (41a) gives

$$\begin{aligned} &\frac{5}{9} f(\Lambda s) = 1 - \xi \\ &\quad \Rightarrow \xi = \sqrt{\frac{3}{5}}\frac{1}{\Sigma_t} f^{-1}\left(\frac{9}{5}(1-\xi)\right). \end{aligned}$$

Equivalently,

$$s = \begin{cases} 0, & 0 \le \xi \le \frac{4}{9}, \\ \sqrt{\frac{3}{5}}\frac{1}{\Sigma_t} f^{-1}\left(\frac{9}{5}(1-\xi)\right), & \frac{4}{9} < \xi \le 1. \end{cases} \tag{42}$$

Again, (42) states that with probability $\frac{4}{9}$, a particle will suffer its next collision at the precise location of the previous one. Each time a particle experiences a collision (whether it moves or not) it is subject to absorption, with probability Σ_a/Σ_t. The functions $\Sigma_t(s)$, $p(s)$, and $\xi(s)$ are shown in Figures 1–3.

5. Simplified P_3 (SP_3). The SP_3 approximation to (6) consists of the following two coupled equations:

$$-\frac{1}{3\Sigma_t}\nabla^2(\phi_0 + 2\phi_2) + \Sigma_t\phi_0 = S, \tag{43a}$$

$$-\frac{9}{35\Sigma_t}\nabla^2\phi_2 + \Sigma_t\phi_2 = \frac{2}{5}(\Sigma_t\phi_0 - S), \tag{43b}$$

where

$$S(\mathbf{x}) = \Sigma_s\phi_0(\mathbf{x}) + Q(\mathbf{x}). \tag{43c}$$

To demonstrate that the SP_3 equations can be represented as a nonclassical transport process, we must calculate the Green's function for (43). These functions satisfy

$$-\frac{1}{3\Sigma_t}\nabla^2(G_0 + 2G_2) + \Sigma_t G_0 = \delta(\mathbf{x}), \tag{44a}$$

$$-\frac{9}{35\Sigma_t}\nabla^2 G_2 + \Sigma_t G_2 - \frac{2}{5}\Sigma_t G_0 = -\frac{2}{5}\delta(\mathbf{x}), \tag{44b}$$

where G_0 and G_2 are functions of $r = |\mathbf{x}|$ and, when found, they enable (43) to be written

$$\phi_0(\mathbf{x}) = \int\int\int G_0(|\mathbf{x} - \mathbf{x}'|)S(\mathbf{x}')dV', \tag{45a}$$

$$\phi_2(\mathbf{x}) = \int\int\int G_2(|\mathbf{x} - \mathbf{x}'|)S(\mathbf{x}')dV'. \tag{45b}$$

Equation (45b) is not needed, but (45a) is needed to show the desired result.

We know that

$$G(r) = \frac{e^{-\Sigma_t \lambda r}}{4\pi r} \tag{46a}$$

is the Green's function for the operator $-\nabla^2 + \Sigma_t^2\lambda^2$, i.e., it satisfies

$$-\nabla^2 G + \Sigma_t^2\lambda^2 G = \delta(\mathbf{x}). \tag{46b}$$

More specifically, we have the following.

1. For $r > 0$, $G(r)$ satisfies

$$-\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial G}{\partial r} + \Sigma_t^2\lambda^2 G = 0. \tag{47a}$$

2. Also, if we integrate (46b) over $|x| \le \varepsilon$,

$$-\int_{|\mathbf{x}|\le\varepsilon} \nabla\cdot\nabla G dV = -\int_{|\mathbf{x}|=\varepsilon} \mathbf{n}\cdot\nabla G dS = -(4\pi\varepsilon^2)\frac{\partial G}{\partial r}(\varepsilon), \tag{47b}$$

and let $\varepsilon \to 0$, we get

$$\lim_{\varepsilon\to 0}\left(-4\pi\varepsilon^2 \frac{\partial G}{\partial r}(\varepsilon)\right) = 1. \tag{47c}$$

The right side of (47b) is the rate at which the δ-function source emits particles at $\mathbf{x} = 0$. The left side of this equation is the net rate at which particles leak away from the point $\mathbf{x} = 0$.

It is easily verified that $G(r)$ defined by (46a) satisfies equations (47a) and (47c).

To solve (44), we seek two functions, $G_0(r)$ and $G_2(r)$, satisfying

1. for $0 < r < \infty$,

$$-\frac{1}{3\Sigma_t}\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}(G_0 + 2G_2) + \Sigma_t G_0 = 0, \tag{48a}$$

$$-\frac{9}{35\Sigma_t}\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} G_2 + \Sigma_t G_2 - \frac{2}{5}\Sigma_t G_0 = 0; \tag{48b}$$

2.

$$-\frac{1}{3\Sigma_t}\lim_{\varepsilon\to 0}\left[(4\pi\varepsilon^2)\left(\frac{\partial G_0}{\partial r}(\varepsilon) + 2\frac{\partial G_2}{\partial r}(\varepsilon)\right)\right] = 1, \tag{49a}$$

$$-\frac{9}{35\Sigma_t}\lim_{\varepsilon\to 0}\left[(4\pi\varepsilon^2)\frac{\partial G_2}{\partial r}(\varepsilon)\right] = -\frac{2}{5}. \tag{49b}$$

Note that (49a) and (49b) were obtained by operating on (44) by

$$\lim_{\varepsilon\to 0}\int_{|\mathbf{x}|\le\varepsilon}(\cdot)dV.$$

To satisfy (48), we seek solutions of these equations of the form

$$G_0(r) = \frac{e^{-\Sigma_t\lambda r}}{4\pi r}, \tag{50a}$$

$$G_2(r) = a\frac{e^{-\Sigma_t\lambda r}}{4\pi r}, \tag{50b}$$

where λ and a are constants to be determined. Using

$$\nabla^2 \left(\frac{e^{-\Sigma_t \lambda r}}{4\pi r} \right) = \Sigma_t^2 \lambda^2 \left(\frac{e^{-\Sigma_t \lambda r}}{4\pi r} \right),$$

(48a) and (48b) yield

$$-\frac{1}{3\Sigma_t}[\Sigma_t^2 \lambda^2 + 2a\Sigma_t^2 \lambda^2] + \Sigma_t = 0,$$
$$-\frac{9}{35\Sigma_t}[\Sigma_t^2 \lambda^2 a] + \Sigma_t a - \frac{2}{5}\Sigma_t = 0,$$

or

$$-\frac{1}{3}(1+2a)\lambda^2 + 1 = 0,$$
$$-\frac{9}{35} a\lambda^2 + a = \frac{2}{5}.$$

The second of these equations gives

(51a) $$a = \frac{14}{35 - 9\lambda^2},$$

and then the first gives

(51b) $$-\frac{1}{3}\left(1 + \frac{28}{35 - 9\lambda^2}\right)\lambda^2 + 1 = 0.$$

Simple manipulations of (51b) give

$$0 = 3\lambda^4 - 30\lambda^2 + 35.$$

This equation has two solutions:

$$(\lambda^\pm)^2 = 5 \pm 2\sqrt{\frac{10}{3}} \approx 5 \pm 3.651484.$$

Taking the positive square roots, we get

(52a) $$\lambda^+ = 2.941340,$$

(52b) $$\lambda^- = 1.161256.$$

Note that for the classical diffusion equation treated in section 3, $\lambda = \sqrt{3}$, and

$$\mu = \frac{1}{\lambda} = \frac{1}{\sqrt{3}} = 0.577350$$

is the positive value of μ in the S_2 Gauss–Legendre quadrature set. For (52a) arising from the SP_3 equations,

$$\mu^+ = \frac{1}{\lambda^+} = 0.339981,$$
$$\mu^- = \frac{1}{\lambda^-} = 0.861137$$

are the two positive values of μ in the S_4 Gauss–Legendre quadrature set.

Introducing (52) into (51a), we get

$$a^+ = \frac{14}{35 - 9(2.941340)^2} = -0.326619, \tag{53a}$$

$$a^- = \frac{14}{35 - 9(1.161256)^2} = 0.612334. \tag{53b}$$

Thus, we have found two solutions of (48) of the form defined by (50): one for λ^+ and a^+ defined by (52a) and (53a); the other for λ^- and a^- defined by (52b) and (53b). The general solution is a linear combination of these two solutions, e.g.,

$$G_0(r) = \Sigma_t A^+ \left(\frac{e^{-\Sigma_t \lambda^+ r}}{4\pi r} \right) + \Sigma_t A^- \left(\frac{e^{-\Sigma_t \lambda^- r}}{4\pi r} \right), \tag{54a}$$

$$G_2(r) = \Sigma_t A^+ a^+ \left(\frac{e^{-\Sigma_t \lambda^+ r}}{4\pi r} \right) + \Sigma_t A^- a^- \left(\frac{e^{-\Sigma_t \lambda^- r}}{4\pi r} \right), \tag{54b}$$

where the constants A^+ and A^- are determined by (49). Inserting (54) into (49), we get

$$A^+ a^+ + A^- a^- = -\frac{14}{9}, \tag{55a}$$

$$A^+ + A^- = \frac{55}{9}. \tag{55b}$$

Solving these equations for A^+ and A^-, we obtain

$$A^+ = 5.642025. \tag{56a}$$

$$A^- = 0.469086. \tag{56b}$$

Thus, the Green's function for the scalar flux $G_0(r)$ is given by (54a), with $\lambda^\pm$ defined by (52) and $A^\pm$ by (56):

$$G_0(r) = \frac{\Sigma_t}{4\pi r} \left[A^+ e^{-\Sigma_t \lambda^+ r} + A^- e^{-\Sigma_t \lambda^- r} \right]. \tag{57}$$

Equation (45a) now gives

$$\begin{aligned} \Sigma_t \phi_0(\mathbf{x}) &= \int\int\int \Sigma_t G_0(|\mathbf{x} - \mathbf{x}'|) S(\mathbf{x}') dV' \\ &= \int\int\int \frac{\Sigma_t^2 |\mathbf{x} - \mathbf{x}'| \left[A^+ e^{-\Sigma_t \lambda^+ |\mathbf{x} - \mathbf{x}'|} + A^- e^{-\Sigma_t \lambda^- |\mathbf{x} - \mathbf{x}'|} \right] S(\mathbf{x}')}{4\pi |\mathbf{x} - \mathbf{x}'|^2} dV', \end{aligned}$$

and this agrees with (18) if we define

$$p(s) = \Sigma_t^2 s \left(A^+ e^{-\Sigma_t \lambda^+ s} + A^- e^{-\Sigma_t \lambda^- s} \right), \qquad 0 \le s < \infty. \tag{58}$$

To confirm that this legitimately defines a distribution function, we can easily calculate

$$\int_0^\infty \Sigma_t^2 s \left(A^+ e^{-\Sigma_t \lambda^+ s} + A^- e^{-\Sigma_t \lambda^- s} \right) ds = \frac{A^+}{(\lambda^+)^2} + \frac{A^-}{(\lambda^-)^2} = 1.$$

Thus,

$$\int_0^\infty p(s)ds = 1,$$

as required.

Next, one can easily obtain

$$\begin{aligned}\int_s^\infty p(s')ds' &= \int_s^\infty \Sigma_t^2 s' \left(A^+ e^{-\Sigma_t\lambda^+ s'} + A^- e^{-\Sigma_t\lambda^- s'}\right) ds' \\ &= A^+ \left(\frac{1+\Sigma_t\lambda^+ s}{(\lambda^+)^2}\right) e^{-\Sigma_t\lambda^+ s} + A^- \left(\frac{1+\Sigma_t\lambda^- s}{(\lambda^-)^2}\right) e^{-\Sigma_t\lambda^- s}.\end{aligned}$$

Therefore,

$$\Sigma_t(s) = \frac{p(s)}{\int_s^\infty p(s')ds'} = \frac{A^+(\Sigma_t^2 s)e^{-\Sigma_t\lambda^+ s} + A^-(\Sigma_t^2 s)e^{-\Sigma_t\lambda^- s}}{A^+\left(\frac{1+\Sigma_t\lambda^+ s}{(\lambda^+)^2}\right)e^{-\Sigma_t\lambda^+ s} + A^-\left(\frac{1+\Sigma_t\lambda^- s}{(\lambda^-)^2}\right)e^{-\Sigma_t\lambda^- s}}. \tag{59}$$

For $\Sigma_t s \gg 1$,

$$e^{-\Sigma_t\lambda^+ s} \ll e^{-\Sigma_t\lambda^- s},$$

and (59) reduces to

$$\Sigma_t(s) = \frac{\Sigma_t^2 s}{1+\Sigma_t\lambda^- s}(\lambda^-)^2 \approx \Sigma_t\lambda^- \approx 1.161256\Sigma_t \qquad (s\to\infty). \tag{60}$$

This result is more accurate than the "diffusion" value of $\sqrt{3}\Sigma_t = 1.732051\Sigma_t$.

The SP_3 mean free path is

$$\begin{aligned}\bar{s} &= \int_0^\infty sp(s)ds = \int_0^\infty \Sigma_t^2 s^2 \left(A^+ e^{-\Sigma_t\lambda^+ s} + A^- e^{-\Sigma_t\lambda^- s}\right) ds \\ &= \frac{1}{\Sigma_t}\left(\frac{2A^+}{(\lambda^+)^3} + \frac{2A^-}{(\lambda^-)^3}\right) \\ &= \frac{1.042533}{\Sigma_t}.\end{aligned} \tag{61}$$

This result is much closer to the "correct" value of Σ_t^{-1} than either the diffusion result (28) or the SP_2 result (40).

Finally, the distance-to-collision s can be sampled by the formula

$$\begin{aligned}\xi &= \int_0^s p(r)dr = \int_0^s \left[\Sigma_t^2 r \left(A^+ e^{-\Sigma_t\lambda^+ r} + A^- e^{-\Sigma_t\lambda^- r}\right)\right] dr \\ &= \frac{A^+}{(\lambda^+)^2}\left[1-(1+\Sigma_t\lambda^+ s)e^{-\Sigma_t\lambda^+ s}\right] + \frac{A^-}{(\lambda^-)^2}\left[1-(1+\Sigma_t\lambda^- s)e^{-\Sigma_t\lambda^- s}\right] \\ &= F(\Sigma_t s), \qquad 0 < s < \infty.\end{aligned} \tag{62}$$

The function F can be tabulated to efficiently give

$$s = \frac{1}{\Sigma_t} F^{-1}(\xi). \tag{63}$$

Again, the functions $\Sigma_t(s)$, $p(s)$, and $\xi(s)$ are shown in Figures 1–3.

6. Discussion. In this paper we have shown that for an infinite homogeneous medium, three diffusion-based approximations to the standard steady-state linear Boltzmann equation (classical diffusion, SP_2, and SP_3) can each be represented *exactly* by a nonclassical transport equation with a nonconstant $\Sigma_t(s)$. (For the standard Boltzmann equation, $\Sigma_t(s) = \Sigma_t =$ constant, independent of s.) The practical value of the approximate diffusion-based methods is that they are traditionally formulated without use of the angular variable $\mathbf{\Omega}$, making them much less expensive to simulate than the original Boltzmann equation. For each diffusion approximation, we derived an explicit expression for the path-length distribution $p(s)$ and showed that as one progresses from diffusion to SP_2 to SP_3, the corresponding scattering cross section $\Sigma_t(s)$ increasingly better approximates the constant Σ_t of the Boltzmann equation (see Figure 1). This is because the classical exponential distribution is approximated better and better (see Figure 2). As a result, we have seen that the mean free path is approximated with increasing accuracy. As a side note, we remark that the second moment of the path length distribution $\int_0^\infty s^2 p(s) ds$ for all diffusion approximations gives the exact transport value $\frac{2}{\Sigma_t^2}$. However, we do not see a systematic reason why this should be the case.

These results give theoretical insight into the properties of the approximate methods. The results also make it possible—in principle—to consistently simulate diffusion, SP_2, and SP_3 problems using a Monte Carlo method in which the distance-to-collision is determined by a nonexponential distribution function. However, before this can be done for realistic problems, the theory in this paper must be generalized in two ways.

First, the theory must be extended to heterogeneous media in such a way that the interface conditions for the nonclassical Boltzmann equation at material interfaces are consistent with the interface conditions used for the relevant diffusion approximations. The "natural" interface condition for the nonclassical Boltzmann equation would seem to be that for each $\mathbf{x}$ and $\mathbf{\Omega}$, the nonclassical angular flux should be a continuous function of s. Presumably, this (or some other) condition is consistent with the standard approximate interface conditions.

Second, the theory in this paper must be extended to finite media. For such problems, boundary conditions for the nonclassical angular flux on the outer boundary of the system must be formulated in a way that is consistent with standard outer boundary conditions to the relevant diffusion approximation. Specifically, what should the assigned value of s be for particles that enter the system from the exterior? The choice $s = 0$ is intuitively appealing but is not necessarily correct.

This work must be done in order for the representation of the diffusion-based approximations to the Boltzmann equation by nonclassical Boltzmann equations to become "complete." When this happens, it will be possible to interpret these approximations as being fully equivalent to nonclassical transport processes, and to employ Monte Carlo methods to directly simulate them. However, these remaining tasks must be left for future work.

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