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The Milne problem with Fresnel reflection

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Abstract

The Milne problem, with internally reflecting boundary conditions as required by Fresnel theory, is solved exactly by the method of Wiener and Hopf. In addition to the specular case we also solve for diffuse reflection, since this provides a useful comparison. The results are also compared with those of Aronson (1995 *J. Opt. Soc. Am.* **12** 2532) and excellent agreement is obtained. The Wiener–Hopf procedure makes it possible to find an expression for the value of refractive index such that the extrapolated endpoint no longer exists. Tables for this critical value of refractive index are given for both specular and diffuse reflection. The reflected and transmitted surface angular distributions are also given for a range of refractive indices. Some comments are made about the nature of the solution as the reflection becomes perfectly specular. The equivalent diffusion theory results have also been obtained and it is seen that this approximation is reasonable for very small absorption, but rapidly becomes inaccurate for large absorption and large refractive index.

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1. Introduction

The burgeoning interest in the use of near infra-red radiation for the detection of abnormalities in neo-natal brain tissue has led to further developments in the associated radiative transfer problem. In particular we cite the work of Aronson (1995), who has considered the modification of the diffusion theory boundary conditions when some degree of internal reflection is present at a plane boundary. This work has shown that the usual classical diffusion equation boundary conditions undergo major changes according to the value of the refractive index. Aronson has also shown that the extrapolated endpoint has limited value for such problems, because it ceases to exist for a given absorption ratio at a critical value of the refractive index. A more useful boundary condition is based upon the extrapolation distance which always exists. Further work on this general problem can be found in Freund and Berkovits (1990), Zhu *et al* (1991), Freund (1992) and Nieuwenhuizen and Luck (1993). The latter work has some bearing on the mathematical methods we shall employ in this paper although the basic ideas were already available in Williams (1975), whose work was further developed by Razi Naqvi *et al* (1991), Razi Naqvi (1993), Abdel Krim and Degheidy (1998) and Atalay (2000). More will be said about these papers in our concluding section. A further significant contribution to this subject is due to Kuznetsov (1942, 1945), Sobolev (1948) and van de Hulst (1948). Full details can be found in Sobolev (1963), but essentially the above authors have used the method of invariant imbedding to obtain integral equations for the surface angular distribution for arbitrary reflection coefficient. They have not, however, considered the matter of the extrapolated endpoint.

The purpose of the present work is to give a rigorous treatment to the Milne problem where the photons obey the Fresnel conditions at the vacuum-medium boundary with a certain fraction reflected and the balance transmitted by refraction. The physical mechanism of photon interaction at the boundary is by specular reflection, but for completeness we shall also discuss diffuse reflection because it has a surprisingly simple solution. There is also some physical interest in discussing the diffuse scattering solution since it can describe to some extent the influence of an optically rough surface. Indeed, one could consider a linear combination of specular and diffuse scattering and thereby study the transitional behaviour between a smooth and a rough surface. Specular reflection is a reflection of the same type as is caused by a smooth surface: it is directional and obeys the laws of physical optics; diffuse scattering on the other hand has little directivity and takes place over a larger area of surface than the first Fresnel zone. Its phase is incoherent and its fluctuations have large amplitudes. These two types of surfaces and their properties have been discussed in some detail by Beckmann and Spizzichino (1963).

It should be noted that the use of the Fresnel conditions with a radiative transfer equation (Chandrasekhar 1960) involves a hybrid argument in the sense that in the region near the boundary, within a photon mean free path, electromagnetic effects dominate. This is in contrast to neutron transport where the neutron passes through a boundary unhindered. Also, in situations where the photon energy is high, refractive index unity, e.g. nuclear reactor shielding, one can neglect internal reflection. However, for the case of infra-red radiation passing through a tissue–air interface (refractive index around 1.5), it is essential to include refraction and reflection.

The main contributions of the present work are to give a complete solution for the angular distribution at the surface and the spatial distribution throughout the medium. Also to give a precise condition at which the extrapolated endpoint ceases to exist. A further contribution is the assessment of the accuracy of diffusion theory.

2. General theory

Let $\phi(x, \mu)$ be the flux (velocity $\times$ density) of the radiation at position x which is travelling in the direction $\vartheta = \cos^{-1}(\mu)$ with respect to the x-axis. Then, the equation of radiative transfer may be written (Chandrasekhar 1960, Williams 1971) as

$$\mu \frac{\partial \phi(x, \mu)}{\partial x} + \phi(x, \mu) = \frac{c}{2} \int_{-1}^{1} \mathrm{d}\mu' \, \phi(x, \mu') \equiv \frac{c}{2} \phi_0(x) \tag{1}$$

where x is in units of the photon mean free path and $c = \Sigma_s/\Sigma$. The symbol Σ_s is the scattering cross section (coefficient) and $\Sigma = \Sigma_s + \Sigma_a$, where Σ_a is the absorption cross section.

We shall consider a half-space $x > 0$ with a vacuum in $x < 0$. There is a source of photons at $x = \infty$ such that at large distances from the boundary

$$\phi(x, \mu) \sim \frac{e^{\nu x}}{1 + \nu\mu}. \tag{2}$$

The classical Milne problem arises if the boundary condition at $x = 0$ is given by

$$\phi(0, \mu) = 0, \qquad 0 \leqslant \mu \leqslant 1 \tag{3}$$

i.e. no photons cross the boundary from the void into the medium. In the present case, however, the physics of the medium requires that internal reflection be accounted for (Born and Wolf 2002). Thus the boundary condition (3) now becomes

$$\phi(0, \mu) = \int_0^1 d\mu' \, R(\mu, \mu')\phi(0, -\mu'), \qquad 0 \leqslant \mu \leqslant 1. \tag{4}$$

We note that the reflection is specular at the surface and hence

$$R(\mu, \mu') = r(\mu)\delta(\mu - \mu') \tag{5}$$

leading to

$$\phi(0, \mu) = r(\mu)\phi(0, -\mu), \qquad 0 \leqslant \mu \leqslant 1. \tag{6}$$

The Fresnel reflection coefficient is given by

$$\begin{aligned} r(\mu) &= \frac{1}{2}\left[\left(\frac{\mu - n\mu_0}{\mu + n\mu_0}\right)^2 + \left(\frac{\mu_0 - n\mu}{\mu_0 + n\mu}\right)^2\right], \qquad \mu_c \leqslant \mu \leqslant 1 \\ &= 1, \qquad 0 \leqslant \mu \leqslant \mu_c \end{aligned} \tag{7}$$

with $\mu_0^2 = 1 - n^2 + n^2\mu^2$ (μ_0 is the angle of refraction) and the critical angle for internal reflection is given by

$$\mu_c = \frac{\sqrt{n^2 - 1}}{n} \tag{8}$$

or $\vartheta_c = \sin^{-1}(1/n)$, n being the refractive index of the medium in $x > 0$. We note from equation (5) that if $n = 1$, $\mu_c = 0$ and $r(\mu) = 0$, i.e. all photons are transmitted as in the classical case. In the case of a tissue–air interface and infra-red photons, the boundary condition is far more complicated and consequently the Milne problem becomes far richer in content.

In order to make the problem more general, we also consider the case of diffuse reflection in which

$$R(\mu, \mu') = 2\mu' r(\mu) \tag{9}$$

leading to the boundary condition

$$\phi(0, \mu) = 2r(\mu) \int_0^1 d\mu' \, \mu'\phi(0, -\mu'), \qquad 0 \leqslant \mu \leqslant 1. \tag{10}$$

The factor of 2 is a convenient normalization factor which maintains particle balance when $r(\mu) = 1$.

It would, of course, be possible to consider a combination of specular and diffuse reflection as we did in Williams (1975) but for simplicity we consider the cases separately.

2.1. Solution by the Wiener–Hopf technique

We define the Laplace transform of the angular flux as

$$\bar{\phi}(s,\mu) = \int_0^\infty \mathrm{d}x\, \mathrm{e}^{-sx}\phi(x,\mu). \tag{11}$$

Apply the transform to equation (1), divide by $(1+s\mu)$ and integrate over $\mu(-1, 1)$ to get

$$\int_{-1}^{0} \frac{\mathrm{d}\mu\,\mu\phi(0,\mu)}{1+s\mu} + \int_0^1 \frac{\mathrm{d}\mu\,\mu\phi(0,\mu)}{1+s\mu} = V(s)\bar{\phi}_0(s) \tag{12}$$

where

$$V(s) = 1 - \frac{c}{2s}\log\left(\frac{1+s}{1-s}\right). \tag{13}$$

We define

$$g_-(s) = \int_{-1}^{0} \frac{\mathrm{d}\mu\,\mu\phi(0,\mu)}{1+s\mu} \tag{14}$$

$$g_+(s) = \int_0^1 \frac{\mathrm{d}\mu\,\mu\phi(0,\mu)}{1+s\mu} \tag{15}$$

whence (12) becomes

$$g_-(s) + g_+(s) = V(s)\bar{\phi}_0(s). \tag{16}$$

We now follow the well-established Wiener–Hopf procedure (Williams 1971) whereby we define the function

$$\tau(s) = \frac{V(s)(s^2-1)}{s^2-\nu^2} = \frac{\tau_+(s)}{\tau_-(s)}. \tag{17}$$

The quantities $\pm\nu$ are the roots of $V(s) = 0$. Thus $\tau(s)$ has no zeros in the range $s(-1, 1)$ and tends to unity as $|s| \to \infty$. The functions $\tau_\pm(s)$ are defined as

$$\log\tau_\pm(s) = \frac{1}{2\pi\mathrm{i}}\int_{\pm\eta-\mathrm{i}\infty}^{\pm\eta+\mathrm{i}\infty} \frac{\log\tau(u)}{u-s}\,\mathrm{d}u. \tag{18}$$

$\tau_+(s)$ is analytic for $\mathrm{Re}(s) < \eta$ and $\tau_-(s)$ for $\mathrm{Re}(s) > -\eta$, where $\eta < 1$. We also note that $g_-(s)$ is analytic for $\mathrm{Re}(s) < 1$ and $g_+(s)$ for $\mathrm{Re}(s) > -1$. $\bar{\phi}_0(s)$ is analytic for $\mathrm{Re}(s) > \nu$. Rearranging the terms in equation (16) we find

$$\frac{(s-1)}{\tau_+(s)}\{g_-(s) + g_+(s)\} = \frac{s^2-\nu^2}{s+1}\frac{1}{\tau_-(s)}\bar{\phi}_0(s). \tag{19}$$

Now the purpose of the Wiener–Hopf technique is to arrange equation (19) such that each side is analytic in overlapping half-spaces. Each side is therefore the analytic continuation of the other and is an entire function. In the present case, the right-hand side is analytic in $\mathrm{Re}(s) > \nu$. The first term on the left-hand side is analytic in $\mathrm{Re}(s) < \eta$, but the second term is only analytic in the strip $-1 < \mathrm{Re}(s) < \eta$. Thus, we must decompose this term as follows by Cauchy's principle, namely:

$$\frac{g_+(s)}{\tau_+(s)} = F_+(s) - F_-(s) \tag{20}$$

where

$$F_\pm(s) = \frac{1}{2\pi\mathrm{i}}\int_{\pm\eta-\mathrm{i}\infty}^{\pm\eta+\mathrm{i}\infty} \frac{\mathrm{d}u}{u-s}\frac{g_+(u)}{\tau_+(u)} \tag{21}$$

and F_+ and F_- have the same regions of analyticity as τ_+ and τ_-, respectively.

Equation (19) may now be written as

$$\frac{(s-1)}{\tau_+(s)}g_-(s) + (s-1)F_+(s) = (s-1)F_-(s) + \frac{s^2-\nu^2}{s+1}\frac{1}{\tau_-(s)}\bar{\phi}_0(s). \tag{22}$$

The right-hand side of equation (22) is analytic in $\mathrm{Re}(s) > \nu$ and the left-hand side in $\mathrm{Re}(s) < \eta$; hence, we have our common strip of analyticity and the necessary conditions are satisfied. The limit of each side of equation (22) as $|s| \to \infty$ is equal to a constant A_0, thus according to Liouville's theorem (Titchmarsh 1937)

$$(s-1)F_-(s) + \frac{s^2-\nu^2}{s+1}\frac{1}{\tau_-(s)}\bar{\phi}_0(s) = A_0. \tag{23}$$

We may now evaluate $F_-(s)$ by interchanging orders of integration and using Cauchy's residue theorem to get

$$F_-(s) = -\int_0^1 \frac{\mathrm{d}\mu\, \mu\tau_-(1/\mu)}{1+s\mu}\phi(0,\mu) \tag{24}$$

$\phi(0,\mu)$ in (24) can be replaced by either one of the boundary conditions (6) or (10). Equation (23) is now written as

$$\bar{\phi}_0(s) = \frac{(s+1)\tau_-(s)}{s^2-\nu^2}\left[A_0 + (s-1)\int_0^1 \frac{\mathrm{d}\mu\, \mu\tau_-(1/\mu)}{1+s\mu}\phi(0,\mu)\right]. \tag{25}$$

This could be inverted to get the spatial distribution $\phi_0(x)$; however, we do not yet know $\phi(0,-\mu)$. To get this, we can integrate equation (1) over $x(0,\infty)$ and find

$$\phi(0,-\mu) = \frac{c}{2\mu}\int_0^\infty \mathrm{d}x\, \mathrm{e}^{-x/\mu}\phi_0(x) = \frac{c}{2\mu}\bar{\phi}_0(1/\mu). \tag{26}$$

Setting $s = 1/\mu$ in equation (25), using (26) and noting that Chandrasekhar's H-function is given by

$$H(\mu) = \frac{(1+\mu)\tau_-(1/\mu)}{1+\nu\mu}. \tag{27}$$

we find the following integral equation for $\phi(0,-\mu)$,

$$\frac{c}{2}\frac{H(\mu)}{1-\nu\mu}A_0 = \phi(0,-\mu) - \frac{(1-\mu)H(\mu)}{1-\nu\mu}\frac{c}{2}\int_0^1 \frac{\mathrm{d}\mu'\, \mu'(1+\nu\mu')}{(\mu+\mu')(1+\mu')}\phi(0,\mu')H(\mu'). \tag{28}$$

There are two special cases to consider: (1) specular and (2) diffuse reflection.

(1) *Specular.* In this case, we use equation (6) to get

$$\frac{c}{2}\frac{H(\mu)}{1-\nu\mu}A_0 = \phi(0,-\mu) - \frac{(1-\mu)H(\mu)}{1-\nu\mu}\frac{c}{2}\int_0^1 \frac{\mathrm{d}\mu'\, \mu'(1+\nu\mu')r(\mu')}{(\mu+\mu')(1+\mu')}\phi(0,-\mu')H(\mu'). \tag{29}$$

This is a Fredholm equation for the angular distribution $\phi(0,-\mu)$. It must be solved numerically and this will be done in a later section.

(2) *Diffuse*. Using equation (10), we find

$$\phi(0,-\mu) = \frac{c}{2}\frac{H(\mu)}{1-\nu\mu}A_0 + \frac{(1-\mu)H(\mu)}{1-\nu\mu}\frac{c}{2}J_0\int_0^1 \frac{\mathrm{d}\mu'\, \mu'(1+\nu\mu')r(\mu')}{(\mu+\mu')(1+\mu')}H(\mu') \tag{30}$$

where

$$J_0 = 2\int_0^1 \mathrm{d}\mu\, \mu\phi(0,-\mu). \tag{31}$$

Equation (30) is an explicit result for $\phi(0, -\mu)$ except for the unknown J_0. To get J_0, we multiply equation (30) by μ and integrate over $\mu(0, 1)$. The result, obtained after using the properties of the H-function, is

$$\frac{A_0}{J_0} = \frac{\nu}{\sqrt{1-c}}\left(\frac{1}{2} - r_1\right) + \int_0^1 \frac{\mathrm{d}\mu}{1+\mu}\mu r(\mu)(1+\nu\mu)H(\mu) \tag{32}$$

where

$$r_1 = \int_0^1 \mathrm{d}\mu\, \mu r(\mu). \tag{33}$$

Thus, we have an explicit result for $\phi(0, -\mu)$ and hence from equation (25) for $\phi_0(x)$.

2.2. The extrapolation distance and extrapolated endpoint

A convenient boundary condition for diffusion theory is to set the extrapolated solution to zero at a specified distance beyond the surface. This means that

$$\phi_{\mathrm{asy}}(-z_0) = 0 \tag{34}$$

where $x = -z_0$ is the distance beyond $x = 0$ in $x < 0$ where the photon flux would 'mathematically' go to zero. An alternative boundary condition is

$$d = \frac{\phi_{\mathrm{asy}}(0)}{\phi'_{\mathrm{asy}}(0)} \tag{35}$$

where $\phi_{\mathrm{asy}}(x)$ is the solution of the transport equation at several mean free paths from the boundary. To explain these matters, we return to equation (25) and invert the Laplace transform $\bar{\phi}_0(s)$. To do this requires a knowledge of the singularities of $\bar{\phi}_0(s)$. Clearly, we can see that there are simple poles at $s = \pm\nu$. Also, there is a branch point at $s = -1$ which requires a cut in the complex plane extending from -1 to $-\infty$. But, in addition, there is a pole at $s = -1/\mu$ embedded in the cut, and because $\mu(0, 1)$ this pole moves along the cut. We shall delay discussion of this more complicated aspect of the problem until later. The cut contribution will introduce a term in $\phi_0(x)$ which decays rapidly away from the boundary. The important part of the solution which determines the extrapolated endpoint and the extrapolation distance is the asymptotic part which arises from the pole contributions. Thus, we can readily show by Cauchy's residue theorem that

$$\phi_{\mathrm{asy}}(x) = \frac{1+\nu}{2\nu}\tau_-(\nu)A_0^+\,\mathrm{e}^{\nu x} - \frac{1-\nu}{2\nu}\tau_-(-\nu)A_0^-\,\mathrm{e}^{-\nu x} \tag{36}$$

where

$$A_0^+ = A_0 - (1-\nu)\int_0^1 \frac{\mathrm{d}\mu}{1+\mu}\mu H(\mu)\phi(0,\mu) \tag{37}$$

$$A_0^- = A_0 - (1+\nu)\int_0^1 \frac{\mathrm{d}\mu\,(1+\nu\mu)}{(1+\mu)(1-\nu\mu)}\mu H(\mu)\phi(0,\mu). \tag{38}$$

Now we can write the asymptotic solution in the form

$$\phi_{\mathrm{asy}}(x) = B\sinh\nu(x+z_0) \tag{39}$$

where z_0 is, by definition, the extrapolated endpoint. Comparing coefficients of $\exp(\pm\nu x)$ between (36) and (39), we find

$$z_0 = \frac{1}{2\nu}\log\left(\frac{1+\nu}{1-\nu}\frac{\tau_-(\nu)}{\tau_-(-\nu)}\right) + \frac{1}{2\nu}\log\left(\frac{A_0^+}{A_0^-}\right). \tag{40}$$

But the first term on the right-hand side of (40) is simply the classic Milne problem extrapolated endpoint, which we denote by $z_0(c)$ (Davison 1957). The other term arises from reflection; we denote this term by $z_0^*(R)$.

For completeness, we note that for $c = 1$, $\nu = 0$, i.e. zero absorption,

$$z_0 = 0.71044\ldots + z_0^*(R) \tag{41}$$

where

$$z_0^*(R) = \frac{\int_0^1 \mathrm{d}\mu\, \mu H(\mu)\phi(0,\mu)}{1 - \int_0^1 \frac{\mathrm{d}\mu}{1+\mu}\mu H(\mu)\phi(0,\mu)}. \tag{42}$$

The extrapolation distance, d, is defined by equation (35), hence

$$d = \frac{1}{\nu}\frac{A_0^+ - A_0^-\,\mathrm{e}^{-2\nu z_0(c)}}{A_0^+ + A_0^-\,\mathrm{e}^{-2\nu z_0(c)}}. \tag{43}$$

We further note from equations (37) and (38) that

$$A_0^- = A_0^+ - \frac{2\nu}{1-\nu}\int_0^1 \frac{\mathrm{d}\mu}{1-\nu\mu}\mu H(\mu)\phi(0,\mu) \tag{44}$$

i.e. $A_0^+ > A_0^-$. If we set $\phi(0,\mu) = r(\mu)\phi(0,-\mu)$, it transpires numerically that for a given $r(\mu)$, A_0^- decreases as c decreases. At a particular value of refractive index n, $A_0^- = 0$ and $z_0 = \infty$. Thereafter z_0 ceases to exist. At this value of n, the extrapolation distance $d = 1/\nu$, as can be seen from equation (43). The critical values of n and related quantities will be calculated in the next section.

2.3. *Diffusion theory results*

It is useful to examine the accuracy of diffusion theory for this problem. In order to do this, we must construct an appropriate boundary condition. First, consider the case of specular reflection when according to equation (6) we may write

$$\phi(0,\mu) = r(\mu)\phi(0,-\mu), \qquad 0 \leqslant \mu \leqslant 1. \tag{45}$$

Now in the spirit of diffusion theory, we can write (Davison 1957),

$$\phi(0,\mu) = \tfrac{1}{2}\phi_0(0) + \tfrac{3}{2}\mu\phi_1(0) \tag{46}$$

where $\phi_1(0) = -D\phi_0'(0)$. If we insert (46) into (45), multiply by μ and integrate over $\mu(0, 1)$, we find

$$\phi_0(0) = \lambda_\mathrm{s}\phi_0'(0) \tag{47}$$

where

$$\lambda_\mathrm{s} = \frac{2}{3}\left(\frac{1+3r_2}{1-2r_1}\right) \tag{48}$$

and

$$r_2 = \int_0^1 \mathrm{d}\mu\, \mu^2 r(\mu). \tag{49}$$

Similarly, if we assume diffuse reflection, the boundary condition is, from (10),

$$\phi(0,\mu) = 2r(\mu)\int_0^1 \mathrm{d}\mu'\, \mu'\phi(0,-\mu'), \qquad 0 \leqslant \mu \leqslant 1. \tag{50}$$

Using (46), multiplying by μ and integrating over $\mu(0, 1)$, we find

$$\phi_0(0) = \lambda_\mathrm{d}\phi_0'(0) \tag{51}$$

where

$$\lambda_{\rm d} = \frac{2}{3}\left(\frac{1+2r_1}{1-2r_1}\right). \tag{52}$$

Equations (47) and (51) show that the extrapolation distances for specular and diffuse reflection are $\lambda_{\rm s}$ and $\lambda_{\rm d}$, respectively and, moreover, that they are independent of absorption, i.e. the value of c.

To find the extrapolated endpoint, we assume a solution of the diffusion equation in the form

$$\phi_0(x) = A_0\,{\rm e}^{\nu x} + B_0\,{\rm e}^{-\nu x} \tag{53}$$

where $\nu^2 = \Sigma_{\rm a}/D$. Using either boundary condition we find that

$$z_0 = \frac{1}{2\nu}\log\left(\frac{1+\nu\lambda}{1-\nu\lambda}\right) \tag{54}$$

with the appropriate value of λ. Note also that z_0 with zero absorption is identically equal to λ, i.e. the extrapolation distance. These values will be compared with the transport theory values in the next section.

3. Numerical calculations and discussion

Here, we shall describe the methods used to solve the integral equation (29) and the critical values of refractive index for both specular and diffuse reflection.

3.1. Diffuse reflection

While this particular mechanism is not the most realistic physically, it does have the advantage of mathematical simplicity in the sense that the solution of the associated integral equation is relatively easy to obtain as seen in equation (32). Before discussing the case where $r(\mu)$ takes the Fresnel form, let us consider a much simpler case in which $r(\mu) = \gamma$, where $\gamma \leqslant 1$ and is independent of μ. This case was considered by Williams (1975) for $c = 1$, i.e. no absorption. For $r(\mu) = \gamma$, we can evaluate all the integrals in both (32) and (40) by using the properties of the H-function. We find

$$\frac{A_0}{J_0} = \frac{\nu}{2\sqrt{1-c}} + \gamma\left[\nu h_1 + \frac{2}{c}\frac{(1-\nu)}{H(1)} - \frac{2}{c}(1-\nu)\sqrt{1-c} - \frac{\nu}{2\sqrt{1-c}}\right] \tag{55}$$

where

$$h_1 = \int_0^1 {\rm d}\mu\,\mu H(\mu) \tag{56}$$

and

$$z_0 = z_0(c) + \frac{1}{2\nu}\log\left[\frac{1-\gamma(1-2h_1\sqrt{1-c})}{1-\gamma\left(1-2h_1\sqrt{1-c}+\frac{8(1-c)}{c\nu}\right)}\right]. \tag{57}$$

The critical value of γ at which z_0 no longer exists occurs when

$$\frac{1}{\gamma_{\rm c}} = 1 - 2h_1\sqrt{1-c} + \frac{8(1-c)}{c\nu}. \tag{58}$$

This function is given in table 1 for a range of values of c. Thus, as c varies between 0 and 1, $\gamma_{\rm c}$ also varies between 0 and 1.

Table 1. Critical value of reflection coefficient.

c	γ_c	c	γ_c
1	1	0.9	0.4609
0.9999	0.9772	0.8	0.3167
0.999	0.9294	0.5	0.1176
0.99	0.7918	0.2	0.0312
0.95	0.5861	0.0	0

Table 2. Critical values of refractive index for diffuse reflection.

c	n_c	c	n_c	c	n_c
1	∞	0.96	1.616	0.6	1.214
0.9999	4.980	0.94	1.517	0.5	1.194
0.999	3.189	0.92	1.455	0.4	1.180
0.99	2.055	0.90	1.410	0.3	1.168
0.98	1.815	0.8	1.296	0.2	1.154
0.97	1.694	0.7	1.244	0	1

Let us return now to the case of the Fresnel reflection coefficient as in equation (30). After some algebra, we can write

$$z_0 = z_0(c) + \frac{1}{2\nu}\log\left(\frac{A_0^+}{A_0^-}\right) \tag{59}$$

where

$$A_0^+ = \frac{1}{2} - r_1 + \sqrt{1-c}\int_0^1 \mathrm{d}\mu\,\mu r(\mu)H(\mu) \tag{60}$$

$$A_0^- = \frac{1}{2} - r_1 - \sqrt{1-c}\int_0^1 \mathrm{d}\mu\,\mu r(\mu)\frac{(1+\nu\mu)}{(1-\nu\mu)}H(\mu). \tag{61}$$

For $c = 1$,

$$z_0 = 0.71044\ldots + \frac{2}{\sqrt{3}\,(1-2r_1)}\int_0^1 \mathrm{d}\mu\,\mu r(\mu)H(\mu). \tag{62}$$

The critical value of the refractive index n_c is given by the root of

$$\frac{1}{2} - r_1 = \sqrt{1-c}\int_0^1 \mathrm{d}\mu\,\mu r(\mu)\frac{(1+\nu\mu)}{(1-\nu\mu)}H(\mu). \tag{63}$$

The associated value of the extrapolation distance d is obtained from equation (43). Table 2 shows the critical values of the refractive index versus c.

Table 3 shows values of the extrapolated endpoint for a range of values of c. Table 4 shows values of the extrapolation distance which continues to be meaningful for $n > n_c$.

3.2. *Specular reflection*

Specular reflection is the more realistic case and requires the solution of the integral equation (29) for $\phi(0, -\mu)$. With this knowledge, we may use equations (37) and (38) to get

Table 3. Extrapolated endpoint for diffuse reflection × c.

n	$c = 1.0$	0.99	0.98	0.97	0.96	0.94	0.92	0.90
1	0.7104	0.7104	0.7104	0.7104	0.7104	0.7104	0.7105	0.7106
1.1	0.9390	0.9386	0.9382	0.9378	0.9373	0.9364	0.9353	0.9342
1.2	1.2407	1.2446	1.2485	1.2525	1.2566	1.2651	1.2740	1.2833
1.3	1.5961	1.6143	1.6338	1.6547	1.6773	1.7282	1.7892	1.8648
1.4	2.0006	2.0521	2.1106	2.1781	2.2574	2.4712	2.8390	3.9328
1.5	2.4531	2.5707	2.7179	2.9113	3.1853	4.7092	–	–
1.6	2.9533	3.1945	3.5471	4.1581	6.0525	–	–	–
1.7	3.5020	3.9692	4.8742	–	–	–	–	–
1.8	4.1000	4.9884	9.0726	–	–	–	–	–
1.9	4.7487	6.4940	–	–	–	–	–	–
2.0	5.4492	9.5589	–	–	–	–	–	–

Table 4. Extrapolation distance for diffuse reflection.

n	$c = 1.0$	0.99	0.98	0.97	0.96	0.94	0.92	0.90
1	0.7104	0.7140	0.7175	0.7211	0.7248	0.7321	0.7396	0.7472
1.1	0.9390	0.9397	0.9405	0.9411	0.9419	0.9432	0.9446	0.9460
1.2	1.2407	1.2378	1.2348	1.2317	1.2285	1.2220	1.2151	1.2079
1.3	1.5961	1.5890	1.5816	1.5740	1.5663	1.5501	1.5333	1.5157
1.4	2.0006	1.9887	1.9764	1.9637	1.9507	1.9235	1.8949	1.8650
1.5	2.4531	2.4358	2.4180	2.3995	2.3804	2.3405	2.2983	2.2541
1.6	2.9533	2.9302	2.9062	2.8812	2.8553	2.8008	2.7431	2.6823
1.7	3.5020	3.4725	3.4416	3.4093	3.3757	3.3048	3.2293	3.1495
1.8	4.1000	4.0635	4.0250	3.9846	3.9425	3.8530	3.7572	3.6557
1.9	4.7487	4.7044	4.6576	4.6083	4.5565	4.4462	4.3274	4.2011
2.0	5.4492	5.3966	5.3407	5.2814	5.2189	5.0851	4.9403	4.7860

$$A_0^+ = A_0 - (1-\nu)\int_0^1 \frac{\mathrm{d}\mu}{1+\mu}\mu H(\mu) r(\mu)\phi(0,-\mu) \tag{64}$$

$$A_0^- = A_0 - (1+\nu)\int_0^1 \frac{\mathrm{d}\mu\,(1+\nu\mu)}{(1+\mu)(1-\nu\mu)}\mu H(\mu) r(\mu)\phi(0,-\mu). \tag{65}$$

Thus we calculate z_0 and d from equations (40) and (43).

To solve equation (29) we employ the NAG Library routine D05ABF for Fredholm integral equations. This procedure expands the solution as an N-term Chebyshev series and solves for the coefficients. An interpolation method then gives the solution at any desired point. Having found the solution we can then calculate the reflected photon flux

$$\phi_{\mathrm{ref}}(0,\mu) = r(\mu)\phi(0,-\mu). \tag{66}$$

The transmitted photon flux must take into account the refraction angle thus we have, after using Snell's law

$$\phi_{\mathrm{trans}}(0,\mu_0) = (1-r(\mu))\phi(0,-\mu)/n^2. \tag{67}$$

In equation (67), $\mu_0 = \sqrt{1-n^2+n^2\mu^2}$ and $\mu_c \leqslant \mu \leqslant 1$, $0 \leqslant \mu_0 \leqslant 1$.

Table 5 shows the critical values of the refractive index at which the extrapolated endpoint ceases to exist. Interestingly, the values are close to those for diffuse reflection.

Table 5. Critical values of refractive index for specular reflection.

c	n_c	c	n_c
0.9999	4.992	0.95	1.617
0.999	3.206	0.94	1.556
0.99	2.090	0.93	1.544
0.98	1.859	0.92	1.522
0.97	1.745	0.91	1.500
0.96	1.670	0.90	1.482

Table 6. Extrapolated endpoint for specular reflection $\times$ c.

n	$c = 1.0$	0.99	0.98	0.97	0.96	0.94	0.92	0.90
1	0.7104	0.7104	0.7104	0.7105	0.7105	0.7105	0.7106	0.7106
1.1	0.8810	0.8780	0.8751	0.8721	0.8692	0.8634	0.8576	0.8518
1.2	1.1455	1.1415	1.1373	1.1330	1.1285	1.1192	1.1094	1.0992
1.3	1.4747	1.4764	1.4780	1.4793	1.4805	1.4823	1.4831	1.4828
1.4	1.8595	1.8813	1.9046	1.9297	1.9567	2.0183	2.0929	2.1869
1.5	2.2972	2.3653	2.4447	2.5392	2.6549	3.0007	3.8389	–
1.6	2.7859	2.9468	3.1597	3.4649	3.9743	–	–	–
1.7	3.3252	3.6613	4.2126	5.5269	–	–	–	–
1.8	3.9145	4.5790	6.3135	–	–	–	–	–
1.9	4.5565	5.8703	–	–	–	–	–	–
2.0	5.2525	8.1148	–	–	–	–	–	–

Table 7. Extrapolation distance for specular reflection.

n	$c = 1.0$	0.99	0.98	0.97	0.96	0.94	0.92	0.90
1	0.7104	0.7140	0.7175	0.7211	0.7248	0.7321	0.7396	0.7472
1.1	0.8810	0.8800	0.8792	0.8784	0.8777	0.8766	0.8759	0.8754
1.2	1.1455	1.1380	1.1307	1.1235	1.1164	1.1028	1.0897	1.0773
1.3	1.4747	1.4593	1.4441	1.4291	1.4143	1.3855	1.3576	1.3307
1.4	1.8595	1.8350	1.8108	1.7869	1.7633	1.7171	1.6721	1.6284
1.5	2.2972	2.2625	2.2281	2.1942	2.1606	2.0947	2.0304	1.9679
1.6	2.7859	2.7399	2.6943	2.6492	2.6045	2.5168	2.4311	2.3476
1.7	3.3252	3.2666	3.2087	3.1513	3.0945	2.9828	2.8736	2.7670
1.8	3.9145	3.8424	3.7710	3.7003	3.6302	3.4924	3.3575	3.2257
1.9	4.5565	4.4696	4.3835	4.2982	4.2138	4.0474	3.8845	3.7253
2.0	5.2525	5.1495	5.0475	4.9464	4.8463	4.6490	4.4558	4.2667

Table 6 shows the values of the extrapolated endpoint, and table 7 shows the extrapolation distance. All values are in close agreement with those of Aronson (1995).

In order to illustrate the form taken by the angular distributions at the surface of the half-space, we show figures 1 and 2. In figure 1, we show the reflected distribution for $c = 0.99$ and four values of refractive index. The large 'bite' taken out of the curve is due to the internal reflection and transmission. The abrupt discontinuity at $\vartheta = \vartheta_c$ arises from the onset of internal reflection. This discontinuity causes some numerical difficulty when solving the integral equation (29). It is found necessary to set $N = 500$ in the NAG routine to obtain satisfactory accuracy. Figure 2 shows the transmitted flux. This has no discontinuity since the

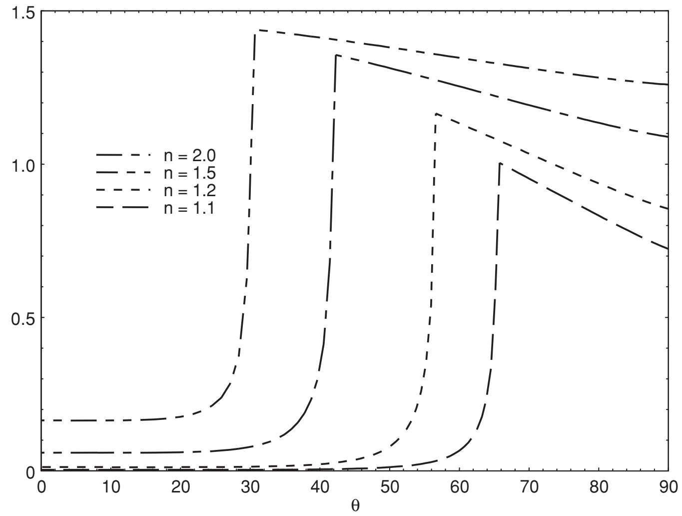

Figure 1. Reflected angular distribution at surface for $c = 0.99$.

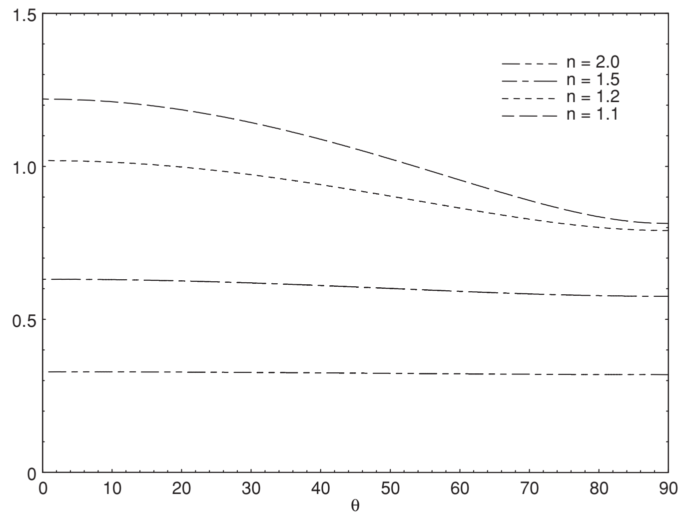

Figure 2. Transmitted angular distribution at surface for $c = 0.99$.

refracted ray bends away from the normal when going from a dense to a less dense medium thus when the internal critical angle is reached the refracted ray moves parallel to the surface.

The numerical results for diffusion theory are given in tables 8 and 9 for diffuse reflection, and in tables 10 and 11 for specular reflection. We note that the values of the critical refractive index at which the extrapolated endpoint ceases to exist are within 8% of the transport values for $c > 0.99$. This is a remarkable achievement for diffusion theory. In addition, the extrapolation distance is within 6% for $c > 0.99$ but deteriorates rapidly as c decreases. The extrapolated endpoint is not reproduced well except for very small values of $1 - c$, especially as n approaches its critical value. In figure 3, we compare diffusion and transport theory, with specular reflection, for the extrapolation distance d. The full line is diffusion theory, which is

Table 8. Critical values of refractive index for diffuse reflection (diffusion theory).

c	n_c	c	n_c	c	n_c
1	∞	0.96	1.550	0.6	1.077
0.9999	4.971	0.94	1.442	0.5	1.048
0.999	3.168	0.92	1.372	0.4	1.025
0.99	2.012	0.90	1.322	0.3	1.007
0.98	1.762	0.8	1.186	0.2	1.000
0.97	1.633	0.7	1.119	0	1

Table 9. Extrapolated endpoint for diffuse reflection × c and extrapolation distance[a] d (diffusion theory).

n	$c = 1.0$	0.99	0.98	0.97	0.96	0.94	0.92	0.90
1	0.6667	0.6630	0.6592	0.6555	0.6518	0.6442	0.6367	0.6290
1.1	0.9883	0.9881	0.9881	0.9883	0.9887	0.9900	0.9923	0.9958
1.2	1.3423	1.3536	1.3662	1.3802	1.3958	1.4330	1.4808	1.5445
1.3	1.7334	1.7706	1.8135	1.8636	1.9229	2.0836	2.3535	3.0001
1.4	2.1641	2.2522	2.3616	2.5025	2.6942	3.4943	–	–
1.5	2.6365	2.8183	3.0729	3.4725	4.2875	–	–	–
1.6	3.1524	3.5020	4.1037	5.7867	–	–	–	–
1.7	3.7137	4.3650	6.1037	–	–	–	–	–
1.8	4.3221	5.5431	–	–	–	–	–	–
1.9	4.9793	7.4465	–	–	–	–	–	–
2.0	5.6871	13.967	–	–	–	–	–	–

[a] Extrapolation distance is the same as extrapolated endpoint for $c = 1$.

Table 10. Critical values of refractive index for specular reflection (diffusion theory).

c	n_c	c	n_c
0.9999	4.981	0.95	1.534
0.999	3.189	0.94	1.487
0.99	2.048	0.93	1.449
0.98	1.803	0.92	1.417
0.97	1.676	0.91	1.390
0.96	1.594	0.90	1.367

Table 11. Extrapolated endpoint for specular reflection × c and extrapolation distance[a] d (diffusion theory).

n	$c = 1.0$	0.99	0.98	0.97	0.96	0.94	0.92	0.90
1	0.6667	0.6630	0.6592	0.6555	0.6518	0.6442	0.6367	0.6290
1.1	0.9002	0.8986	0.8970	0.8954	0.8940	0.8914	0.8892	0.8875
1.2	1.2039	1.2096	1.2159	1.2229	1.2307	1.2491	1.2720	1.3009
1.3	1.5604	1.5841	1.6109	1.6414	1.6763	1.7644	1.8906	2.0920
1.4	1.9657	2.0269	2.1001	2.1896	2.3025	2.6609	3.7283	–
1.5	2.4186	2.5514	2.7262	2.9725	3.3640	–	–	–
1.6	2.9193	3.1828	3.5907	4.3888	–	–	–	–
1.7	3.4683	3.9683	5.0191	–	–	–	–	–
1.8	4.0666	5.0064	12.481	–	–	–	–	–
1.9	4.7154	6.5556	–	–	–	–	–	–
2.0	5.4161	9.8425	–	–	–	–	–	–

[a] Extrapolation distance is the same as extrapolated endpoint for $c = 1$.

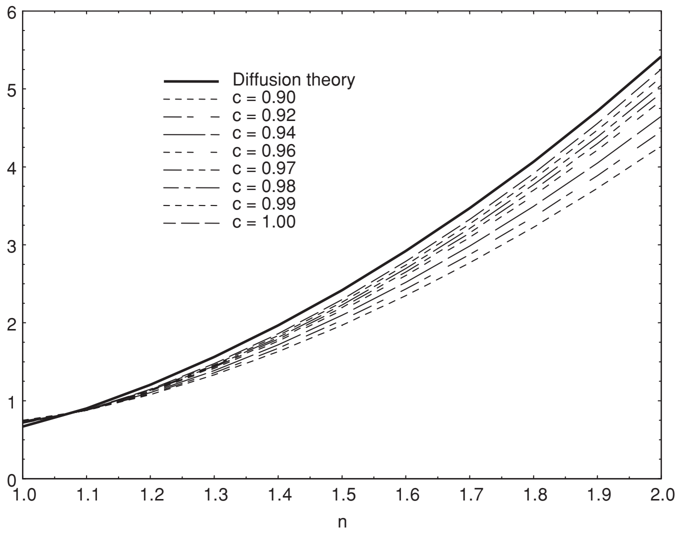

Figure 3. Extrapolation distance for specular reflection. Transport versus diffusion theory.

independent of c; the other lines denote transport theory for the associated values of c. We note that for $c < 0.99$ the agreement is good over the range of refractive index given. It deteriorates, however, for smaller c and larger n. One can draw the conclusion that the use of the extrapolated endpoint as a boundary condition for this type of problem should be avoided and the more useful boundary condition involving the extrapolation distance used.

Finally, we wish to comment on the nature of the shape of $\phi_0(x)$ in $x > 0$. We have already found the asymptotic part of $\phi_0(x)$ due to the poles at $s = \pm\nu$ and this is given by equation (36). However, there still remains the contribution from the cut and the embedded pole. It is straightforward, if tedious, to obtain this term and we give it below as

$$\phi_{\mathrm{trans}}(x) = -A_0 \int_0^1 \frac{\mathrm{d}\mu\, \mathrm{e}^{-x/\mu} g(c,\mu)}{(1+\nu\mu)H(\mu)} + \int_0^1 \mathrm{d}\mu\, \mathrm{e}^{-x/\mu} \left(1 - \frac{c\mu}{2}\log\left(\frac{1+\mu}{1-\mu}\right)\right) g(c,\mu)\phi(0,\mu)$$
$$+ \frac{c}{2}\int_0^1 \frac{\mathrm{d}w\,(1+w)\,\mathrm{e}^{-x/w} g(c,w)}{(1+\nu w)H(w)} P\int_0^1 \frac{\mathrm{d}\mu\, \mu\phi(0,\mu)H(\mu)(1+\nu\mu)}{(1+\mu)(w-\mu)}. \tag{68}$$

The term $\phi(0,\mu) = r(\mu)\phi(0,-\mu)$ for specular reflection and $\phi(0,\mu) = r(\mu)J_0$ for diffuse reflection. The function $g(c,\mu)$ is given by

$$\frac{1}{g(c,\mu)} = \left(1 - \frac{c\mu}{2}\log\left(\frac{1+\mu}{1-\mu}\right)\right)^2 + \left(\frac{c\pi\mu}{2}\right)^2. \tag{69}$$

It is instructive to note that in the case of specular reflection with $r(\mu) = 1$, we have perfect reflection and therefore there should be a mirror image of $\phi_0(x)$ in $x < 0$. Although it is not easy to see this from (36) and (68), it may readily be shown from equation (25), and we obtain

$$\phi(x,\mu) = \phi(-x,-\mu) = \frac{\lambda c}{2}\left[\frac{\mathrm{e}^{\nu x}}{1+\nu\mu} + \frac{\mathrm{e}^{-\nu x}}{1-\nu\mu}\right]. \tag{70}$$

Alternatively, we may convert the integro-differential equation into integral form for $\phi_0(x)$. Using both diffuse and specular reflection we find, with $r(\mu) = \gamma_{\mathrm{s}}$ for specular and $r(\mu) = \gamma_{\mathrm{d}}$ for diffuse, the following integral equation

$$\phi_0(x) = \frac{c}{2}\int_0^\infty \mathrm{d}x'\, H(x,x')\phi_0(x') \tag{71}$$

Table 12. Extrapolated endpoint for diffuse and specular reflection using a variational method.

n	$z_0(s)$	$z_0^*(s)$	$z_0(d)$	$z_0^*(d)$
1.1	0.8799	0.8810	0.9431	0.9390
1.2	1.1391	1.1455	1.2476	1.2407
1.3	1.4625	1.4747	1.6044	1.5961
1.4	1.8428	1.8595	2.0097	2.0006
1.5	2.2765	2.2972	2.4626	2.4531
1.6	2.7620	2.7859	2.9631	2.9533
1.7	3.2990	3.3252	3.5119	3.5020
1.8	3.8875	3.9145	4.1101	4.1000
1.9	4.5284	4.5565	4.7588	4.7487
2.0	5.2224	5.2525	5.4593	5.4492

where

$$H(x,x') = E_1(|x-x'|) + 2\gamma_d E_2(x)E_2(x') + \gamma_s E_1(|x-x'|). \tag{72}$$

This equation was first derived by Williams (1975). For $\gamma_d = 0$, $\gamma_s = 1$, i.e. pure specular reflection, we can write equation (71) as

$$\phi_0(x) = \frac{c}{2}\int_0^\infty dx'\, E_1(|x-x'|)\phi_0(x') + \frac{c}{2}\int_{-\infty}^0 dx'\, E_1(|x-x'|)\phi_0(-x'). \tag{73}$$

Then if $\phi_0(x) = \phi_0(-x)$, we have an infinite medium equation and can show that $\phi_0(x) = \cosh(\nu x)$ is a solution, i.e. a mirror image. On the other hand, when $\gamma_s = 0$ and $\gamma_d = 1$, i.e. pure diffuse reflection, no such solution exists. This too is to be expected and the appropriate form for $\phi_0(x)$ for this case must be obtained from equation (68).

As a postscript, it is worth noting that in Williams (1975), we introduced a variational method to solve for the extrapolated endpoint in the special case of $c = 1$. We have repeated those calculations using the Fresnel form of $r(\mu)$ and a simple trial function of the form $\phi_0(x) \sim x + z_0$. We present the results in table 12 for specular and diffuse reflection, where the exact values are also given for comparison. Considering the crudity of the trial function the accuracy of the variational method is very high. In the table, $z_0(s)$ and $z_0(d)$ are the variational results for specular and diffuse reflection, respectively. $z_0^*(s)$ and $z_0^*(d)$ are the exact values.

In conclusion, we should like to comment on the results of some earlier workers. The papers by Razi Naqvi *et al* (1991), Razi Naqvi (1993) and Abdel Krim *et al* (1998) extend the variational work of Williams (1975) by using an improved trial function. The paper by Atalay (2000) is of particular interest, however, since it is an attempt to produce an exact solution for the specular case with a constant value of the reflection coefficient and with $c < 1$. For a constant specular reflection coefficient, Atalay uses the singular eigenfunction technique (Williams 1971) and obtains an integral equation which is analogous to equation (29) with $r(\mu) = \gamma$, $(0 \leqslant \gamma \leqslant 1)$. But he does not solve it exactly. Instead he simply uses the inhomogeneous term as a first iterate and inserts this in the equivalent expressions to (37) and (38). As a result, his numerical values are not as accurate as those obtained by using the methods reported here but are nevertheless very close. Atalay has also extended the work to include linear anisotropic scattering.

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References

Abdel Krim M S and Degheidy A R 1998 Variational approach to the Milne problem with a specular and diffuse reflecting boundary *Ann. Nucl. Energy* **25** 317

Aronson R 1995 Boundary conditions for diffusion of light *J. Opt. Soc. Am.* **12** 2532

Atalay M A 2000 Milne problem for linearly anisotropic scattering and a specularly reflecting boundary *Ann. Nucl. Energy* **27** 1483

Beckmann P and Spizzichino A 1963 *The Scattering of Electromagnetic Waves from Rough Surfaces* (Oxford: Pergamon)

Born M and Wolf E 2002 *Principles of Optics* (Cambridge: Cambridge University Press)

Chandrasekhar S 1960 *Radiative Transfer* (New York: Dover)

Davison B 1957 *Neutron Transport Theory* (Oxford: Oxford University Press)

Freund I 1992 Surface reflections and boundary conditions for diffusive photon transport *Phys. Rev.* A **45** 8854

Freund I and Berkovits R 1990 Surface reflection and optical transport through random media: coherent backscattering, optical memory effect and dynamical correlation *Phys. Rev.* B **41** 496

Kuznetsov E S 1942 Light scattering in a medium in contact with a reflecting wall of given albedo *Izv. AN SSSR Ser. Geor.-Geophys.* **5**

Kuznetsov E S 1945 On the computation of diffusely reflected light by the earth surface in the problem of light scattering in the atmosphere *Izv. AN SSSR Ser. Geor.-Geophys.* **8**

Nieuwenhuizen Th M and Luck J M 1993 Skin layer of diffusive media *Phys. Rev.* E **48** 569

Razi Naqvi K 1993 Milne's problem for a non-capturing medium: accurate analytic approximations for particle density and emergent angular distribution *J. Quant. Spectrosc. Radiat. Transfer* **50** 59

Razi Naqvi K, El-Shahat A and Mork K J 1991 Variational approach to the Milne problem with a gray boundary *Phys. Rev.* A **44** 994

Sobolev V V 1948 On brightness coefficients on a plane layer in a turbid medium *DAN SSSR* **61**

Sobolev V V 1963 *A Treatise on Radiative Transfer* (Princeton, NJ: Van Nostrand)

Titchmarsh E C 1937 *Introduction to the Theory of Fourier Integrals* (Oxford: Clarendon)

Van de Hulst H 1948 Scattering in planetary atmospheres *Astrophys. J.* **107** 220

Williams M M R 1971 *Mathematical Methods in Particle Transport Theory* (London: Butterworths)

Williams M M R 1975 The influence of specular and diffuse reflection on the extrapolation distance *Atomkernenergie* **25** 19

Zhu J X, Pine D J and Weitz D A 1991 Internal reflection of diffusive light in random media *Phys. Rev.* A **44** 3948