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The Equivalence of "Forward" and "Backward" Nonclassical Particle Transport Theories

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Abstract - *In this paper, two distinct "nonclassical" particle transport theories – in which the distribution function $P(s)$ for the distance s between collisions is not exponential – are discussed. The two nonclassical theories were developed to describe different physical problems, and the mathematical transport equations that arise from the two theories are different. Nonetheless, we show in this paper that by means of a physically-motivated transformation, it is possible to derive one of the theories from the other. Our analysis also includes boundary conditions for finite media; previous publications on nonclassical transport have usually only considered infinite media.*

I. INTRODUCTION

During the previous decade, two distinct "nonclassical" theories of particle transport – in which the distance-to-collision is not exponential – have been independently and almost simultaneously developed. Both new theories require an "expanded" phase space that includes an extra independent variable $s \geq 0$, having the dimension of space. In this paper, we show that under certain circumstances, the two theories are mathematically equivalent.

The two nonclassical theories were developed to mathematically model different problems. One of the theories was proposed to model an ensemble-averaged particle transport process in a statistically random medium [1, 2, 3, 4, 5, 6, 7, 8]. [An often-considered random medium consists of a specific solid material containing randomly-distributed holes, or "voids," which can have random sizes and shapes. Systems of this type would be (i) a block of Swiss cheese, (ii) a container of boiling water at an instant in time, or (iii) a large dense fog or cloud. This is the type of random system considered in this paper.] For each specific realization of this system, the distance-to-collision is a piecewise exponential function, but the ensemble-averaged distance-to-collision distribution function $P(s)$, where s is the distance between collisions, is not exponential or piecewise-exponential. The idea underlying this theory is to develop a particle transport equation in which the distribution function for the distance-to-collision is equal to the non-exponential $P(s)$, while the collision process is consistent with the correct physics. [If a particle experiences a collision in the solid-with-random-voids, the collision must occur in the solid. Therefore, the scattering law for the solid should determine the scattering term in the nonclassical transport equation.]

The resulting nonclassical theory preserves the correct ensemble-averaged $P(s)$ and the correct scattering physics, but in no other sense is this theory known to be exact. The nonclassical transport equation arising from this approach was hypothesized; it was not derived by a rigorous mathematical procedure. In this nonclassical equation, s is interpreted as the distance *from the previous* collision, so we refer to this theory as the *backward* nonclassical transport theory.

The other nonclassical theory arose by examining particle transport problems in which the locations of the scattering centers are not random – but instead, are located on a fixed, spatially periodic grid – and taking a suitable "Boltzmann-Grad" limit in which the the size of the scattering centers and the distance between them simultaneously shrink to zero [9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. In the resulting theory, s is physically interpreted as the distance *to the next* collision, so we refer to this theory as the *forward* nonclassical transport theory. The stated motivation for the development of this theory was that the researchers wanted to understand the effect that would occur in kinetic theory if it could not be assumed that the locations of the scattering centers occur randomly in space, but rather, are strongly correlated: "The periodic Lorentz gas ... is one example of this type of situation. Assuming that heavy particles [scattering centers] are located at the vertices of some lattice in the Euclidean space clearly introduces about the maximum amount of correlation between these heavy particles. This periodicity assumption entails a dramatic change in the structure of the equation that one obtains under the same scaling limit that would otherwise lead to a linear Boltzmann equation" [16]. The new equation obtained in this work is sometimes called a "generalized" Boltzmann equation. In this paper, we refer to it as the "forward nonclassical" Boltzmann equation.

(*Note*: The Boltzmann-Grad limit of a periodic Lorentz gas does not perfectly model any common physical system. Presumably, one could consider more realistic intermediate scenarios in which the positions of the scattering centers are random but correlated. However, this more difficult problem has not been studied yet.)

Mathematically, the forward and backward nonclassical transport theories are described by (different) linear transport equations on an expanded phase space that includes the extra independent variable s, which has a different interpretation in the two theories. In a recent PhD thesis [19], Krycki showed that for infinite medium problems, the backward nonclassical problem is similar to the adjoint of the forward nonclassical problem. However, the forward and backward nonclassical equations are not strict adjoints of each other, and until now, it was not known whether these two equations were related to each other in a precise way.

The purpose of this paper is to go beyond Krycki's result and show that for finite-medium problems with suitably prescribed internal sources and incident boundary fluxes, (i) the forward nonclassical transport problem can be directly derived from the backward nonclassical transport problem, by means of a physically-motivated transformation, and (ii) the solutions of the forward and backward problems yield the same physical reaction rates at which particles collide with the scattering centers.

Thus, the analysis in this paper shows that although the forward and backward problems are described by different mathematical equations that have different solutions, the two theories are basically equivalent. Also, this paper is the first to consider boundary conditions for nonclassical transport. Previous papers on nonclassical transport methods have treated only infinite media. (The analysis in this paper does not require a finite medium; the medium can be infinite.)

The remainder of this paper is organized as follows. In Section II we establish notation by describing a "classical" transport problem for a homogeneous, monoenergetic, isotropically-scattering system. For this problem, the distribution function for distance-to-collision is exponential [see Eq. (3)]. In Section III we describe the "backward" nonclassical transport equation, which is based on the classical problem from Sec. II but contains the extra independent variable s and the non-exponential distribution function $P(s)$. Section IV presents the "forward" nonclassical transport equation, which also contains s and $P(s)$. In Section V, we show that when $P(s)$ is exponential, the two nonclassical Eqs. (8) and (13) reduce to the classical transport Eqs. (1). In Section VI we formulate and use a physically-motivated transformation to derive the Forward Nonclassical Transport Problem [Eqs. (13)] from the Backward Nonclassical Transport Problem [Eqs. (8)]. A concluding discussion is given in Section VII.

II. A CLASSICAL TRANSPORT PROBLEM

To set the stage, let us consider a specified 3D physical domain V, containing a known internal isotropic source $Q(\boldsymbol{x})$ and a known incident boundary angular flux $\Psi^b(\boldsymbol{x},\boldsymbol{\Omega})$. For simplicity, the transport process in V is assumed to be monoenergetic, with isotropic scattering. (The inclusion of energy-dependence and anisotropic scattering would be straightforward.) If Σ_t = total cross section and Σ_s = scattering cross section, the classical Boltzmann transport equation and boundary condition for the angular flux $\Psi(\boldsymbol{x},\boldsymbol{\Omega})$ are given by:

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\Psi(\boldsymbol{x},\boldsymbol{\Omega})+\Sigma_t\Psi(\boldsymbol{x},\boldsymbol{\Omega})=\frac{1}{4\pi}\Big[\Sigma_s\Phi(\boldsymbol{x})+Q(\boldsymbol{x})\Big]\,,\quad \boldsymbol{x}\in V\,,\ \ \boldsymbol{\Omega}\in 4\pi\,, \tag{1a}$$

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega})=\Psi^b(\boldsymbol{x},\boldsymbol{\Omega})\,,\qquad \boldsymbol{x}\in\partial V\,,\ \ \boldsymbol{\Omega}\cdot\boldsymbol{n}<0\,, \tag{1b}$$

where

$$\Phi(\boldsymbol{x})=\int_{4\pi}\Psi(\boldsymbol{x},\boldsymbol{\Omega}')d\Omega'=\text{scalar flux}\,. \tag{2}$$

For the classic transport process described by Eqs. (1), the distribution function for the distance-to-collision s is easily shown to be exponential:

$$P_0(s)=\Sigma_t e^{-\Sigma_t s}\,,\quad 0\le s<\infty\,. \tag{3}$$

If V were to consist of disjoint homogeneous subregions, the only change to Eq. (1a) would be that Σ_t and Σ_s would become piecewise constant functions of $\boldsymbol{x}$. In this situation, the distribution function for distance-to-collision would become piecewise-exponential, and space- and angle-dependent:

$$P_0(\boldsymbol{x},\boldsymbol{\Omega},s)=\Sigma_t(\boldsymbol{x}+s\boldsymbol{\Omega})e^{-\int_0^s\Sigma_t(\boldsymbol{x}+s'\boldsymbol{\Omega})ds'}\,. \tag{4}$$

III. "BACKWARD" NONCLASSICAL PROBLEM

If the physical system V were to become a random union of disjoint homogeneous subregions, and the distribution function $P_0(\boldsymbol{x},\boldsymbol{\Omega},s)$ were to be ensemble-averaged over all possible realizations of the random system, the resulting distribution function would become a non-piecewise-exponential function:

$$P(s)=\langle P_0(\boldsymbol{x},\boldsymbol{\Omega},s)\rangle\,, \tag{5}$$

where $\langle\cdot\rangle$ denotes "ensemble average," and we have assumed that the ensemble-averaging process is sufficiently random and uniform to remove all space and angle-dependence from $\langle P_0(\boldsymbol{x},\boldsymbol{\Omega},s)\rangle$.

It has been shown [1, 2] that a particle transport process, having (non-exponential) $P(s)$ as its distribution function for distance to collision, has an s-dependent total cross section $\Sigma_t(s)$ satisfying:

$\Sigma_t(s)ds$ = the probability that a particle, having traveled path length s since initiating a flight path, will collide with a scattering center while traveling the extra path length ds . (6)

Here, a particle specifically "initiates a flight path" at the instant (i) it is born in V from the internal source Q, (ii) it enters V through the outer boundary ∂V, or (iii) it scatters. At these instants, s = the path length the particle has traveled = 0, and s increases in a timelike manner as the particle streams along its flight path. The path-length-dependent $\Sigma_t(s)$ and non-exponential $P(s)$ are related by:

$$\Sigma_t(s)=\frac{P(s)}{\int_s^\infty P(s')ds'}\,, \tag{7a}$$

and

$$P(s)=\Sigma_t(s)e^{-\int_0^s\Sigma_t(s')ds'}\,. \tag{7b}$$

A "nonclassical" transport problem describing this transport process, applied to the problem described by Eqs. (1), was formulated in [1, 2] as:

$$\frac{\partial f}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s)+\boldsymbol{\Omega}\cdot\nabla f(\boldsymbol{x},\boldsymbol{\Omega},s)+\Sigma_t(s)f(\boldsymbol{x},\boldsymbol{\Omega},s)=\frac{\delta(s)}{4\pi}F(\boldsymbol{x})\,,\quad \boldsymbol{x}\in V\,,\ \ \boldsymbol{\Omega}\in 4\pi\,,\ \ 0<s\,, \tag{8a}$$

$$F(\boldsymbol{x})=c\int_{4\pi}\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega}')}\Sigma_t(s')f(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'd\Omega'+Q(\boldsymbol{x})\,. \tag{8b}$$

This equation is supplemented with the boundary condition:

$$f(\boldsymbol{x},\boldsymbol{\Omega},s)=\Psi^b(\boldsymbol{x},\boldsymbol{\Omega})\delta(s)\,,\quad \boldsymbol{x}\in\partial V\,,\ \ \boldsymbol{\Omega}\cdot\boldsymbol{n}<0\,,\ \ 0<s\,. \tag{9}$$

In Eqs. (8a) and (9), $\delta(s)$ is the usual delta function. In Eq. (8b),

$$c = \text{scattering ratio} = \text{probability that when a particle collides with a scattering center, the particle will scatter} \ , \qquad (10)$$

and

$$\ell(\boldsymbol{x}, \boldsymbol{\Omega}) = \text{the distance from } \boldsymbol{x} \text{ to } \partial V \text{ in the direction of } -\boldsymbol{\Omega} \ \ [\text{see Fig. 1}] \ . \qquad (11)$$

In Eqs. (8), all particles initiate flight paths (from either the boundary source, the internal source, or the scattering source) with $s = 0$. As a particle streams away from the beginning of its flight path, the path-length traveled s increases in a timelike manner, and $\Sigma_t(s)ds$ = the probability that a particle has an interaction with a scattering center between s and $s + ds$. When a particle collides with a scattering center, classical transport physics applies: the particle scatters isotropically with probability c.

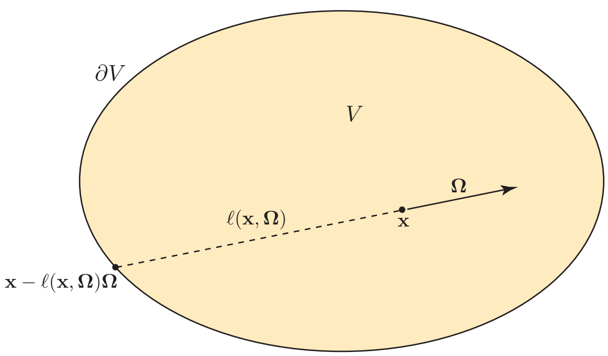

Figure 1: The System V and the Function $\ell(\boldsymbol{x}, \boldsymbol{\Omega})$

In Eq. (8b), c is assumed to be independent of s. [If c depended on s, $c(s')$ would occur within the integral in Eq. (8b).] We refer to Eqs. (8) as the "backward" nonclassical version of the classical problem defined by Eqs. (1), because for any phase space point $(\boldsymbol{x}, \boldsymbol{\Omega}, s)$, the variable s refers "backward" to the spatial point $\boldsymbol{x} - s\boldsymbol{\Omega}$ at which the particle initiated its flight path.

Remark: Previous papers on the backward nonclassical transport equation have usually considered steady-state problems in an infinite medium with a localized source, in which the neutron flux $\to 0$ as $|\boldsymbol{x}| \to \infty$. Here we consider steady-state backward nonclassical transport in a bounded system V, in which particles that enter the system through the outer boundary ∂V are treated by the same random process to determine distance-to-collision as particles that are born internally (due to the source Q) or that scatter.

IV. "FORWARD" NONCLASSICAL PROBLEM

An alternative nonclassical theory has also been formulated. The extra independent variable $s > 0$ occurs in this theory as well, but it has a different physical interpretation. The alternative theory arises by considering a macroscopic transport process in which macroscopic scattering centers are placed in a 2D or 3D system at fixed, regular positions. (The scattering centers form a periodic lattice, called a "Lorentz gas.") Then a macroscopic "ball" or "sphere" is set in motion between the scattering centers. The ball travels in a straight line until it collides with a scattering center. When a collision occurs, the ball reflects specularly away from the scattering center, with no loss of energy. (In 2D, the resulting transport process would resemble the one generated by a pinball machine.) After the mathematical equations are set up to describe this process, a "Boltzmann-Grad" limit is taken in which (i) the size of the scattering centers, (ii) the size of the "ball" or "sphere", and (iii) the distance between the scattering centers all limit to 0. The result of performing this strict mathematical limit is the following particle transport equation:

$$-\frac{\partial \psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega}, s) + \boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \frac{P(s)}{4\pi}\left[c\int_{4\pi}\psi(\boldsymbol{x}, \boldsymbol{\Omega}', 0)d\Omega' + Q(x)\right] \ , \quad \boldsymbol{x} \in V \ , \ \ \boldsymbol{\Omega} \in 4\pi \ , \ \ 0 < s \ . \qquad (12a)$$

This equation is supplemented with the boundary condition

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \Psi^b(\boldsymbol{x}, \boldsymbol{\Omega})P(s) \ , \quad \boldsymbol{x} \in \partial V \ , \ \ \boldsymbol{\Omega} \cdot \boldsymbol{n} < 0 \ , \ \ 0 < s \ . \qquad (12b)$$

In Eqs. (12), particles do not initiate a flight path with $s = 0$, but rather with $s \geq 0$ randomly determined by the distribution function $P(s)$. (This is the case for particles that enter the system through the outer boundary, particles that are born from the internal source, and particles that scatter.) As a particle streams along its flight path, s decreases, and at the instant when $s = 0$, the particle collides with a scattering center. When this collision occurs, the physical scattering physics applies: the particle isotropically scatters with probability c.

We refer to Eqs. (12) as the "forward" nonclassical version of the classical problem defined by Eqs. (1), because at any phase space point $(\boldsymbol{x}, \boldsymbol{\Omega}, s)$, the variable s refers "forward" to the spatial point $\boldsymbol{x} + s\boldsymbol{\Omega}$ where the particle will experience its next collision.

Remark: Previous papers on the forward nonclassical transport equation have usually considered a time-dependent problem in an infinite medium, with no internal sources. Here we consider a steady-state problem for a finite medium containing internal and boundary sources. In the forward transport Eq. (12a), particles that are born from Q or scatter begin their flight paths by sampling the distance to collision s from the distribution function $P(s)$. The boundary condition (12b) treats particles that enter the system through ∂V the same way: their flight paths in V begin with s sampled from $P(s)$.

V. EXPONENTIAL PATH LENGTH DISTRIBUTION

If $P(s)$ is exponential:

$$P(s) = \Sigma_t e^{-\Sigma_t s} \ , \qquad (13)$$

where Σ_t = constant, then Eq. (7a) gives

$$\Sigma_t(s) = \Sigma_t = \text{ constant} ,$$

and the backward nonclassical Eqs. (8) and (9) become:

$$\frac{\partial f}{\partial s}(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} f(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \Sigma_t f(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \frac{\delta(s)}{4\pi}\left[c\Sigma_t \int_{4\pi}\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega}')} f(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'd\Omega' + Q(\boldsymbol{x})\right] ,$$
$$\boldsymbol{x} \in V , \quad \boldsymbol{\Omega} \in 4\pi , \quad 0 < s < \ell(\boldsymbol{x}, \boldsymbol{\Omega}) , \qquad (14a)$$

$$f(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \Psi^b(\boldsymbol{x}, \boldsymbol{\Omega})\delta(s) ,$$
$$\boldsymbol{x} \in \partial V , \quad \boldsymbol{\Omega} \cdot \boldsymbol{n} < 0 , \quad 0 < s . \qquad (14b)$$

Operating on these equations by

$$\lim_{\epsilon\to 0} \int_{-\epsilon}^{\ell(\boldsymbol{x},\boldsymbol{\Omega})+\epsilon} (\cdot)ds ,$$

using

$$f(\boldsymbol{x}, \boldsymbol{\Omega}, -\epsilon) = f(\boldsymbol{x}, \boldsymbol{\Omega}, \ell(\boldsymbol{x}, \boldsymbol{\Omega}) + \epsilon) = 0 ,$$

and defining

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})} f(\boldsymbol{x}, \boldsymbol{\Omega}, s)ds , \qquad (15)$$

we obtain:

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\Psi(\boldsymbol{x}, \boldsymbol{\Omega}) + \Sigma_t\Psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \frac{1}{4\pi}\left[\Sigma_s \int_{4\pi} \Psi(\boldsymbol{x}, \boldsymbol{\Omega}')d\Omega' + Q(\boldsymbol{x})\right] ,$$
$$\boldsymbol{x} \in V , \quad \boldsymbol{\Omega} \in 4\pi , \qquad (16a)$$

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \Psi^b(\boldsymbol{x}, \boldsymbol{\Omega}) , \quad \boldsymbol{x} \in \partial V , \quad \boldsymbol{\Omega} \cdot \boldsymbol{n} < 0 . \qquad (16b)$$

Eqs. (16) are identical to Eqs. (1). Therefore, when $P(s)$ is exponential, the solution $f(\boldsymbol{x}, \boldsymbol{\Omega}, s)$ of the backward Eqs. (8) yields the solution Ψ of Eqs. (1).

Also, if $P(s)$ is exponential [Eq. (13)], then it is very easy to show that the exact solution $\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)$ of the forward nonclassical Eqs. (12) is:

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \Psi(\boldsymbol{x}, \boldsymbol{\Omega})P(s) , \qquad (17)$$

where $\Psi(\boldsymbol{x}, \boldsymbol{\Omega})$ is the solution of Eqs. (1).

Thus, if $P(s)$ is exponential, then the solutions of both the forward and the backward nonclassical transport equations become fully consistent with the solution of the classical transport Eqs. (1).

Next, we show that (i) a physically-motivated transformation allows one to directly derive the forward nonclassical problem from the backward nonclassical problem, and (ii) the physical reaction rates predicted by the backward Eqs. (8) and the forward Eqs. (13) are identical. This transformation effectively shows that the forward and the backward nonclassical transport problems (13) and (8) are equivalent.

VI. ANALYSIS

We begin the analysis with the backward nonclassical transport problem, Eqs. (8). The operator on the left side of Eq. (8a) is a standard first-order partial differential operator, so Eqs. (8) can be solved for f by the method of characteristics. For $0 \le s' \le \ell(\boldsymbol{x}, \boldsymbol{\Omega})$, this solution is:

$$f(\boldsymbol{x},\boldsymbol{\Omega}, s') = \frac{1}{4\pi}F(\boldsymbol{x} - s'\boldsymbol{\Omega})e^{-\int_0^{s'}\Sigma_t(s'')ds''} + \Psi^b(\boldsymbol{x} - \ell(\boldsymbol{x}, \boldsymbol{\Omega})\boldsymbol{\Omega}, \boldsymbol{\Omega})\delta(s' - \ell(\boldsymbol{x}, \boldsymbol{\Omega}))e^{-\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})}\Sigma_t(s'')ds''} . \qquad (18)$$

In Eq. (18), we replace s' by $s' + s$, $\boldsymbol{x}$ by $\boldsymbol{x} + s\boldsymbol{\Omega}$, and $\ell(\boldsymbol{x}, \boldsymbol{\Omega})$ by $\ell(\boldsymbol{x} + s\boldsymbol{\Omega}, \boldsymbol{\Omega}) = \ell(\boldsymbol{x}, \boldsymbol{\Omega}) + s$ to obtain

$$f(\boldsymbol{x} + s\boldsymbol{\Omega}, \boldsymbol{\Omega}, s' + s) = \frac{1}{4\pi}F(\boldsymbol{x} - s'\boldsymbol{\Omega})e^{-\int_0^{s'+s}\Sigma_t(s'')ds''} + \Psi^b(\boldsymbol{x} - \ell(\boldsymbol{x}, \boldsymbol{\Omega})\boldsymbol{\Omega}, \boldsymbol{\Omega})\delta(s' - \ell(\boldsymbol{x}, \boldsymbol{\Omega}))e^{-\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})+s}\Sigma_t(s'')ds''} . \qquad (19)$$

Next, we multiply Eq. (19) by $\Sigma_t(s' + s)$ and operate by $\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})}(\cdot)ds'$, obtaining:

$$\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})} \Sigma_t(s' + s)f(\boldsymbol{x} + s\boldsymbol{\Omega}, \boldsymbol{\Omega}, s' + s)ds' = \frac{1}{4\pi}\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})} F(\boldsymbol{x} - s'\Omega)P(s' + s)ds' + \Psi^b(\boldsymbol{x} - \ell(\boldsymbol{x}, \boldsymbol{\Omega})\boldsymbol{\Omega}, \boldsymbol{\Omega})P(\ell(\boldsymbol{x}, \boldsymbol{\Omega}) + s) . \qquad (20)$$

At this point, we define the left side of Eq. (20) to be $\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)$:

$$\boxed{\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) \equiv \int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})} \Sigma_t(s' + s)f(\boldsymbol{x} + s\boldsymbol{\Omega}, \boldsymbol{\Omega}, s' + s)ds'} . \qquad (21)$$

The integral in Eq. (21) is representative of the collision rate at the point $\boldsymbol{x} + s\boldsymbol{\Omega}$, due to particles that initiated their flight paths on the line $\boldsymbol{x} - s'\boldsymbol{\Omega}, 0 \le s' \le \ell(\boldsymbol{x}, \boldsymbol{\Omega})$. [See Figure 2.] All these particles would of necessity stream through the point $\boldsymbol{x}$. Therefore, $\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)$ represents the particles at $\boldsymbol{x}$, traveling in direction $\boldsymbol{\Omega}$, that will collide with a scattering center at $\boldsymbol{x} + s\boldsymbol{\Omega}$ (i.e. after traveling a further path length s). This interpretation is consistent with the interpretation of the solution of the forward nonclassical transport problem.

We now show that $\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)$, defined by Eq. (21), satisfies the forward nonclassical transport Eqs. (12).

First, we set $s = 0$ in Eq. (21):

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, 0) = \int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})} \Sigma_t(s')f(\boldsymbol{x}, \boldsymbol{\Omega}, s')ds' ,$$

and then we operate by $\int_{4\pi}(\cdot)d\Omega'$, obtaining

$$\int_{4\pi} \psi(\boldsymbol{x},\boldsymbol{\Omega}', 0)d\Omega' = \int_{4\pi}\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega}')} \Sigma_t(s')f(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'd\Omega' . \qquad (22)$$

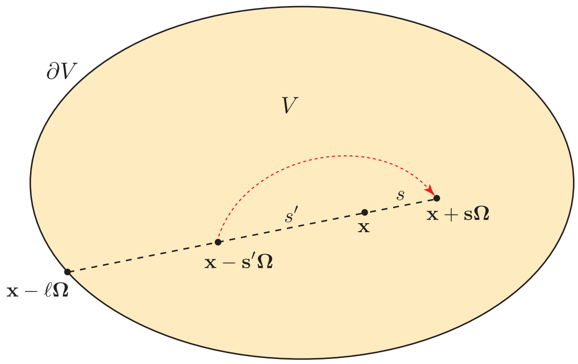

Figure 2: Streaming from $\boldsymbol{x} - s'\boldsymbol{\Omega}$ to $\boldsymbol{x} + s\boldsymbol{\Omega}$

This shows that the physical scattering rate terms (the rates at which particles collide with scattering centers) in the backward Eq. (8b) and the forward Eq. (12a) are equal. Eqs. (8b) and (22) allow us to write for both the forward and backward problems:

$$F(\boldsymbol{x}) = c\int_{4\pi}\psi(\boldsymbol{x},\boldsymbol{\Omega}',0)d\Omega' + Q(\boldsymbol{x}) \,. \tag{23}$$

We now combine Eqs. (20) and (21) to get

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \frac{1}{4\pi}\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})} F(\boldsymbol{x}-s'\boldsymbol{\Omega})P(s'+s)ds' + \Psi^b(\boldsymbol{x}-\ell(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega},\boldsymbol{\Omega})P(\ell(\boldsymbol{x},\boldsymbol{\Omega})+s) \,, \tag{24}$$

where $F(x)$ is defined in terms of ψ by Eq. (23).

Replacing $\boldsymbol{x}$ by $\boldsymbol{x} - s\boldsymbol{\Omega}$ in Eq. (24), we get

$$\begin{aligned}\psi(\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega},s) &= \frac{1}{4\pi}\int_0^{\ell(\boldsymbol{x},\boldsymbol{\Omega})-s} F(\boldsymbol{x}-s\boldsymbol{\Omega}-s'\boldsymbol{\Omega})P(s'+s)ds' \\ &\quad + \Psi^b(\boldsymbol{x}-\ell(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega},\boldsymbol{\Omega})P(\ell(\boldsymbol{x},\boldsymbol{\Omega})) \\ &= \frac{1}{4\pi}\int_s^{\ell(\boldsymbol{x},\boldsymbol{\Omega})} F(\boldsymbol{x}-s''\boldsymbol{\Omega})P(s'')ds'' \\ &\quad + \Psi^b(\boldsymbol{x}-\ell(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega},\boldsymbol{\Omega})P(\ell(\boldsymbol{x},\boldsymbol{\Omega})) \,.\end{aligned}$$

Operating on this result by $-\frac{d}{ds}$ yields

$$-\frac{d}{ds}\psi(\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega},s) = \frac{1}{4\pi}F(\boldsymbol{x}-s\boldsymbol{\Omega})P(s) \,,$$

or

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega},s) - \frac{\partial\psi}{\partial s}(\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega},s) = \frac{1}{4\pi}F(\boldsymbol{x}-s\boldsymbol{\Omega})P(s) \,.$$

Replacing $\boldsymbol{x}$ by $\boldsymbol{x} + s\boldsymbol{\Omega}$, we obtain:

$$-\frac{\partial\psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \frac{1}{4\pi}F(\boldsymbol{x})P(s) \,. \tag{25}$$

This is the forward nonclassical transport Eq. (12a), with $F(\boldsymbol{x})$ defined by Eq. (23).

Finally, we set $\boldsymbol{x} \in \partial V$ in Eq. (24), with $\boldsymbol{\Omega}\cdot\boldsymbol{n} < 0$. Then $\ell(\boldsymbol{x},\boldsymbol{\Omega}) = 0$, and Eq. (24) simplifies to

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \Psi^b(\boldsymbol{x},\boldsymbol{\Omega})P(s) \,. \tag{26}$$

This is the forward nonclassical boundary condition (12b).

Thus, the preceding analysis shows that if $f(\boldsymbol{x},\boldsymbol{\Omega},s)$ is the solution of the backward nonclassical transport Eqs. (8), and $\psi(\boldsymbol{x},\boldsymbol{\Omega},s)$ is defined in terms of f by Eq. (21), then ψ satisfies the forward nonclassical transport Eqs. (12). Also, the physical scattering rates obtained for the two problems are identical. [This follows from Eq. (22).]

Alternatively, if we are given the forward problem defined by Eqs. (12), then using the same geometry, the same $Q(\boldsymbol{x})$, and the same $P(s)$, we can define the backward problem defined by Eqs. (8). Then all of the above results again hold, and the forward problem can (as before) be re-derived from the backward problem. In this way, a backward problem can be derived from a forward problem, and the solutions of these two problems yield the same physical reaction rates.

Thus, the forward and backward nonclassical transport problems are fully equivalent. The forward problem can be derived from the backward problem, and vice versa.

VII. DISCUSSION

To summarize, the physically-motivated transformation given by Eq. (21) yields:

- Eq. (22), which shows that the rates at which particles experience collisions in the backward Eqs. (8) and the forward Eqs. (12) are identical.
- Eq. (25), which is the forward nonclassical transport equation (12a) for ψ.
- Eq. (26), which is the forward nonclassical boundary condition (12b) for ψ.

Therefore, Eq. (21) explicitly (i) defines the solution of the forward nonclassical problem ψ in terms of the backward nonclassical problem f, and (ii) shows that the solutions of the forward and backward problems yield the same physical rate at which particles collide with scattering centers. In effect, Eq. (21) allows one to show that the forward and backward problems are equivalent.

We have assumed that the path-length distribution $P(s)$ is identical for scattered, internal source, and boundary source particles. In more general problems, this assumption may not be valid. (The topic of boundary – and material interface – conditions for nonclassical transport problems has received scant attention in the literature.) For example, particles that scatter or are born by the internal source might have path length distributions determined by $P(s)$, while particles that enter V through ∂V might be subject to a different path length distribution $P^b(s)$. It is currently an open question as to whether the equivalence between the forward and backward theories holds when $P^b(s) \neq P(s)$.

Another point is that in previous papers, the forward nonclassical theories have usually been considered for time-dependent problems, while the backward nonclassical theory has been considered only for steady-state problems. It would be of interest to develop a time-dependent backward theory, and then to show whether (or not) this theory is equivalent to the corresponding forward theory.

If the forward and backward nonclassical transport theories for a given problem are equivalent, then is there any benefit to working with one theory versus the other? The answer to this question may depend on the nature of the work being contemplated. The backward theory has the possible disadvantage of being more "singular"; the backward Eqs. (8) and its boundary condition Eq. (9) both contain delta functions, while the forward Eqs. (12) do not. On the other hand, the backward nonclassical problem is quite similar to a time-dependent classical problem, and numerical methods for the classical problem might be more easily adaptable to the nonclassical backward problem.

To briefly pursue this line of thought, a deterministic simulation of a nonclassical transport problem would probably be analogous in difficulty and cost to solving a time-dependent classical transport problem. [The distance from (or to) collision variable s in the nonclassical theories would be analogous to time t in a classical theory.] Monte Carlo could be the most straightforward way to numerically simulate nonclassical problems. One "simply" has to take an existing Monte Carlo code and change $P(s)$ from its currently exponential form to its non-exponential form. A practical issue is that it is also necessary to find an efficient way to sample from the non-exponential $P(s)$. First experiments in this effort are described in a companion paper [20].

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