

Exact interface conditions for photon diffusion

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ABSTRACT

An exact interface condition for photon diffusion is derived. The condition involves a single parameter, which depends on the index of refraction. Exact formulas are given for this parameter, which is also plotted.

1 INTRODUCTION

The imaging of subsurface features is a difficult and complicated process. In the analysis of such problems diffusion theory has found a place. It is an approximate theory, often quite bad, but often remarkably good. Its prime virtue is that calculations with diffusion theory are relatively easy. We have presented in these proceedings a series of papers studying the use of near-infrared radiation for subsurface imaging for medical applications¹⁻⁴. The prime calculational method we have used is Monte Carlo. Because the Monte Carlo calculations are long and expensive, we have made diffusion calculations to compare with Monte Carlo, and to replace it where feasible. Other groups have used diffusion theory for the same purpose.

In using diffusion theory to obtain particle distributions, one must specify boundary conditions. Since the diffusion equation is a second-order partial differential equation in space, one boundary condition is required at the exterior boundary and two conditions are required at any interior interface between two media. For particle diffusion, these conditions are that the intensity and flux are continuous across the interface. Continuity of flux is demanded by the diffusion equation itself, if one integrates it across the narrow interface region. From the physical point of view, the diffusion equation is a continuity equation for the particles. Continuity of flux expresses the same thing—a finite number of particles can't be absorbed in an infinitesimally small region. The intensity is taken continuous across an interface because the diffusing particles don't recognize an interface when they cross it. The collision probabilities change on the other side, but there are no road signs at the interface itself.

For photons the situation is different. The reasoning that requires the flux to be continuous applies here, too. If the index of refraction is different on the two sides of the interface, though, that is a definite road sign to photons. Light, unlike molecules or neutrons, is reflected and refracted wherever the index of refraction changes. In this paper we give the boundary condition for photons that replaces continuity of intensity.

The problem has been considered previously^{5,6}. In this paper we give an exact formula for this second interface condition. Just as the interface conditions for particles are not suitable at an exterior vacuum boundary, so with the results we discuss here. What is required in that case is a modified extrapolated end point condition.

2 PARTICLE DIFFUSION

In this section we give a standard elementary kinetic theory discussion of diffusion, which gives (1) the diffusion coefficient, and (2) the interface conditions for particles⁷. This stresses the physical (as distinguished from mathematical) approximations involved and also makes clear what has to be modified for photons.

We make the standard diffusion theory assumptions:

- (1). Plane geometry
- (2). Isotropic scattering
- (3). Slowly varying particle distribution.

Assumption (2) can be modified, if the differential cross section is not too anisotropic, by replacing the total cross section by the transport cross section. We do not discuss this further here.

Taking the stratification perpendicular to the z -axis, we compute the downward flux across the xy -plane to be

$$J_- = \int_{z>0} \frac{\Sigma_s \phi(z) e^{-\Sigma_t r}}{4\pi r^2} d\mathbf{r}, \quad (1)$$

where

Σ_t = macroscopic total cross section

Σ_s = macroscopic scattering cross section

$\phi(z)$ = intensity at z

r = distance of last scattering point from point of flux measurement.

We take the point of the flux measurement as the origin. The integral is taken over the half-space $z > 0$.

In evaluating this expression one generally ignores the absorption as being negligibly small, so that Σ_s is replaced by Σ_t . Expanding $\phi(z)$ to first order gives

$$\phi(z) = \phi + z\phi' = \phi + r \cos \theta \phi', \quad (2)$$

where ϕ and $\phi' = \partial\phi/\partial z$, are both evaluated at $z = 0$, and θ is the angle between the ray to the last scattering point and the z -axis. Note that this describes a Lambertian distribution. That is not something we assume for convenience or for lack of anything better. It follows when the spatial variation of the intensity is weak enough so that the first-order expansion is valid.

Putting Eq. (2) into Eq. (1) and performing the indicated integrations results in

$$J_- = (\phi/2) \int_0^1 \mu d\mu + (\phi'/2\Sigma_t) \int_0^1 \mu^2 d\mu = \phi/4 + \phi'/6\Sigma_t. \quad (3)$$

Similarly, the upward flux through the plane $z = 0$ is

$$J_+ = (\phi/2) \int_0^1 \mu d\mu - (\phi'/2\Sigma_t) \int_0^1 \mu^2 d\mu = \phi/4 - \phi'/6\Sigma_t. \quad (4)$$

The *net* upward flux is

$$J = J_+ - J_-. \quad (5)$$

Away from an interface, where ϕ is continuous, this gives

$$J = -(1/3\Sigma_t)\phi'. \quad (6)$$

The basic approximation of diffusion is Fick's law:

$$\mathbf{J} = -D\nabla\phi. \quad (7)$$

Comparison with Eq. (6) gives the usual formula for the diffusion coefficient:

$$D = -1/3\Sigma_t. \quad (8)$$

Thus we may rewrite Eqs. (3) and (4) as

$$J_- = (1/4)\phi + (1/2)D\phi' = (1/4)\phi - (1/2)J \quad (9)$$

$$J_+ = (1/4)\phi - (1/2)D\phi' = (1/4)\phi + (1/2)J. \quad (10)$$

If there is a material boundary at the interface, so that the cross sections are different on the two sides, then D is discontinuous. J is continuous, so ϕ' is discontinuous.

3 PHOTON DIFFUSION

For photons, one is concerned also with a change in the index of refraction. The assumption in this paper is that the index of refraction changes over a distance small compared to a mean free path. In that case it can be regarded as discontinuous. The big difference from the analysis for particles is that there is now reflection and refraction at the interface. The reflection coefficient R will depend on which medium the light is coming from and on the angle of incidence, and therefore on its cosine, μ .

Let the total cross section, diffusion coefficient and index of refraction be Σ_{t1} , D_1 and n_1 respectively for $z > 0$, and Σ_{t2} , D_2 and n_2 for $z < 0$. The relative index of refraction in going from the upper medium to the lower one is $n = n_2/n_1$. The only necessary modification to the previous section is that a factor $1 - R$ must appear in the integrand in Eq. (1) and in the corresponding integral for J_+ . This factor persists into Eqs. (3) and (4). We must also take into account the discontinuity of ϕ at the interface, taking $\phi = \phi_1$ in the expressions for J_- and $\phi = \phi_2$ in the expressions for J_+ .

In all generality we can take $n > 1$. For convenience we write the cosine of the angle with the normal in the lower medium as μ' . Snell's law can be written as

$$1 - \mu^2 = n^2(1 - \mu'^2). \quad (11)$$

Writing the reflection coefficient for radiation incident from above as $R(\mu, n)$ and that for radiation incident from below as $R(\mu', 1/n)$, we have

$$J_- = (\phi_1/2) \int_0^1 [1 - R(\mu, n)]\mu d\mu + (\phi'_1/2\Sigma_{t1}) \int_0^1 [1 - R(\mu, n)]\mu^2 d\mu \quad (12)$$

$$J_+ = (\phi_2/2) \int_0^1 [1 - R(\mu', 1/n)]\mu d\mu - (\phi'_2/2\Sigma_{t2}) \int_0^1 [1 - R(\mu', 1/n)]\mu^2 d\mu, \quad (13)$$

or finally,

$$J_- = (1/2)A_1\phi_1 - (1/2)B_1J \quad (14)$$

$$J_+ = (1/2)A_2\phi_2 + (1/2)B_2J, \quad (15)$$

where J , of course, is the same in both equations.

Here

$$A_1 = \int_0^1 [1 - R(\mu, n)]\mu d\mu \quad (16)$$

$$A_2 = \int_{\mu_c}^1 [1 - R(\mu', 1/n)] \mu' d\mu' \quad (17)$$

$$B_1 = 3 \int_0^1 [1 - R(\mu, n)] \mu^2 d\mu \quad (18)$$

$$B_2 = 3 \int_{\mu_c}^1 [1 - R(\mu', 1/n)] \mu'^2 d\mu', \quad (19)$$

where μ_c is the cosine of the critical angle, beyond which there is total reflection:

$$\mu_c = \sin^{-1}(1/n). \quad (20)$$

Subtracting Eq. (14) from Eq. (15) gives

$$J = (1/2)[A_2\phi_2 - A_1\phi_1 + (B_1 + B_2)J]. \quad (21)$$

The reflection coefficient is obtained directly from the Fresnel relations giving the amplitude of reflected and transmitted light at an interface⁸. In accord with the randomizing nature of diffusion, we must take the light incident on the interface to be unpolarized. The appropriate reflection coefficient is then an average of those for the two possible plane polarizations. It is

$$R(\mu, n) = (1/2) \left[\left(\frac{\mu - n\mu'}{\mu + n\mu'} \right)^2 + \left(\frac{n\mu - \mu'}{n\mu + \mu'} \right)^2 \right]. \quad (22)$$

Keijzer et. al.⁶ approximated the reflection coefficient by an exponential function and integrated the resulting expressions for A_1 , A_2 and $B_1 + B_2$. We demonstrate an exact integration here.

4 EXACT BOUNDARY CONDITION

It is apparent from Eq. (22) that $R(\mu, n) = R(\mu', 1/n)$. From Eq. (11), $\mu d\mu = n^2 \mu' d\mu'$. It follows immediately that $A_1 = n^2 A_2$. This result has previously been obtained by Cohen⁵ in the case in which there is no net flux, and it is also perhaps implicit in some work of Preisendorfer⁹. We find the result here in complete generality. Then from Eq. (21),

$$\phi_2 - n^2 \phi_1 = C(n)J, \quad (23)$$

where

$$C(n) = (2 - B_1 - B_2)/A_2. \quad (24)$$

The necessary integrals can be performed analytically. The substitutions $a = \sqrt{n^2 - 1}$, $t = \sqrt{a^2 + \mu^2}/a$, $g = (n^2 - 1)/(n^2 + 1)$, $q = (n - 1)/(n + 1)$, $p = \sqrt{q}$ and $y = t^2$ give

$$A_1 = 1/2 - \frac{a^2}{16} \int_q^1 \left[y^2 + \left(\frac{y - g}{1 - gy} \right)^2 \right] \frac{1 - y^2}{y^2} dy \quad (25)$$

$$B_1 = 1 - \frac{3a^3}{16} \int_p^1 \left[t^4 + \left(\frac{t^2 - g}{1 - gt^2} \right)^2 \right] \frac{1 - t^2 - t^4 + t^6}{t^3} dt. \quad (26)$$

$$B_2 = 1 - \left(\frac{a}{n} \right)^3 - \frac{3}{16} \left(\frac{a}{n} \right)^3 \int_p^1 \left[t^4 + \left(\frac{t^2 - g}{1 - gt^2} \right)^2 \right] \frac{1 + t^2 - t^4 - t^6}{t^3} dt. \quad (27)$$

The integrands are rational functions of y or t and the integrals can be performed exactly. The results are

$$A_1 = \frac{5n^6 + 8n^5 + 6n^4 - 5n^3 - n - 1}{3(n^2 + 1)^2(n^2 - 1)(n + 1)} - \frac{4n^4(n^4 + 1)}{(n^2 + 1)^3(n^2 - 1)^2} \log n + \frac{n^2(n^2 - 1)^2}{2(n^2 + 1)^3} \log \frac{n + 1}{n - 1} \quad (28)$$

$$B_1 = 1 - \frac{3(n^2 - 1)^{3/2}}{16}(I_0 - I_1 - I_2 + I_3) \quad (29)$$

$$B_2 = 1 - \frac{(n^2 - 1)^{3/2}}{n^3} \left[1 + \frac{3}{16}(I_0 + I_1 - I_2 - I_3) \right], \quad (30)$$

where

$$I_n = (1 - p^{2n+1})/(2n + 1) + J_n \quad (31)$$

$$J_0 = \frac{16n^4}{(n^2 + 1)^4} K_2 - \frac{8n^2(n^2 - 1)^2}{(n^2 + 1)^4} K_1 - \frac{8n^2(n^2 - 1)}{(n^2 + 1)^3} \left(\frac{1}{p} - 1 \right) + \frac{(n^2 - 1)^2}{3(n^2 + 1)^2} \left(\frac{1}{p^3} - 1 \right) \quad (32)$$

$$J_1 = \frac{16n^4}{(n^2 + 1)^3(n^2 - 1)} K_2 - \frac{8n^2(n^4 + 1)}{(n^2 + 1)^3(n^2 - 1)} K_1 + \frac{(n^2 - 1)^2}{(n^2 + 1)^2} \left(\frac{1}{p} - 1 \right) \quad (33)$$

$$J_2 = \frac{16n^4}{(n^2 + 1)^2(n^2 - 1)^2} K_2 - \frac{8n^2}{(n^2 + 1)^3(n^2 - 1)} K_1 + \frac{(n^2 + 1)^2}{(n^2 - 1)^2} (1 - p) \quad (34)$$

$$J_3 = \frac{16n^4}{(n^2 + 1)(n^2 - 1)^3} K_2 - \frac{8n^2(n^4 + 4n^2 + 1)}{(n^2 + 1)(n^2 - 1)^3} K_1 + \frac{8n^2(n^2 + 1)}{(n^2 - 1)^3} (1 - p) + \frac{(n^2 + 1)^2}{3(n^2 - 1)^2} (1 - p^3) \quad (35)$$

$$K_1 = \sqrt{\frac{n^2 + 1}{n^2 - 1}} \left(\log \frac{\sqrt{n^2 + 1} + \sqrt{n^2 - 1}}{\sqrt{n^2 + 1} + n - 1} + \frac{1}{2} \log n \right) \quad (36)$$

$$K_2 = \frac{n^2 + 1}{4} \left(1 - \frac{p}{n} \right) + \frac{1}{2} K_1 \quad (37)$$

$$p = \sqrt{\frac{n - 1}{n + 1}}. \quad (38)$$

The result for A_1 , in somewhat different form, was known to Walsh¹⁰ in 1926.

5 RESULTS

The results of evaluating Eqs. (28)-(30), together with $A_2 = n^2 A_1$, are shown graphically in Fig. 1 as functions of n . We have used Eqs. (32)-(38) to compute the J_k and have checked the results with a 92-point Gaussian integration. Note that A_i and B_i go to the correct limits when n goes to unity. Figure 2 shows $C(n)$. It is zero, as expected, when $n = 1$ and goes as n^2 for large n .

6 CONCLUSION

We have demonstrated the consistent diffusion interface condition for photons at a discontinuity, in the form of Eq. (23), and evaluated the coefficient $C(n)$ of the flux exactly. This approach is not adequate at a vacuum boundary for the usual reasons that vacuum boundaries require special conditions in diffusion theory. The proper approach is to derive a modified extrapolated end point. Work is in progress on this problem.

7 ACKNOWLEDGEMENTS

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8 REFERENCES

1. H. L. Graber, R. L. Barbour, J. Lubowsky, R. Aronson, B. B. Das, K. M. Yoo and R. Alfano, "Evaluation of Steady-State, Time- and Frequency Domain Data for the Problem of Optical Diffusion Tomography," *SPIE* vol. 1641, accompanying paper in these proceedings, 1992.
2. R. L. Barbour, H. L. Graber, J. Lubowsky, R. Aronson, B. B. Das, K. M. Yoo and R. Alfano, "Imaging of Diffusing Media by a Progressive Iteration Backprojection Method Using Time-Domain Data," *SPIE* vol. 1641, accompanying paper in these proceedings, 1992.
3. Y. Wang, J-H. Chang, R. Aronson, R. L. Barbour, H. L. Graber and J. Lubowsky, "Imaging of Scattering Media by Diffusion Tomography: An Iterative Perturbation Approach," *SPIE* vol. 1641, accompanying paper in these proceedings, 1992.
4. F. H. Schlereth, J. M. Fossaceca, A. D. Keckler and R. L. Barbour, "Imaging of Diffusing Media with a Neural Net Formulation: A Problem in Large-Scale Computation," *SPIE* vol. 1641, accompanying paper in these proceedings, 1992.
5. Arnon Cohen, Ph. D. Dissertation, Carnegie-Mellon University, 1969.
6. Marleen Keijzer, Willem M. Star and Pascal R. M. Storch, "Optical Diffusion in Layered Media," *Appl. Opt.*, vol. 22, pp. 1820-1824, 1988.
7. See, for instance, J. R. Lamarsh, Introduction to Nuclear Reactor Theory, Ch. 5, Addison-Wesley, Reading, MA, 1983.
8. M. Born and E. Wolf, Principles of Optics, Second Edition, Ch. 1, Pergamon Press, New York, 1964.
9. R. W. Preisendorfer, Hydrologic Optics, Sec. 2.6, U. S. Dep't. of Commerce, Nat'l. Oceanic and Atmospheric Administration, 1976.
10. Unpublished report, quoted by J. W. Ryde, *Proc. Roy. Soc. London*, vol. A131, pp. 451-475, 1931.

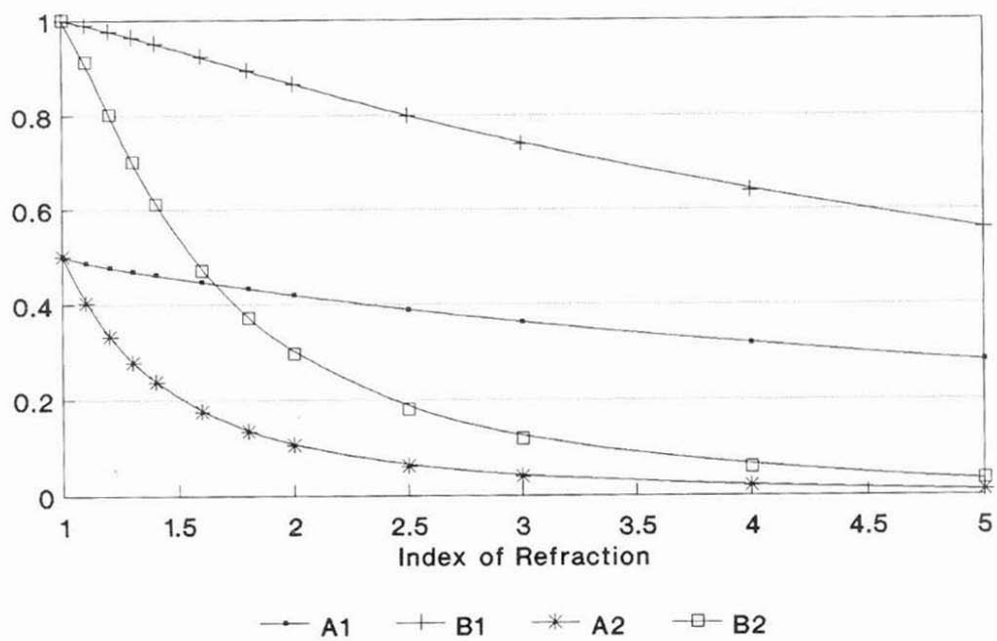


Fig. 1. Boundary Coefficients

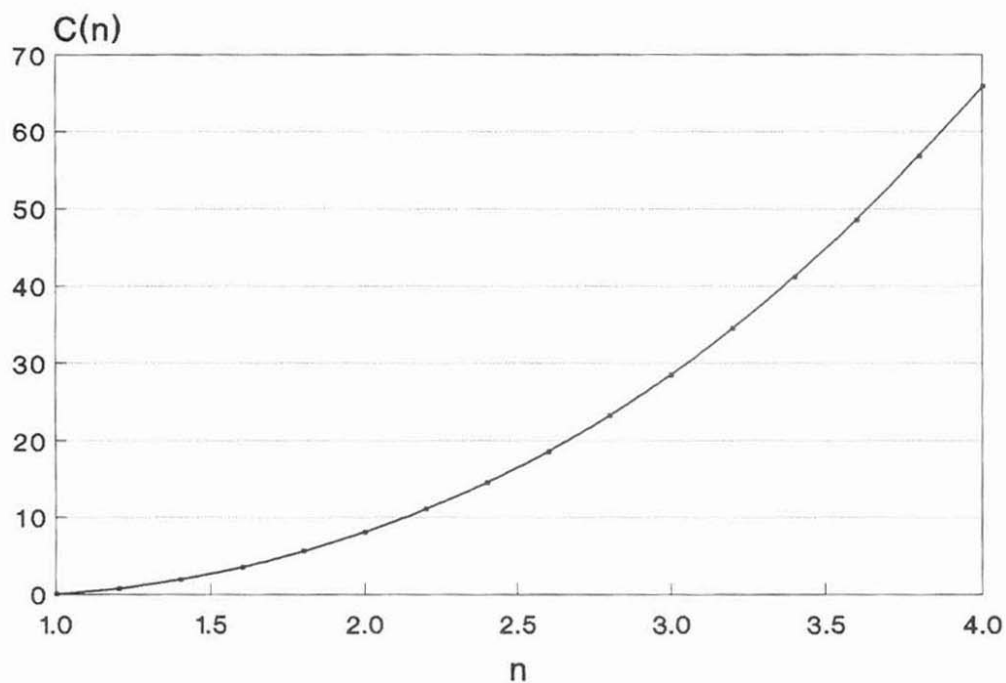


Fig. 2. Boundary Coefficient C(n)