Radiative transfer implies a modified reciprocity relation

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The usual global reciprocity relations of radiative transfer do not hold for two points located in regions of different index of refraction. Modified reciprocity relations that involve the relative index are derived. The result has computational as well as theoretical consequences. © 1997 Optical Society of America

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1. INTRODUCTION

A common article of wisdom both in linear particle transport and in diffusion theory is that global reciprocity holds. That is, if source and detector are interchanged (and, in transport theory, if particle motions are reversed), the new detector readings are the same as the old ones, with no assumptions about the spatial arrangement of material. This paper will demonstrate that this reciprocity property fails for light when source and detector sit in regions of different index of refraction. Instead, it must be replaced by a modified reciprocity relation.

There are requirements on the scattering, such as that detailed balance hold. Here we consider the case of elastic scattering, in the sense used by astrophysicists, in which the recoil energy of the scatterers is negligible. The discussion here will be restricted to time-independent problems.

The major applications of linear particle transport (and of diffusion, which is an approximation to linear transport) have been in neutron transport and in radiative transfer. In neutron transport the difficulty does not arise; in radiative transfer it evidently has not been considered before now. The motivation for the present work is the burgeoning application to medical imaging by light. In the regime of interest in most of that work, one deals with monoenergetic photons (that is, Newtonian particles) subject to random collisions but obeying the laws of geometrical optics. Thus at discontinuities in the index of refraction, the reflection is specular and the refraction obeys Snell’s law. A tool in frequent use is perturbation theory, which requires for its application solution of an adjoint problem. The results of this paper are relevant to the usual procedure of obtaining the adjoint solution by solving a direct problem and using reciprocity.

The reciprocity relation can be stated as a symmetry property of the Green’s function. In diffusion theory, this is
g(r, r’) = G(r’, r),
where G(r, r’) is the intensity at r resulting from a unit isotropic source at r’. In transport theory it is

G(r, Ω; r’, Ω’) = G(r’, −Ω’; r, −Ω),
(2)
where G(r, Ω; r’, Ω’) is the angular intensity at r in direction Ω due to a unit monodirectional source at r’ in direction Ω’. That is, interchanging source and detector and simultaneously reversing particle directions does not change the detector reading. This reciprocity is a global consequence of time-reversal invariance.

Equation (1) arises from the fact that the diffusion problem is self-adjoint. It is well known that the Green’s functions of self-adjoint operators are Hermitian. The transport operator is not self-adjoint. In general, there need be no reciprocity relation for the Green’s function of a non-self-adjoint operator, as in the case, for instance, of the transport equation for neutrons in the slowing-down region. When the scattering kernel is symmetric, as in the situation discussed here, or when it can be symmetrized, as, for instance, for thermal neutrons, one can still obtain a reciprocity relation for the transport Green’s function.

In the presence of nonuniform index of refraction the diffusion operator is no longer self-adjoint and Eq. (1) fails. Likewise, Eq. (2) fails in transport theory. The finding of this paper is that nevertheless, one can find generalized reciprocity relations, in which Eqs. (1) and (2) must be replaced respectively by the relations

G(r’, r) = n G(r, r’)
(3)
and

G(r’, Ω; r, Ω) = n^2 G(r, −Ω; r’, −Ω),
(4)
where n is the relative index of refraction from r to r’. It is not G but G/n^2(r) that is symmetric, where n(r) is the index at the field point.

Equation (1) follows from Eq. (2), as does Eq. (3) from Eq. (4), by averaging the transport theory results over initial direction and integrating over final direction. It must be proved separately for diffusion theory, however, because both the diffusion equation and the diffusion interface conditions are approximations to the transport results.
First diffusion theory and then transport theory is considered for two-region systems. The results are then extended to arbitrary variations in the index of refraction. The result is illustrated with a discussion of collisionless transport in two half-spaces, which allows an explicit solution. Finally, computational consequences of using the generalized reciprocity relations are discussed.

2. DIFFUSION THEORY

First consider diffusion theory because it is simpler. The diffusion Green’s function satisfies the equation

$$\nabla \cdot D(r)\nabla G(r, r') + \Sigma_a(r)G(r, r') = \delta(r - r'), \quad (5)$$

in some volume \(V\), where \(D\) is the diffusion coefficient and \(\Sigma_a\) is the macroscopic absorption cross section at \(r\). The usual boundary condition, whether the boundary is free or whether Fresnel reflection holds, is that \(G\) satisfies a linear boundary condition when \(r\) is on the surface \(S\). The standard proof of reciprocity is to multiply Eq. (5) by \(G(r, r')\), subtract from it the corresponding relation with \(r'\) and \(r''\) interchanged, integrate over the volume, and use Green’s theorem to change the term with the divergence into a surface integral. The result is

$$\int_S dS \hat{\mathbf{e}} \cdot D(r)[G(r, r')\nabla G(r, r') - G(r, r'')\nabla G(r, r'')] = G(r', r'') - G(r'', r'). \quad (6)$$

The unit vector in the outward normal direction is written here as \(\hat{\mathbf{e}}\) to avoid confusion with the index of refraction \(n\). The left-hand side vanishes for homogeneous linear boundary conditions of the form \(aG + b\partial G/\partial n = 0\), where \(\partial G/\partial n\) is a normal derivative, and Eq. (1) follows. The self-adjointness of the diffusion operator has been invoked here explicitly to prove the result.

Now suppose that \(V\) is composed of two regions, \(V_1\) and \(V_2\), with index of refraction \(n_1\) and \(n_2\), respectively. The procedure in the last paragraph must be done separately for \(V_1\) and \(V_2\) because the Green’s function is discontinuous on the interface \(S\). The surface integrals still vanish on the exterior portion of \(S\) but not on \(S\). For \(V_i\), Eq. (6) must be replaced by

$$I_i = \int_{S_i} dS \hat{\mathbf{e}} \cdot D(r)[G(r_i, r', r'')\nabla G(r_i, r')] - G(r_i, r)\nabla G(r, r'),

= H_i(r')G(r', r'') - H_i(r'')G(r', r'), \quad (7)$$

where \(I_i\) designates the surface integral evaluated on the \(V_i\) side of \(S\) and \(\hat{\mathbf{e}}_i\) is the unit normal pointing outward from \(V_i\) (so that \(\hat{\mathbf{e}}_1 = -\hat{\mathbf{e}}_2\)). The symbol \(\mathbf{r}_i\) in the arguments explicitly designates a surface point with the function defined on the \(V_i\) side. The symbol \(H_i(r)\) represents the step function for \(V_i\). It is unity if \(r \in V_i\) and zero otherwise. While the diffusion operator in each region is self-adjoint, the problem is not; the discontinuity in the Green’s function spoils the self-adjointness, which would require that \(I_1 = -I_2\).

The flux due to a unit source at \(r'\) is given by \(J(r, r') = -D(r)\nabla G(r, r')\) and must be continuous everywhere, including interfaces. For particles, the second interface condition is that \(G\) be continuous. For photons obeying geometrical optics, the flux is still continuous, since this is just a statement of energy conservation. The appropriate second interface condition here is

$$n^2G(r_1, r') - G(r_2, r') = C(n)\hat{\mathbf{e}}_1 \cdot J(r, r'), \quad (8)$$

where \(n\) is the relative index of refraction from \(V_1\) to \(V_2\) and \(C(n)\) is a constant depending on \(n\) alone. The symbol \(\mathbf{r}\) rather than \(r_1\) or \(r_2\) appears on the right-hand side of Eq. (8) because the expression is continuous. This relation was derived by a generalization of the simple kinetic theory argument that leads to Fick’s law. Then

$$\int_S dS \hat{\mathbf{e}}_2 \cdot D(r_2)G(r_2, r'')\nabla G(r_2, r') = \int_S dS \hat{\mathbf{e}}_1 \cdot J(r, r')[n^2G(r_1, r') - C(n)\hat{\mathbf{e}}_1 \cdot J(r, r')]. \quad (9)$$

It follows that \(I_2 = -n^2I_1\), and so

$$[n^2H_1(r') + H_2(r')]G(r', r') = [n^2H_1(r'') + H_2(r'')]G(r'', r'). \quad (10)$$

Equation (3) follows immediately.

3. TRANSPORT THEORY

The linear transport equation for the Green’s function is

$$\hat{\Omega} \cdot \nabla G(r, \hat{\Omega}; r', \hat{\Omega}') + \Sigma_a(r)G(r, \hat{\Omega}; r', \hat{\Omega}') = \int d\Omega' \Sigma_s(r, \hat{\Omega}'; \hat{\Omega} - \hat{\Omega}') G(r, \hat{\Omega}; r', \hat{\Omega}') + \delta(r - r')\delta(\hat{\Omega} - \hat{\Omega}'). \quad (11)$$

In the usual proof of reciprocity, one multiplies this equation by \(G'(r, \hat{\Omega}') = G(r, -\hat{\Omega}; r', -\hat{\Omega}')\), subtracts from it \(G'(r, \hat{\Omega}) = G(r, \hat{\Omega}; r', \hat{\Omega}')\) multiplied by the equation for \(G''(r, -\hat{\Omega})\), and integrates over all \(r\) and \(\hat{\Omega}\). The second term on the left makes no contribution. Neither does the scattering term, by virtue of the reciprocity of the differential scattering cross section required by time-reversal invariance, to wit: \(\Sigma_s(r, \hat{\Omega} \to \hat{\Omega}') = \Sigma_s(r, \hat{\Omega}'; \hat{\Omega} - \hat{\Omega}')\). The result is

$$\int d\Omega \int d\Omega' \hat{\Omega}G''(r, -\hat{\Omega}') G'(r, \hat{\Omega}) = G''(r', -\hat{\Omega}') - G'(r', \hat{\Omega}). \quad (12)$$

The left-hand side vanishes for both a free surface (no radiation incident from the outside) and for specular reflection. In the former case, the boundary condition is \(G(r, \hat{\Omega}) = 0\) when \(r \in S\) and \(\hat{\mathbf{e}} \cdot \hat{\Omega} < 0\), where the generic \(G\) is introduced to represent either \(G'\) or \(G''\) and the argument \(\mathbf{r}\) in \(G\) is suppressed for surface points. Thus either \(G''(r, -\hat{\Omega})\) or \(G'(r, \hat{\Omega})\) vanishes on the surface for all \(\hat{\Omega}\). For specular reflection,

$$G(-\hat{\Omega}) = r(\hat{\mathbf{e}} \cdot \hat{\Omega})G(\hat{\Omega}), \quad r \in S, \quad \hat{\mathbf{e}} \cdot \hat{\Omega} > 0, \quad (13)$$
where \( \hat{\Omega}_{r} \) is the direction of the reflected ray for incident direction \( \hat{\Omega} \), and \( r(\hat{\mathbf{e}} \cdot \hat{\Omega}) \) is the reflection probability. The surface integral in Eq. (12) can thus be rewritten as

\[
J_2 = \int_{\hat{\mathbf{e}} \cdot \hat{\Omega} > 0} \text{d} \hat{\mathbf{e}} \cdot \hat{\mathbf{e}} \cdot \hat{\Omega} \cdot [G^*(\hat{\Omega}_{r})G'({\hat{\Omega}}) - G^*(\hat{\Omega})G'({\hat{\Omega}_{r}})].
\]

(14)

Since \( \hat{\mathbf{e}} \cdot \hat{\Omega} = \hat{\mathbf{e}} \cdot \hat{\Omega}_{r} \) and \( \hat{\Omega} \) and \( \hat{\Omega}_{r} \) are 180° apart in azimuth about \( \hat{\mathbf{e}} \), the integral vanishes.

For the two-region problem, again there is a surface contribution only from \( S' \), so

\[
I_i = \int_{S'} \text{d}r J_i(r, r', \hat{\Omega}', r'', \hat{\Omega}'') = H_i(r')G'(r', -\hat{\Omega}') - H_i(r'')G'(r'', \hat{\Omega}''),
\]

(15)

where

\[
J_i = \int \text{d} \hat{\Omega}_{r} \hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r} G^*(\hat{\Omega}_{r})G'({\hat{\Omega}}).
\]

(16)

The arguments on \( J_i \) have been suppressed here.

While reflection contributes nothing to these integrals, transmission does. Conservation of energy gives the interface condition

\[
\text{d} \hat{\Omega}_{r} \hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r} G(\hat{\Omega}_{r}) = \text{d} \hat{\Omega}_{r} \hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r} t_{i-j}(\hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r})G(\hat{\Omega}_{r}),
\]

(17)

Here \( \hat{\Omega}_{r} \) is the direction vector of a ray on the \( V_i \) side of the interface, \( \hat{\Omega}_{t} \) is the direction vector of the same ray (refracted) on the \( V_j \) side of the interface, and \( t_{i-j}(\hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r}) \) is the fraction of the energy incident on the interface at \( r \) in direction \( \hat{\Omega}_{r} \) transmitted from \( V_i \) to \( V_j \). The minus sign comes from the fact that \( \hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r} \) and \( \hat{\mathbf{e}}_j \cdot \hat{\Omega}_{r} \) have opposite signs, since \( \hat{\mathbf{e}}_i = -\hat{\mathbf{e}}_j \). Local reciprocity demands that

\[
t_{i-j}(\hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r}) = t_{j-i}(-\hat{\mathbf{e}}_j \cdot \hat{\Omega}_{r}).
\]

(18)

The Fresnel formulas explicitly obey this reciprocity.\(^6\)

From Snell’s law one derives that

\[
\text{d} \hat{\Omega}_{r} \hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r} = -n^2 \text{d} \hat{\Omega}_{r} \hat{\mathbf{e}}_2 \cdot \hat{\Omega}_{r}.
\]

(19)

This, together with Eq. (17), gives the \( n^2 \) law of radiance,

\[
G(\hat{\Omega}_{r}) = n^2 t_{i-j}(\hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r})G(\hat{\Omega}_{r}),
\]

where \( \hat{\mathbf{e}}_i \cdot \hat{\Omega}_{r} > 0 \). It follows that

\[
J_2 = \int_{\hat{\mathbf{e}} \cdot \hat{\Omega} > 0} \text{d} \hat{\mathbf{e}} \cdot \hat{\mathbf{e}} \cdot \hat{\Omega} \cdot [G^*(\hat{\Omega}_{r})G'({\hat{\Omega}}) - G^*(\hat{\Omega})G'({\hat{\Omega}_{r}})]
\]

\[
= -\int_{\hat{\mathbf{e}} \cdot \hat{\Omega} > 0} \text{d} \hat{\mathbf{e}} \hat{\mathbf{e}} \cdot \hat{\Omega} t_{1-2}(\hat{\mathbf{e}} \cdot \hat{\Omega})G(\hat{\Omega})
\]

\[
\times [G^*(\hat{\Omega})G'({\hat{\Omega}_{r}}) - G^*(\hat{\Omega}_{r})G'({\hat{\Omega}})].
\]

(20)

The first equality here comes from writing the integral in Eq. (16) in terms of directions such that \( \hat{\mathbf{e}}_1 \cdot \hat{\Omega}_1 > 0 \); the second uses Eq. (17); the third, Eq. (18); the fourth replaces \( \hat{\Omega} \) with \( -\hat{\Omega} \); the fifth uses Eq. (19); the sixth, Eq. (17) again; and the seventh equality extends the integral to all \( \hat{\Omega} \). It follows from Eq. (20) that \( n^2 I_1 + I_2 = 0 \) and thus that

\[
[n^2 H_1(r') + H_2(r')]G'(r', -\hat{\Omega}') = [n^2 H_1(r'') + H_2(r'')]G'(r'', \hat{\Omega}''),
\]

(21)

which gives Eq. (4).

A. Generalization to General Geometries

To extend the diffusion theory results beyond a simple two-region geometry, consider any closed surface \( S \) with local outward normal \( \hat{\mathbf{e}} \) and define

\[
K = \int_S \text{d}S \hat{\mathbf{e}} \cdot D(r)[G(\mathbf{r}, \mathbf{r}') \nabla G(\mathbf{r}, \mathbf{r}')]
\]

\[
- G(\mathbf{r}, \mathbf{r}') \nabla G(\mathbf{r}, \mathbf{r}')]n^2(r),
\]

(22)

where \( n(r) \) is the local index of refraction at \( r \). It follows from the results above that while \( n(r) \) may not be continuous, the surface integral \( K \) is invariant for surfaces \( S \) that can be deformed into one another by a continuous transformation without passing through \( \mathbf{r}' \) or \( \mathbf{r}'' \). Let \( S \) enclose both points. It was shown above that when \( S \) is taken as the outer boundary of the system, \( K = 0 \). Deform the surface to two infinitesimal spheres, one sur-
rounding \( r' \) and one surrounding \( r'' \). On the first sphere, \( n(r) = n(r') \) and on the second, \( n(r) = n(r'') \), while \( K = 0 \). Thus

\[
G(r', r'')/n^2(r') - G(r'', r')/n^2(r'') = 0. \tag{23}
\]

Since the relative index of refraction is \( n = n(r'')/n(r') \), Eq. (3) follows. The same argument leads to Eq. (4) in transport theory, where here one defines

\[
K = \int_S d\hat{r}/n^2(\hat{r}) \cdot \hat{\Omega} G'(\hat{r}, -\hat{\Omega})G'(\hat{r}, \hat{\Omega}). \tag{24}
\]

B. Example: Collisionless Transport for Two Halff-spaces

The results of this paper are hardly intuitive. One can perhaps see better how the modified reciprocity comes about by examining the result of explicit calculation in a simple case, for example, for purely absorbing media in plane geometry.

Consider two uniform nonscattering half-spaces with interface at \( x = 0 \). For \( x > 0 \) the index of refraction is unity and the macroscopic absorption cross section is \( \Sigma \); for \( x < 0 \) the index is \( n \) and the cross section \( \Sigma' \). A plane source at \( x' < 0 \) emits 1 photon/s into a small solid angle \( \Delta\Omega' \) making angle \( \cos^{-1} \mu' \) with the positive \( x \) axis, and a collimated detector at \( x > 0 \) accepts photons in a small solid angle \( \Delta\Omega \) centered about the direction given by \( \cos^{-1} \mu \). Let us examine first the case of no absorption. If the photons from the source do not enter the detector, the Green’s function is zero, and clearly, this is also the result is the same, as it is if transport theory is used instead.

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