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Analytic Reduction of the Monostatic Lidar Multiple Backscattering Integral

by Daniel T. Gillespie *Research Department*

AUGUST 1985

NAVAL WEAPONS CENTER CHINA LAKE, CA 93555-6001



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FOREWORD

An article by D. T. Gillespie entitled "Stochastic-Analytic Approach to the Calculation of Multiply Scattered Lidar Returns" was published in the *Journal of the Optical Society of America (JOSA) A*, Vol. 2, August 1985, pp. 1307-24. That article derived a formal integral expression for the intensity of laser radiation backscattered from a cloud as a function of the number of cloud particle scatterings. This report reduces that *formal* integral expression to a *computable* integral expression; i.e., an expression that can be numerically evaluated on a digital computer. This reduction of the backscattering integral is an intricate, purely mathematical task, the length of which made its inclusion in the JOSA article impractical.

This work was done at the Naval Weapons Center during 1983 and 1984. It was funded jointly by the Naval Weapons Center Independent Research Program (Program Element 61152N, Task Area ZR000-01-01, Work Unit 138070) and by the Air Force Office of Scientific Research Chemical and Atmospheric Sciences Program (AFOSR-MIPR-84-00007).

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Contents

1. In	troduction
2. EI	iminating the x- and y-Delta Functions
3. El	iminating the <i>t</i> -Delta Function
4. Bo	ounding the Integrand and Integration Domain
5. Ci	ubing the Integration Domain
Refe	rences
Appe	endix: Components of the Vectors \mathbf{e}_i in the xyz-Frame
Figu	res
1	. Trajectory of an <i>n</i> -Scattered Photon
2	2. Geometric Interpretation of the Relations Among the Principle
	Variables in Eqs. (46) and (47) for $n = 2, 3$ and $4 \dots 24$
3	B. Geometric Interpretation of the Relations Among the Principle
	Variables in Eqs. (53), (60) and (62) for <i>n</i> = 2, 3 and 4
4	6. Geometric Interpretation of the Variable v_t defined in Eq. (54) 26
A1	Relative Orientation of the xyz -Frame and the $x'y'z'$ -Frame 30

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1. INTRODUCTION

This report is essentially an appendix to Ref. 1. We shall show here how Eqs. (44) and (49) of Ref. 1 are derived from Eq. (43) of Ref. 1. The derivation is a lengthy, purely mathematical exercise, which requires no assumptions or approximations not already implicit in Eq. (43) of Ref. 1.

The article in Ref. 1 addresses the problem of theoretically calculating the instantaneous power backscattered from a cloud in a so-called "monostatic lidar system." Such a system consists of essentially two components: a pulse-type *laser*, which fires a short, highly collimated pulse into the cloud at time t = 0; and a colocated, conically baffled *receiver*, which measures backscattered radiation at times t > 0. The ultimate quantity to be calculated is $J_n(t)$, the power measured by the receiver at any time t due to photons that have been scattered exactly n times by the cloud particles, where n is any positive integer. In Ref. 1 it was shown that, for a sufficiently small receiver, $J_n(t)$ is completely determined by a certain function $P_n(t,0,0)$ [see Eqs. (19), (21)-(23) of Ref. 1]. It was further shown that $P_n(t,0,0)$ has the following formal representation [see Eq. (43) and Eqs. (30)-(33) of Ref. 1]:

$$P_{n}(t,0,0) = \beta_{s}^{n} \exp(-\beta ct) \int_{0}^{\infty} du_{0} \cdots \int_{0}^{\infty} du_{n-1} \int_{0}^{n} d\theta_{1} \int_{0}^{2n} d\phi_{1} \cdots \int_{0}^{n} d\theta_{n} \int_{0}^{2n} d\phi_{n}$$

$$\times \exp\{\beta b(1 - (\mathbf{z} \cdot \mathbf{e}_{n})^{-1})\} \prod_{i=1}^{n} \left[f(\theta_{i}) \sin\theta_{i} I\left(\sum_{j=0}^{i-1} u_{j}(\mathbf{z} \cdot \mathbf{e}_{j}) > b\right) \right] I(-\mathbf{z} \cdot \mathbf{e}_{n} > \cos\varphi_{0})$$

$$\times \delta\left(t - c^{-1} \sum_{i=0}^{n-1} u_{i} \left[1 - (\mathbf{z} \cdot \mathbf{e}_{i})(\mathbf{z} \cdot \mathbf{e}_{n})^{-1}\right]\right) \delta\left(\sum_{i=0}^{n-1} u_{i} \left[(\mathbf{x} \cdot \mathbf{e}_{i}) - (\mathbf{z} \cdot \mathbf{e}_{i})(\mathbf{z} \cdot \mathbf{e}_{n})^{-1}\right]\right)$$

$$\times \delta\left(\sum_{i=0}^{n-1} u_{i} \left[(\mathbf{y} \cdot \mathbf{e}_{i}) - (\mathbf{z} \cdot \mathbf{e}_{i})(\mathbf{y} \cdot \mathbf{e}_{n})(\mathbf{z} \cdot \mathbf{e}_{n})^{-1}\right]\right). \tag{1}$$

The *mathematical* meanings of the various quantities in this formula are as follows: β_s , β , b and ψ_0 are any constants satisfying

$$0 \le \beta_s \le \beta, \quad b \ge 0, \quad 0 \le \psi_0 \le u/2; \tag{2a}$$

f is any function satisfying

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$$0 \le f(\theta) < \infty$$
 for $0 \le \theta \le u$; (2b)

 δ is the Dirac delta function, defined by the pair of equations

$$\delta(x - x_0) = 0, \quad \text{if } x \neq x_0 \,. \tag{3a}$$

$$\int_{-\infty}^{\infty} g(x) \,\delta(x - x_0) \,dx = g(x_0), \tag{3b}$$

for any function g of x; I is the "inequality function", defined by

$$I("inequality") \equiv \begin{cases} 1, & \text{if "inequality" is satisfied,} \\ 0, & \text{if "inequality" is not satisfied;} \end{cases}$$
(4)

x, **y** and **z** are the basis vectors of a Cartesian coordinate frame, hereinafter referred to as "the *xyz*-frame;" and finally, \mathbf{e}_0 , \mathbf{e}_1 , ..., \mathbf{e}_n are unit vectors given by

$$\mathbf{e}_0 = \mathbf{z}.\tag{5a}$$

$$\mathbf{e}_{i} = \mathbf{x}_{i} \sin\theta_{i} \cos\phi_{i} + \mathbf{y}_{i} \sin\theta_{i} \sin\phi_{i} + \mathbf{z}_{i} \cos\theta_{i}. \quad (i = 1, ..., n)$$
(5b)

where the auxiliary basis vectors x, y, and z, are defined recursively according to

$$\mathbf{x}_1 = \mathbf{x}, \quad \mathbf{y}_1 = \mathbf{y} \quad \text{and} \quad \mathbf{z}_1 = \mathbf{z}, \tag{6a}$$

$$\left. \begin{array}{l} \mathbf{z}_{i} = \mathbf{e}_{i-1} \\ \mathbf{y}_{i} = (\mathbf{z} \times \mathbf{e}_{i-1}) / |\mathbf{z} \times \mathbf{e}_{i-1}| \\ \mathbf{x}_{i} = \mathbf{y}_{i} \times \mathbf{z}_{i} \end{array} \right\} \quad (i = 2, \dots, n)$$
 (6b)

Because of the recursive nature of Eqs. (5) and (6), the xyz-frame components of \mathbf{e}_i will depend on all the angles $\theta_1, \phi_1, \dots, \theta_i, \phi_i$. A computer-oriented procedure for calculating $\mathbf{x} \cdot \mathbf{e}_i$, $\mathbf{y} \cdot \mathbf{e}_i$ and $\mathbf{z} \cdot \mathbf{e}_i$ from these angles is developed in the Appendix [see Eqs. (A7)].

Physically, the vector

$$u_i \mathbf{e}_i \equiv \mathbf{u}_i \equiv \overline{\mathbf{S}_i \mathbf{S}_{i+1}} \quad (i = 0, 1, \dots, n)$$
(7)

may be interpreted as the trajectory of an *n*-scattered photon between its *i*th scattering, at point S_i , and its (i + 1)th scattering, at point S_{i+1} , with S_0 and S_{n+1} both coinciding with the origin O of the *xyz*-frame [see Fig. 1]. Eq. (5a) shows that the photon initially leaves the origin O along the +zaxis, and Eqs. (5b) and (6) show that the direction of u_i for $i \ge 1$ is measured by the polar and azimuthal angles θ_i and ϕ_i in a frame whose polar axis points along u_{i-1} .

Eq. (1) is the starting point for our analysis here. Simply stated, our goal is to "pacify" Eq. (1) — i.e., to reduce it to a form that can be evaluated by standard numerical techniques. The most obvious obstacle to a numerical evaluation of Eq. (1) is the presence of the three delta functions in the integrand; these must be analytically integrated out. An important tool for accomplishing these integrations is the "delta function change-of-variable theorem" (see Ref. 2 for a proof of this theorem): If h is a differentiable function of x whose only zeros are at $x_1, x_2, ..., x_m$, and if $h'(x_i) \neq 0$ for i = 1, ..., m, then

$$\delta(h(x)) = \sum_{i=1}^{m} \frac{\delta(x-x_i)}{|h'(x_i)|}$$
(8)

Before beginning the task of eliminating the delta functions, we shall simplify Eq. (1) slightly by rendering the integration variables dimensionless. To do this, we make the scaling transformation

 $u_i \rightarrow u_i' \equiv u_i/ct.$ (i=0,...,n-1) (9a)

Then

and

 $du_i = ct \, du_i'$ (i = 0,...,n-1)

$$I\left(\sum_{j=0}^{i-1} u_j(\mathbf{z} \cdot \mathbf{e}_j) > b\right) = I\left(\sum_{j=0}^{i-1} u_j'(\mathbf{z} \cdot \mathbf{e}_j) > b/ct\right). \quad (i=1,\dots,n)$$

Furthermore, since Eq. (8) implies that $\delta(ax) = |a|^{-1}\delta(x)$, then

$$\delta\left(t - c^{-1}\sum_{i=0}^{n-1} u_{i}a_{i}\right) = \delta\left(t - c^{-1}ct\sum_{i=0}^{n-1} u_{i}'a_{i}\right) = t^{-1}\delta\left(1 - \sum_{i=0}^{n-1} u_{i}'a_{i}\right)$$
$$\delta\left(\sum_{i=0}^{n-1} u_{i}b_{i}\right) = \delta\left(ct\sum_{i=0}^{n-1} u_{i}'b_{i}\right) = (ct)^{-1}\delta\left(\sum_{i=0}^{n-1} u_{i}'b_{i}\right).$$

and

$$t=0$$
 $t=0$ $t=0$
tituting the above forms into Eq. (1), and then *relabeling* the integration variables u_i'

Substituting the above forms into Eq. (1), and then *relabeling* the integration variables u_i' by removing the prime,

$$u_i' \to u_i, \quad (i=0,...,n-1)$$
 (9b)

we obtain

$$P_{n}(t,0,0) = \beta_{s}^{n} \exp(-\beta ct) (ct)^{n} t^{-1} (ct)^{-2} \int_{0}^{\infty} du_{0} \cdots \int_{0}^{\infty} du_{n-1} \int_{0}^{\pi} d\theta_{1} \int_{0}^{2\pi} d\phi_{1} \cdots \int_{0}^{\pi} d\theta_{n} \int_{0}^{2\pi} d\phi_{n}$$

$$\times \exp[\beta b(1 - (\mathbf{z} \cdot \mathbf{e}_{n})^{-1})] \prod_{i=1}^{n} \left[f(\theta_{i}) \sin \theta_{i} I\left(\sum_{j=0}^{i-1} u_{j} (\mathbf{z} \cdot \mathbf{e}_{j}) > b/ct\right) \right] I(-\mathbf{z} \cdot \mathbf{e}_{n} > \cos \psi_{0})$$

$$\times \delta \left(1 - \sum_{i=0}^{n-1} u_{i} [1 - (\mathbf{z} \cdot \mathbf{e}_{i}) (\mathbf{z} \cdot \mathbf{e}_{n})^{-1}] \right) \delta \left(\sum_{i=0}^{n-1} u_{i} [(\mathbf{x} \cdot \mathbf{e}_{i}) - (\mathbf{z} \cdot \mathbf{e}_{i}) (\mathbf{x} \cdot \mathbf{e}_{n})^{-1}] \right)$$

$$\times \delta \left(\sum_{i=0}^{n-1} u_{i} [(\mathbf{y} \cdot \mathbf{e}_{i}) - (\mathbf{z} \cdot \mathbf{e}_{i}) (\mathbf{y} \cdot \mathbf{e}_{n})^{-1}] \right). \tag{10}$$

For brevity we shall henceforth refer to the three delta functions in Eq. (10) as, reading from left to right, the *t*-delta function, the *x*-delta function and the *y*-delta function [cf. Eq. (43) of Ref. 1]. We turn now to the task of integrating out these delta functions.

2. ELIMINATING THE x- AND y-DELTA FUNCTIONS

We define the vector variables $A_1, A_2, ..., A_n$ by

$$\mathbf{A}_{i} = \sum_{j=0}^{i-1} \mathbf{u}_{j} = \sum_{j=0}^{i-1} u_{j} \mathbf{e}_{j}.$$
 (*i*=1,...,*n*) (11)

Geometrically, \mathbf{A}_i is the (scaled) position vector \overline{OS}_i of the point at which the *i*th scattering occurs [see Fig. 1]. We note in particular that \mathbf{A}_n is independent of \mathbf{e}_n , and hence of the two integration variables θ_n and ϕ_n . In terms of the vectors \mathbf{A}_i , Eq. (10) can be written

$$P_{n}(t,0,0) = \beta_{s}^{n} c(ct)^{n-3} \exp(-\beta ct) \int_{0}^{\infty} du_{0} \cdots \int_{0}^{\infty} du_{n-1} \int_{0}^{n} d\theta_{1} \int_{0}^{2n} d\phi_{1} \cdots \int_{0}^{n} d\theta_{n-1} \int_{0}^{2n} d\phi_{n-1} \\ \times \prod_{i=1}^{n-1} \left[f(\theta_{i}) \sin \theta_{i} l(A_{i,z} > b/ct) \right] L, \qquad (12)$$

where we have defined

$$L = \int_{0}^{n} d\theta_{n} \int_{0}^{2n} d\phi_{n} \exp[\beta b(1 - (\mathbf{z} \cdot \mathbf{e}_{n})^{-1})] f(\theta_{n}) \sin\theta_{n}$$

$$\times I(A_{n,z} > b/ct) I(-\mathbf{z} \cdot \mathbf{e}_{n} > \cos\psi_{0}) \delta\left(1 - \sum_{i=0}^{n-1} u_{i} + A_{n,z}(\mathbf{z} \cdot \mathbf{e}_{n})^{-1}\right)$$

$$\times \delta\left(A_{n,x} - A_{n,z}(\mathbf{x} \cdot \mathbf{e}_{n})(\mathbf{z} \cdot \mathbf{e}_{n})^{-1}\right) \delta\left(A_{n,y} - A_{n,z}(\mathbf{y} \cdot \mathbf{e}_{n})(\mathbf{z} \cdot \mathbf{e}_{n})^{-1}\right).$$
(13)

The quantity L in Eq. (13) is seen to be an integral over all directions of the vector \mathbf{e}_n . Our goal in this section is to evaluate L analytically, and in the process eliminate the x-and y-delta functions. To this end, we first change the integration variables in L from (θ_n, ϕ_n) , the polar and azimuthal angles of \mathbf{e}_n in the $x_n y_n z_n$ -frame [see Eqs. (5) and (6)], to (θ, ϕ) , the polar and azimuthal angles of \mathbf{e}_n in the xyz-frame. This change of variables allows the dot products involving \mathbf{e}_n in the integrand to be written in the relatively simple explicit forms

$$\mathbf{x} \cdot \mathbf{e}_n = \sin\theta \cos\phi, \quad \mathbf{y} \cdot \mathbf{e}_n = \sin\theta \sin\phi, \quad \mathbf{z} \cdot \mathbf{e}_n = \cos\theta.$$
 (14a)

The Jacobian of the transformation $(\theta_n, \phi_n) \rightarrow (\theta, \phi)$ is such that the form of the differential solid angle is preserved, so we have

$$\sin\theta_n \, d\theta_n \, d\phi_n = \sin\theta \, d\theta \, d\phi. \tag{14b}$$

Since θ_n appears as an argument of f in Eq. (13), we will also need a formula for θ_n in terms of θ and ϕ . Such a formula can be obtained by first noting from Eqs. (5b) and (6) that $\cos\theta_n = \mathbf{z}_n \cdot \mathbf{e}_n = \mathbf{e}_{n-1} \cdot \mathbf{e}_n$; expanding the latter dot product in terms of xyz-components, we obtain

 $\theta_n = \theta_n(\theta, \phi) = \arccos[(\mathbf{x} \cdot \mathbf{e}_{n-1}) \sin\theta \cos\phi + (\mathbf{y} \cdot \mathbf{e}_{n-1}) \sin\theta \sin\phi + (\mathbf{z} \cdot \mathbf{e}_{n-1}) \cos\theta].$ (15) Now substituting Eqs. (14) into Eq. (13), we get

 $L = \int_{0}^{n} d\theta \int_{0}^{2\pi} d\phi \exp[\beta b(1 - \sec\theta)] f(\theta_{n}(\theta, \phi)) \sin\theta I(A_{n,z} > b/ct) I(-\cos\theta > \cos\psi_{0})$ $\times \delta \left(1 - \sum_{i=0}^{n-1} u_{i} + A_{n,z} \sec\theta\right) \delta \left(A_{n,x} - A_{n,z} \tan\theta \cos\phi\right) \delta \left(A_{n,y} - A_{n,z} \tan\theta \sin\phi\right), \quad (16)$

in which $\theta_n(\theta, \phi)$ is understood to be the function in Eq. (15). The dependence of the integrand on the integration variables θ and ϕ has now been rendered completely explicit, so we can perform these two integrations. We shall integrate first over ϕ with the help of the y-delta function, and then over θ with the help of the x-delta function.

Since $-\cos\theta \equiv \cos(n-\theta)$, the second *I*-function in Eq. (16) essentially requires that $\theta > n - \psi_0$. This requirement, completed with the fact that $\psi_0 \le n/2$ means that $\theta > n/2$, so we can increase the lower limit on the θ -integration from 0 to n/2. We rewrite Eq. (16) in the iterated form

$$L = \int_{n/2}^{n} d\theta \exp[\beta b(1 - \sec\theta)] \sin\theta I(A_{n,2} > b/ct) I(-\cos\theta > \cos\psi_0) \delta\left(1 - \sum_{i=0}^{n-1} u_i + A_{n,2} \sec\theta\right) L', (17a)$$

where

$$L' = \int_{0}^{2\pi} d\phi f(\theta_{n}(\theta,\phi)) \,\delta(A_{n,x} - A_{n,z} \tan\theta \cos\phi) \,\delta(A_{n,y} - A_{n,z} \tan\theta \sin\phi). \tag{17b}$$

The details of evaluating first L' and then L turn out to depend upon the signs of $A_{n,x}$ and $A_{n,y}$, i.e., upon which quadrant of the xy-plane the vector \overrightarrow{OS}_n projects [see Fig. 1]. But it is clear from symmetry considerations that the final result must be the same in all cases. Therefore, we carry out here the analysis only for the case in which S_n lies above the first quadrant — i.e., the

Case:
$$A_{n,\gamma} > 0$$
 and $A_{n,\gamma} > 0$. (18)

Denoting the argument of the y-delta function in Eq. (17b) by

$$h(\phi) = A_{n,v} - A_{n,v} \tan\theta \sin\phi, \qquad (19)$$

we rewrite that equation as

$$L' = \int_{0}^{2n} d\phi f(\theta_n(\theta, \phi)) \,\delta(A_{n,x} - A_{n,x} \tan \theta \cos \phi) \,I(|A_{n,y}| \le |A_{n,x} \tan \theta|) \,\delta(h(\phi)), \tag{20}$$

where the *I*-function makes explicit a condition that is clearly necessary if *h* is to vanish for some value of ϕ . Assuming that condition is satisfied, it follows from Eq. (19) that there will in general be *two* angles, $\phi^{(1)}$ and $\phi^{(2)}$, for which *h* vanishes, namely those angles for which

$$\sin\phi^{(1)} = \sin\phi^{(2)} = \Lambda_{n,y} / (A_{n,z} \tan\theta).$$
(21a)

Since $A_{n,z} > 0$ and $\theta \in (n/2, n)$ [cf. Eq. (17a)], while $A_{n,y} > 0$ [cf. Eq. (18)], the quantity on the right side of Eq. (21a) is negative. This means that $\phi^{(1)}$ and $\phi^{(2)}$ must lie in the third and fourth quadrants, respectively; thus, using $\cos^2 \phi^{(i)} = 1 - \sin^2 \phi^{(i)}$, we deduce that

$$\cos\phi^{(1)} = (A_{n,z}^{2} \tan^{2}\theta - A_{n,y}^{2})^{1/2} / (A_{n,z} \tan\theta) = -\cos\phi^{(2)}.$$
 (21b)

Now, from Eq. (19) we have $h'(\phi) = -A_{n,z} \tan \theta \cos \phi$, so using Eq. (21b) we deduce that

$$|h'(\phi^{(1)})| = |h'(\phi^{(2)})| = (A_{n,z}^{2} \tan^{2}\theta - A_{n,y}^{2})^{1/2}$$

Therefore, we may use the rule in Eq. (8) to write

$$\delta(h(\phi)) = (A_{n,z}^{2} \tan^{2}\theta - A_{n,y}^{2})^{-1/2} \sum_{i=1}^{2} \delta(\phi - \phi^{(i)}).$$
(22)

Substituting Eq. (22) into Eq. (20), the ϕ - integration becomes trivial [cf. Eq. (3b)]; it yields

$$L' = I(|A_{n,y}| \le |A_{n,z} \tan \theta|) (A_{n,z}^{-2} \tan^2 \theta - A_{n,y}^{-2})^{-1/2} \sum_{i=1}^{2} f(\theta_n(\theta, \phi^{(i)})) \delta(A_{n,x} - A_{n,z} \tan \theta \cos \phi^{(i)}).$$
(23)

When the expressions for $\cos\phi^{(i)}$ in Eq. (21b) are substituted into the delta functions in Eq. (23) we find that, for the case $A_{n,x} > 0$ being considered here, the argument of the i = 2 delta function never vanishes. That term may therefore be dropped, and Eq. (23) reduces to

$$L' = I(|A_{n,y}| \le |A_{n,z}\tan\theta|) (A_{n,z}^{-2}\tan^2\theta - A_{n,y}^{-2})^{-1/2} f(\theta_n(\theta, \phi^{(1)})) \delta(A_{n,x} - |A_{n,z}^{-2}\tan^2\theta - A_{n,y}^{-2}|^{1/2}), \quad (24)$$

where $\theta_{i}(\theta, \phi^{(1)})$ is found from Eqs. (15) and (21) to be

$$\theta_{n}(\theta, \phi^{(1)}) = \arccos\{(\mathbf{x} \cdot \mathbf{e}_{n+1}) \cos\theta A_{n,2}^{-1} (A_{n,2}^{2} \tan^{2}\theta - A_{n,3}^{2})^{1/2} + (\mathbf{y} \cdot \mathbf{e}_{n-1}) \cos\theta A_{n,2}^{-1} A_{n,3} + (\mathbf{z} \cdot \mathbf{e}_{n-1}) \cos\theta\}.$$
(25)

Substituting the above integrated form of L' into Eq. (17a), we obtain

$$L = I(A_{n,2} > b/ct) \int_{n/2}^{n} d\theta \ I(-\cos\theta > \cos\psi_0) \ I(|A_{n,y}| \le |A_{n,2}\tan\theta|) \ \delta\left(1 - \sum_{i=0}^{n-1} u_i + A_{n,2}\sec\theta\right)$$
$$\times \exp[\beta b(1 - \sec\theta)] \ f(\theta_n(\theta, \phi^{(1)})) \sin\theta \ (A_{n,2}^2 \tan^2\theta - A_{n,y}^2)^{-1/2} \ \delta(h(\theta)), \qquad (26)$$

where, in anticipation of using Eq. (8) again, we have redefined h to be

$$h(\theta) = A_{n,x} - (A_{n,x}^{2} \tan^{2} \theta - A_{n,y}^{2})^{1/2}.$$
 (27)

Noting that the integration variable θ is confined to the second quadrant, where the tangent is negative, we see that *h* vanishes only at the angle $\theta^{(1)}$ defined by

$$\tan\theta^{(1)} = -(A_{n,x}^2 + A_{n,y}^2)^{1/2} / A_{n,z}.$$
 (28a)

This fact, coupled with the second quadrant restriction, implies that

$$\sin\theta^{(1)} = (A_{n,x}^2 + A_{n,y}^2)^{1/2} / A_n, \quad \cos\theta^{(1)} = -A_{n,z}^2 / A_n.$$
(28b)

The above formulas in turn imply that

$$\sec\theta^{(1)} = -A_n / A_{n,z}, \quad |A_{n,z} \tan\theta^{(1)}| = (A_{n,x}^2 + A_{n,y}^2)^{1/2}, \quad (A_{n,z}^2 \tan^2\theta^{(1)} - A_{n,y}^2)^{1/2} = A_{n,x}. \quad (28c)$$

Now, the derivative of the function in Eq. (27) is

$$h'(\theta) = -\frac{1}{2} (A_{n,2}^{-2} \tan^2 \theta - A_{n,3}^{-2})^{-1/2} 2A_{n,2}^{-2} \tan \theta \sec^2 \theta.$$

Putting $\theta = \theta^{(1)}$ and using Eqs. (28), we find that

$$|h'(\theta^{(1)})| = (A_{n,x}^2 + A_{n,y}^2)^{1/2} A_n^2 A_{n,x}^{-1} A_{n,z}^{-1}.$$

The rule in Eq. (8) then allows us to write

$$\delta(h(\theta)) = A_{n,x} A_{n,y} A_n^{-2} (A_{n,x}^2 + A_{n,y}^2)^{-1/2} \delta(\theta - \theta^{(1)}).$$
(29)

Substituting Eq. (29) into Eq. (26), the θ – integration is now trivially performed, with the result

$$L = I(A_{n,z} > b/ct) I(-\cos\theta^{(1)} > \cos\psi_0) I(|A_{n,y}| \le |A_{n,z}\tan\theta^{(1)}|) \delta\left(1 - \sum_{i=0}^{n-1} u_i + A_{n,z}\sec\theta^{(1)}\right)$$

 $\times \exp[\beta b(1 - \sec\theta^{(1)})] f(\theta_n(\theta^{(1)}, \phi^{(1)})) \sin\theta^{(1)} (A_{n,z}^2 \tan^2\theta^{(1)} - A_{n,y}^2)^{-1/2}$
 $\times A_{n,x} A_{n,y} A_n^{-2} (A_{n,x}^2 + A_{n,y}^2)^{-1/2}$ (30)

Substituting for $\theta^{(1)}$ from Eqs. (28) and simplifying, we finally obtain

$$L = I(A_{n,z} > b/ct) I(A_{n,z}/A_n > \cos\psi_0) \exp[\beta b(1 + A_n/A_{n,z})] f(\theta_n) A_{n,z} A_n^{-3} \delta\left(1 - \sum_{i=0}^{n-1} u_i - A_n\right), \quad (31)$$

where θ_n is now given by

$$\theta_n = \arccos(-\mathbf{e}_{n-1} \cdot \mathbf{A}_n / A_n). \tag{32}$$

Notice that the result in Eqs. (31) and (32) is manifestly independent of the signs of $A_{n,x}$ and $A_{n,y}$, and hence of the case assumption in Eq. (18); indeed, if the foregoing analysis is repeated for the cases in which either or both of $A_{n,x}$ and $A_{n,y}$ are negative, the final result will still be Eqs. (31) and (32).

Substituting Eq. (31) into Eq. (12), and also putting $\sin\theta_i d\theta_i = -d\cos\theta_i$ for i = 1, ..., n - 1, we obtain the following expression for $P_n(t,0,0)$:

$$P_{n}(t,0,0) = \beta_{s}^{n} c(ct)^{n-3} \exp(-\beta ct) \int_{0}^{x} du_{0} \cdots \int_{0}^{x} du_{n-1} \int_{-1}^{1} d\cos\theta_{1} \int_{0}^{2n} d\phi_{1} \cdots$$

$$\times \int_{-1}^{1} d\cos\theta_{n-1} \int_{0}^{2n} d\phi_{n-1} \Big(\prod_{i=1}^{n-1} I(A_{i,z} > b/ct) \Big) I(A_{n,z} > b/ct) I(A_{n,z}/A_{n} > \cos\psi_{0})$$

$$\times \Big(\prod_{i=1}^{n} f(\theta_{i}) \Big) \exp[\beta b(1 + A_{n}/A_{n,z})] A_{n,z} A_{n}^{-3} \delta\Big(1 - \sum_{i=0}^{n-1} u_{i} - A_{n} \Big).$$
(33)

In this equation, the vectors $\mathbf{A}_1, \dots, \mathbf{A}_n$ are given by Eq. (11), and θ_n is given by Eq. (32).

3. ELIMINATING THE t-DELTA FUNCTION

The task of integrating out the remaining delta function [formerly the delta function involving t in Eq. (1)] is accomplished differently for n = 1 than for $n \ge 2$. We consider first the relatively simple n = 1 case, for which Eq. (33) reads

$$P_{1}(t,0,0) = \beta_{s} c(ct)^{-2} \exp(-\beta ct) \int_{0}^{r} du_{0} I(A_{1,2} > b/ct) I(A_{1,2}/A_{1} > \cos\psi_{0}) \\ \times f(\theta_{1}) \exp[\beta b(1 + A_{1}/A_{1,2})] A_{1,2} A_{1}^{-3} \delta(1 - u_{0} - A_{1})$$
(34)

Since, according to Eqs. (11) and (5a),

$$\mathbf{A}_1 = u_0 \mathbf{e}_0 = u_0 \mathbf{z}$$

then $A_{1,z} = A_1 = u_0$, and Eq. (32) gives

$$\theta_1 = \arccos(-\mathbf{e}_0 \cdot u_0 \mathbf{e}_0 / u_0) = \arccos(-1) = n$$

The condition $A_{1,z}/A_1 > \cos \psi_0$ is just $1 > \cos \psi_0$, which is always satisfied. Eq. (34) therefore simplifies to

$$P_{1}(t,0,0) = \beta_{s} c(ct)^{-2} \exp(-\beta ct) \int_{0}^{\infty} du_{0} I(u_{0} > b/ct) f(\pi) \exp(2\beta b) u_{0}^{-2} \delta(1-2u_{0}).$$

Using the rule in Eq. (8), we have

$$\delta(1 - 2u_0) = 2^{-1} \,\delta(u_0 - 1/2)$$

Therefore, the above equation is

$$P_1(t,0,0) = 2^{-1}\beta_s c(ct)^{-2} \exp[-\beta(ct-2b)]f(u) \int_0^u du_0 f(u_0 > b/ct) u_0^{-2} \delta(u_0 - 1/2).$$

The u_0 -integration is now trivially performed with the aid of Eq. (3b), giving

$$P_{1}(t,0,0) = I(ct>2b) 2c \beta_{s}(ct)^{-2} \exp[-\beta(ct-2b)]f(u).$$
(35)

This result agrees exactly with Eq. (28) of Ref. 1, which was obtained from comparatively simple physical arguments. This agreement constitutes a reassuring, if somewhat limited, consistency check on our calculations thus far.

We now turn to the more interesting and challenging case in which $n \ge 2$. As a prelude to eliminating the remaining delta function in Eq. (33) for that case, we make two more integration variable transformations. The first of these is the transformation

$$(u_{n-1}, \cos\theta_{n-1}, \phi_{n-1}) \to (A_n, \cos\psi, \eta), \tag{36a}$$

where ψ and η are the polar and azimuthal angles of the vector \mathbf{A}_n in the xyz-frame. Since both sets of integration variables in Eq. (36a) simply integrate the point \mathbf{S}_n over all space, we have the differential relation

$$u_{n-1}^{2} du_{n-1} d\cos\theta_{n-1} d\phi_{n-1} = A_{n}^{2} dA_{n} d\cos\psi d\eta.$$
(36b)

Using this relation and the fact that $A_{n,z} = A_n \cos \psi$, Eq. (33) becomes, for $n \ge 2$,

$$P_{n}(t,0,0) = \beta_{s}^{n} c(ct)^{n-3} \exp(-\beta ct) \int_{0}^{\infty} du_{0} \cdots \int_{0}^{\infty} du_{n-2} \int_{0}^{\infty} dA_{n}$$

$$\times \int_{-1}^{1} d\cos\theta_{1} \int_{0}^{2n} d\phi_{1} \cdots \int_{-1}^{1} d\cos\theta_{n-2} \int_{0}^{2n} d\phi_{n-2} \int_{-1}^{1} d\cos\psi \int_{0}^{2n} d\eta$$

$$\times \left(\prod_{i=1}^{n-1} I(A_{i,z} > b/ct)\right) I(A_{n} \cos\psi > b/ct) I(\cos\psi > \cos\psi_{0})$$

$$\times \left(\prod_{i=1}^{n} f(\theta_{i})\right) \exp[\beta b(1 + \sec\psi)] \cos\psi u_{n-1}^{-2} \delta\left(1 - \sum_{i=0}^{n-1} u_{i} - A_{n}\right). \quad (n \ge 2) \quad (37)$$

in which it is understood that the integration variables $\cos\theta_i$ and ϕ_i are absent if n = 2. The quantities appearing in the integrand are given in terms of the integration variables as follows: The (n-1) vectors $\mathbf{e}_0, ..., \mathbf{e}_{n-2}$ are calculated from the recursion relation in Eqs. (A7). The (n-1) vectors $\mathbf{A}_1, ..., \mathbf{A}_{n-1}$ are defined through Eq. (11):

$$\mathbf{A}_{i} \equiv \sum_{j=0}^{i-1} u_{j} \mathbf{e}_{j}, \quad (i=1,...,n-1)$$
(38a)

The vector \mathbf{u}_{n-1} , and its associated magnitude u_{n-1} and unit direction vector \mathbf{e}_{n-1} , are also defined through Eq. (11), but now written for i = n in the form

$$u_{n-1}\mathbf{e}_{n-1} \equiv \mathbf{u}_{n-1} = \mathbf{A}_n - \sum_{j=0}^{n-2} u_j \mathbf{e}_j, \qquad (38b)$$

And finally, θ_{n-1} and θ_n are given by [see Eqs. (5), (6) and (32)]

$$\theta_{n-1} = \arccos(\mathbf{e}_{n-2} \cdot \mathbf{e}_{n-1}), \tag{38c}$$

$$\theta_n = \arccos(-\mathbf{e}_{n-1} \cdot \mathbf{A}_n / \Lambda_n). \tag{38d}$$

Our second transformation of integration variables is another scaling transformation,

$$u_{i} \rightarrow v_{i} \equiv u_{i}/\Lambda_{n}, \quad (i = 0, ..., n - 2)$$
 (39a)

which evidently gives

$$du_0 \cdots du_{n-2} dA_n = A_n^{n-1} dv_0 \cdots dv_{n-2} dA_n.$$
(39b)

This transformation has the effect of making A_{ii} the "unit of length" for all distance vectors. Thus, for i = 0, ..., n - 2, we have $\mathbf{u}_i = A_{ii} \mathbf{v}_i$, where

$$\mathbf{v}_i = v_i \mathbf{e}_i, \quad (i = 0, ..., n - 2)$$
 (40a)

And using Eq. (38b) we see that we can also write $\mathbf{u}_{n-1} = A_n \mathbf{v}_{n-1}$, provided we define \mathbf{v}_{n-1} by

$$v_{n-1}\mathbf{e}_{n-1} \equiv \mathbf{v}_{n-1} = \mathbf{a} - \sum_{j=0}^{n-2} v_j \mathbf{e}_j, \qquad (40\mathbf{b})$$

where **a** is the unit vector in the direction of \mathbf{A}_n :

R

$$\mathbf{a} = \mathbf{A}_n / A_n = \mathbf{x} \sin \psi \cos \eta + \mathbf{y} \sin \psi \sin \eta + \mathbf{z} \cos \psi.$$
(41)

Finally, we see from Eq. (38a) that we can write $\mathbf{A}_i = \mathbf{A}_n \mathbf{B}_i$ for i = 1, ..., n - 1, where

$$\mathbf{B}_{i} \equiv \sum_{j=0}^{i-1} \mathbf{v}_{j} \equiv \sum_{j=0}^{i-1} v_{j} \mathbf{e}_{j}. \quad (i=1,...,n-1)$$
(42)

With Eqs. (39) - (42), the integral in Eq. (37) takes the form

$$P_{n}(t,0,0) = \beta_{s}^{n} c(ct)^{n-3} \exp(-\beta ct) \int_{0}^{t} dv_{0} \cdots \int_{0}^{n} dv_{n-2} \int_{0}^{t} A_{n}^{n-1} dA_{n}$$

$$\times \int_{-1}^{1} d\cos\theta_{1} \int_{0}^{2n} d\phi_{1} \cdots \int_{-1}^{1} d\cos\theta_{n-2} \int_{0}^{2n} d\phi_{n-2} \int_{\cos\psi_{0}}^{1} d\cos\psi \int_{0}^{2n} d\eta$$

$$\times \left(\prod_{i=1}^{n-1} I(A_{n}B_{i,2} > b/ct)\right) I(A_{n}\cos\psi > b/ct)$$

$$\times \left(\prod_{i=1}^{n} f(\theta_{i})\right) \exp[\beta b(1 + \sec\psi)] \cos\psi A_{n}^{-2} v_{n-1}^{-2} \delta\left(1 - A_{n} \left[1 + \sum_{i=0}^{n-1} v_{i}\right]\right). (n \ge 2) \quad (43)$$

Now we define

$$V = 1 + \sum_{i=0}^{n-1} v_i.$$
 (44)

Then the delta function in Eq. (43) can be written

$$\delta\left(1-A_{n}\left|1+\sum_{i=0}^{n-1}v_{i}\right|\right)=\delta(1-VA_{n})=V^{-1}\delta(A_{n}-V^{-1}),$$
(45)

where the last step follows from the rule in Eq. (8). When Eq. (45) is substituted into Eq. (43), the A_n -integration can be trivially accomplished: the delta function is thereby eliminated, and A_n is everywhere replaced by V^{-1} .

Before writing down the result of the A_n -integration, we want to do two more things to Eq. (43). The first is simply to replace $d\cos q$ by $-\sin q dq$. The second is to fix the orientation of the *xz*plane, which thus far has not been specified. Owing to the symmetry of our problem about the *z*-

axis, which exists because the laser and receiver both lie on that axis, we can choose the orientation of the xz-plane freely without affecting the integrand. Let us now stipulate that the xz-plane contains the vector **a**. This implies, firstly, that $\eta = 0$ in Eq. (41), and secondly, that the η -integration in Eq. (43) can be replaced by a simple factor of 2π .

Performing all the operations described above, Eq. (43) becomes

$$P_{n}(t,0,0) = 2\pi \beta_{s}^{n} c(ct)^{n-3} \exp(-\beta ct) \int_{0}^{\infty} dv_{0} \cdots \int_{0}^{\infty} dv_{n-2} \int_{-1}^{1} d\cos\theta_{1} \int_{0}^{2\pi} d\phi_{1} \cdots$$

$$\times \int_{-1}^{1} d\cos\theta_{n-2} \int_{0}^{2\pi} d\phi_{n-2} \int_{0}^{\psi_{0}} d\psi \left(\prod_{i=1}^{n-1} I(V^{-1}B_{i,2} > b/ct) \right) I(V^{-1} \cos\psi > b/ct)$$

$$\times \exp[\beta b(1 + \sec\psi)] \left(\prod_{i=1}^{n} f(\theta_{i}) \right) \cos\psi \sin\psi V^{-(n-2)} v_{n-1}^{-2}, \qquad (n \ge 2)$$
(46)

in which it is understood that, for n = 2, the integration variables $\cos\theta_i$ and ϕ_i are absent. The quantities in the integrand of Eq. (46) are related to the integration variables according to the following specifications: The unit vectors $\mathbf{e}_0, ..., \mathbf{e}_{n-2}$ are found from the recursion relation in Eqs. (A7), while the quantities $\mathbf{e}_{n-1}, v_{n-1}, \theta_{n-1}, \theta_n, \mathbf{B}_1, ..., \mathbf{B}_{n-1}$ and V are determined from the formulas:

$$\mathbf{a} = \mathbf{x}\sin\psi + \mathbf{z}\cos\psi; \tag{47a}$$

$$v_{n-1}\mathbf{e}_{n-1} = \mathbf{a} - \sum_{j=0}^{n-2} v_j \mathbf{e}_j;$$
 (47b)

$$\theta_{n-1} = \arccos(\mathbf{e}_{n-2} \cdot \mathbf{e}_{n-1}); \tag{47c}$$

$$\theta_n = \arccos(-\mathbf{e}_{n-1} \cdot \mathbf{a}); \tag{47d}$$

$$\mathbf{B}_{i} = \sum_{j=0}^{i-1} v_{j} \mathbf{e}_{j}; \quad (i=1,...,n-1)$$
(47e)

$$V = 1 + \sum_{i=0}^{n-1} v_i.$$
 (471)

The content of the above relations is summarized geometrically for the cases n = 2, 3 and 4 by the diagrams in Fig. 2.

4. BOUNDING THE INTEGRAND AND INTEGRATION DOMAIN

In Eq. (46) we have, at last, an expression for $P_n(t,0,0)$ for $n \ge 2$ that is free of delta functions. It is evidently a (3n - 4)-dimensional integral, the complexity of which will usually dictate that it be evaluated numerically rather than analytically. However, Eq. (46) is not suitable for numerical evaluation for two reasons: First, the integration domain is unbounded, since the integration variables v_0, \ldots, v_{n-2} have infinite ranges; and second, the integrand is unbounded, since v_{n-1} can vanish. [Since $\sec \psi \to \infty$ as $\psi \to n/2$, the exponential factor involving $\sec \psi$ in the integrand might also seem to present a boundedness problem; however, the last *I*-function in the integrand imposes the condition $b \sec \psi < ct/V < ct$, where the last inequality follows from the definition of *V*, so the exponential is not a problem.] It must be emphasized that these unbounded features of Eq. (46) do *not* imply that the expression therein is mathematically ill-defined. But they do imply that, if we want to evaluate the integral using conventional numerical techniques, we will have to subject it to some integration variable transformations that render the integrand and the integration domain bounded.

The key to obtaining a set of integration variables for which the integrand and integration domain are bounded turns out to be the set of vectors $\mathbf{C}_0, \mathbf{C}_1, ..., \mathbf{C}_{n-1}$, where \mathbf{C}_i is defined to be the vector from point \mathbf{S}_i to point \mathbf{S}_n (see Fig. 3):

$$\mathbf{C}_{i} \equiv \begin{cases} \mathbf{a}, & \text{if } i = 0, \\ \mathbf{a} - \sum_{j=0}^{i-1} v_{j} \mathbf{e}_{j}, & \text{if } i = 1, ..., n-1. \end{cases}$$
(48)

Notice in particular that

$$C_0 = 1$$
 and $C_{n-1} = v_{n-1} e_{n-1}$. (49)

These vectors \mathbf{C}_{i} will not themselves be our new integration variables, but they will be crucial for defining those new variables. Essentially what we are going to do now is, first, replace each pair of integration variables (θ_{i}, ϕ_{i}) in Eq. (46) by a new pair of variables (θ'_{i}, ϕ'_{i}), and second, replace each length integration variable v_{i} by a new angular variable v_{i} .

The variables θ_i and ϕ_i were defined to be the polar and azimuthal angles respectively of the vector \mathbf{e}_i relative to a coordinate frame whose polar axis is $\mathbf{z}_i = \mathbf{e}_{i-1}$. We now change integration variables according to

$$(\cos\theta_i, \phi_i) \rightarrow (\cos\theta'_i, \phi'_i), \quad (i=1,...,n-2)$$
 (50a)

where θ'_i and ϕ'_i are the polar and azimuthal angles respectively of \mathbf{e}_i relative to a coordinate frame whose polar axis is $\mathbf{z'}_i = \mathbf{C}_i / C_i$. The Jacobian of this transformation is such that each differential solid angle element $d\cos\theta \, d\phi$ is preserved, so we have the differential relation

$$d\cos\theta_{1} d\phi_{1} \cdots d\cos\theta_{n-2} d\phi_{n-2} = d\cos\theta'_{1} d\phi'_{1} \cdots d\cos\theta'_{n-2} d\phi'_{n-2}$$
$$= (\sin\theta'_{1} \cdots \sin\theta'_{n-2}) d\theta'_{1} d\phi'_{1} \cdots d\theta'_{n-2} d\phi'_{n-2}$$

(50b)

Since the integration limits on θ_i and ϕ_i encompass all possible directions of \mathbf{e}_i , it follows that θ'_i and ϕ'_i will have the same respective limits. By definition, θ'_i is the angle between \mathbf{e}_i and \mathbf{C}_i for i = 1, ..., n-2, and we can evidently extend that definition to i = 0 by simply defining

$$\theta'_0 \equiv \psi. \tag{51}$$

The geometrical relations between the old and new polar angles are illustrated in Fig. 3. The orientation of the azimuthal plane that defines the zero of ϕ'_i is open, but there will be a minimum of computational work later on if we take this plane to be the one defined by C_i and z. Thus, we are essentially transforming from the $x_iy_iz_i$ -frame of Eqs. (5) and (6) to the $x'_iy'_iz'_i$ -frame defined by

$$\mathbf{z'}_{i} = \mathbf{C}_{i}/C_{i}$$

$$\mathbf{y'}_{i} = (\mathbf{z} \times \mathbf{C}_{i})/|\mathbf{z} \times \mathbf{C}_{i}|$$

$$\mathbf{x'}_{i} = \mathbf{y'}_{i} \times \mathbf{z'}_{i},$$

$$(i = 1, ..., n-2)$$

$$(52a)$$

relative to which e, has the component representation

$$\mathbf{e}_{i} = \mathbf{x}'_{i} \sin\theta'_{i} \cos\phi'_{i} + \mathbf{y}'_{i} \sin\theta'_{i} \sin\phi'_{i} + \mathbf{z}'_{i} \cos\theta'_{i}, \quad (i = 1, ..., n-2)$$
(52b)

A detailed procedure for calculating the xyz-components of \mathbf{e}_i from the xyz-components of \mathbf{C}_i and the angles θ'_i and ϕ'_i is developed in the Appendix [see Eqs. (A8)].

$$P_{n}(t,0,0) = 2\pi \beta_{s}^{n} c(ct)^{n-3} \exp(-\beta ct) \int_{0}^{t} dv_{0} \int_{0}^{\psi_{0}} d\theta'_{0} \left\{ \prod_{i=1}^{n-2} \int_{0}^{t} dv_{i} \int_{0}^{n} d\theta'_{i} \int_{0}^{2n} d\phi'_{i} \right\}$$

$$\times \left(\prod_{i=1}^{n-1} I(B_{i,2} > Vb/ct) \right) I(\cos\theta'_{0} > Vb/ct) \exp[\beta b(1 + \sec\theta'_{0})]$$

$$\times \left(\prod_{i=1}^{n} f(\theta_{i}) \right) \cos\theta'_{0} \left(\prod_{i=0}^{n-2} \sin\theta'_{i} \right) v_{n-1}^{-2} V^{-(n-2)}, \qquad (n \ge 2) \qquad (53)$$

wherein it is understood that the product in braces is to be omitted in the case n=2.

Next we make the integration variable transformation

$$v_i \rightarrow v_i \equiv \arctan\left(\frac{v_i - C_i \cos\theta'_i}{C_i \sin\theta'_i}\right).$$
 $(i=0,...,n-2)$ (54)

The nature of this transformation can be best appreciated in terms of the geometry of the triangle formed by the three points S_i , S_{i+1} and S_n , as shown in Fig. 4: If the line through S_n perpendicular to the line through S_i and S_{i+1} intersects the latter in the point T_i , then v_i is just the angle between $\overline{S_n T_i}$ and $\overline{S_n S_{i+1}}$. It can be seen from Fig. 4, and it can also be shown from Eq. (54), that as v_i runs from 0 to ∞ , the angle v_i runs from $-(n/2 - \theta'_i)$ to n/2. Therefore, this transformation renders the integration domain bounded; we shall see shortly that it also renders the integrand bounded.

To calculate the Jacobian of the transformation defined in Eq. (54), we begin by solving that equation for v_i :

$$v_i = C_i \sin\theta'_i \tan v_i + C_i \cos\theta'_i.$$
(55)

From this it follows that

$$\frac{\partial v_i}{\partial v_i} = C_i \sin \theta'_i \sec^2 v_i.$$
 (56)

We also note from Fig. 4 that

$$C_{i+1} \cos v_i = T_i S_n = C_i \sin \theta'_i,$$

$$C_{i+1} = C_i \sin \theta'_i \sec v_i.$$
(57)

from which it follows that

Now, a moment's inspection of Eqs. (55) and (57) will show that
$$v_i$$
 depends on v_i and C_i , while C_i in turn depends on C_{i-1} and v_{i-1} , etc., and hence that v_i depends on v_i , v_{i-1} , ..., v_0 , but not on v_{i+1} , v_{i+2} , ..., v_{n-2} . This implies that the Jacobian determinant $\partial(v_i)/\partial(v_i)$ has zero entries everywhere on one side of the main diagonal, and therefore that the determinant is simply equal to the product of its diagonal elements:

$$\frac{\partial (v_0, \dots, v_{n-2})}{\partial (v_0, \dots, v_{n-2})} = \prod_{i=0}^{n-2} \frac{\partial v_i}{\partial v_i}.$$
(58)

Taken together, Eqs. (56) - (58) imply that

$$\frac{\partial (v_0, \dots, v_{n-2})}{\partial (v_0, \dots, v_{n-2})} \left(\prod_{i=0}^{n-2} \sin \theta'_i \right) = \prod_{i=0}^{n-2} \frac{\partial v_i}{\partial v_i} \sin \theta'_i,$$

$$= \prod_{i=0}^{n-2} C_{i} \sin^{2} \theta_{i} \sec^{2} v_{i},$$
$$= \prod_{i=0}^{n-2} C_{i} \left(\frac{C_{i+1}}{C_{i}}\right)^{2},$$
$$= \frac{C_{n-1}^{2}}{C_{0}^{2}} \prod_{i=0}^{n-2} C_{i}.$$

But Eq. (49) implies that $C_{n-1} = v_{n-1}$ and $C_0 = 1$, so we conclude that

$$\frac{\partial(v_0, \dots, v_{n-2})}{\partial(v_0, \dots, v_{n-2})} \left(\prod_{i=0}^{n-2} \sin \theta_i^* \right) v_{n-1}^{-2} = \prod_{i=0}^{n-2} C_i^{-1}$$
(59)

Eq. (59) tells us that the transformation $(v_0, ..., v_{n-2}) \rightarrow (v_0, ..., v_{n-2})$ defined in Eq. (54) brings the integral in Eq. (53) into the form

$$P_{n}(t,0,0) = 2n\beta_{s}^{n}c(ct)^{n-3}\exp(-\beta ct)\int_{0}^{\psi_{0}}d\theta_{0}'\int_{\theta_{0}'-n/2}^{n/2}dv_{0}\left\{\prod_{i=1}^{n-2}\int_{0}^{n}d\theta_{i}'\int_{\theta_{i}'-n/2}^{n/2}dv_{i}\int_{0}^{2n}d\phi_{i}'\right\}$$

$$\times \left(\prod_{i=1}^{n-1}I(B_{i,z} > Vb/ct))I(\cos\theta_{0}' > Vb/ct)\exp[\beta b(1 + \sec\theta_{0}')]$$

$$\times \left(\prod_{i=1}^{n}f(\theta_{i})\right)\cos\theta_{0}'\left(\prod_{i=0}^{n-2}C_{i}'\right)V^{-(n-2)}, \qquad (n \ge 2) \qquad (60)$$

wherein it is understood that the product in braces is to be omitted in the case n = 2.

For n=2 the last two factors in Eq. (60) are both unity (recall that $C_0 = 1$), so the integrand is clearly bounded for n=2. [The exponential involving $\sec\theta'_0$ in the integrand causes no boundedness problems, because the last *I*-function in Eq. (60) imposes the condition $b\sec\theta'_0 < ct/V < ct.$] For $n \ge 3$ the integrand of Eq. (60) contains factors of $C_1, ..., C_{n-2}$, any of which can be arbitrarily large. However, the contribution of these factors to the integrand is moderated by the quantity V according to

$$\left(\prod_{i=0}^{n-2} C_{i}\right) V^{-(n-2)} = \prod_{i=1}^{n-2} (C_{i}/V). \qquad (n \ge 3)$$

The definition of V in Eq. (47f) shows that V is just the perimeter of the figure $OS_1 \cdots S_n O$ [see Fig. 3], and it is obvious that this perimeter cannot be less than twice the length of any cord C_i ; therefore, $C_i/V \le 1/2$ for all *i*, whence

$$\left(\prod_{i=0}^{n-2} C_i\right) V^{-(n-2)} \le (1/2)^{n-2}. \qquad (n \ge 3) \tag{61}$$

We conclude that the integrand in Eq. (60) is bounded for $n \ge 3$.

We collect below, in Eqs. (62), the formulas through which the various quantities in the integrand of Eq. (60) may be calculated in terms of the integration variables. Eq. (62a) follows from Eqs. (48), (47a) and (51); Eq. (62b) follows from Eqs. (55) and (49); Eq. (62c) is Eq. (5a); Eq. (62d) follows from Eqs. (48); Eq. (62e) follows from Eq. (55); the components $e_{i,x}$, $e_{i,y}$ and $e_{i,z}$ in Eq. (62f) are to be calculated from C_i , θ'_i and ϕ'_i according to the formulas in Eqs. (A8); Eq. (62g) follows from Eqs. (48); Eqs. (62h) and (62i) both follow from the second of Eqs. (49); Eqs. (62j) and (62k) both follow from Eq. (47e); Eq. (621) is Eq. (47f); and finally, Eqs. (62m) and (62n) follow from the definition of θ_i as the angle between e_{i-1} and e_i , together with the fact that $e_n = -\mathbf{a} = -\mathbf{C}_0$. The geometric content of the formulas below is summarized in Figs. 3 and 4.

$$C_0 = x \sin\theta'_0 + z \cos\theta'_0 \tag{62a}$$

$$v_0 = \sin\theta'_0 \tan v_0 + \cos\theta'_0 \tag{62b}$$

$$\mathbf{e}_0 = \mathbf{z} \tag{62c}$$

$$C_i = C_{i-1} - v_{i-1} e_{i-1}$$
 (62d)

$$v_i = C_i \sin{\theta'}_i \tan{v_i} + C_i \cos{\theta'}_i \qquad (n \ge 3; i = 1, ..., n - 2)$$
(62e)

$$e_i = \mathbf{x} e_{i,x} + \mathbf{y} e_{i,y} + \mathbf{z} e_{i,z}$$
(621)

$$\mathbf{C}_{n-1} = \mathbf{C}_{n-2} - v_{n-2} \,\mathbf{e}_{n-2} \tag{62g}$$

$$P_{n-1} = C_{n-1}$$
 (62h)

$$\mathbf{e}_{n-1} = \mathbf{C}_{n-1} / C_{n-1}$$
(62i)

$$\mathbf{B}_1 = v_0 \, \mathbf{e}_0 \tag{62j}$$

$$\mathbf{B}_{i} = \mathbf{B}_{i-1} + v_{i-1} \mathbf{e}_{i-1} \qquad (n \ge 3; i = 1, ..., n-1)$$
(62k)

$$V = 1 + \sum_{i=0}^{n-1} v_i$$
(621)

$$\theta_i = \arccos(\mathbf{e}_{i-1} \cdot \mathbf{e}_i) \qquad (i = 1, ..., n-1)$$
(62m)

$$\theta_{n} = \arccos(-\mathbf{e}_{n-1} \cdot \mathbf{C}_{0}) \tag{62n}$$

Notice that Eqs. (62d,e,f) and Eq. (62k) are not used if n=2. The interrelated, recursive structure of the formulas for C_i , v_i and e_i in Eqs. (62a – i) would make the derivation of explicit formulas for those quantities quite complicated, especially if $n \ge 3$; fortunately, explicit formulas are not needed for computational methods that utilize a digital computer.

Eqs. (60), (62) and (A8) are quoted in Ref. 1 as Eqs. (44), (45) and (46), respectively.

5. CUBING THE INTEGRATION DOMAIN

The integral expression in Eq. (60) is free of delta functions and has a bounded integrand and a bounded integration domain. It is therefore amenable to direct evaluation by standard numerical methods. However, many numerical methods are easier to implement if the integration domain is the *unit cube*. In this section we shall make a final change of integration variables to bring Eq. (60) into the form of an integral over the (3n - 4)-dimensional unit cube.

Each of the integration variables θ'_{i} , v_{i} and ϕ'_{i} in Eq. (60) measures an angle that has a clear physical interpretation in terms of the geometry of the path of an *n*-scattered photon [see Figs. 3 and 4]. We are now going to change from these integration variables to a new set of variables, p_{i} , q_{i} and w_{i} , whose physical interpretations are quite obscure but whose lower and upper integration limits are all 0 and 1, respectively. The particular transformation that we shall use for this purpose also has the convenient property that *its Jacobian is a constant*; this means that, apart from a different factor in front of the integral, the integrand in Eq. (60) will be unchanged by the transformation. The actual derivation of our transformation equations uses a special analytical technique in Monte Carlo theory called the "generalized inversion generating method." This analytical technique is discussed in detail in Secs. 2-5, 2-6 and 4-6 of Ref. 3. The derivation, although not particularly difficult, is moderately lengthy; therefore, we shall be content here simply to state the result and then verify that the transformation indeed has the special properties claimed.

With κ_0 defined by

$$\kappa_0 = \psi_0 (2n - \psi_0) / n^2, \tag{63a}$$

we define the variables p_0 and q_0 so that

$$\theta'_{0} = n[1 - (1 - \kappa_{0}p_{0})^{1/2}], \qquad (63b)$$

$$\mathbf{v}_0 = n[1/2 - q_0(1 - \kappa_0 p_0)^{1/2}]. \tag{63c}$$

We also define the variables p_i , q_i and w_j for i = 1, ..., n - 2 so that

$$\theta'_{i} = n(1 - p_{i}^{1/2}),$$
 (63d)

$$v_t = n(1/2 - q_t p_t^{1/2}), \qquad (n \ge 3; \ i = 1, ..., n - 2)$$
 (63e)

$$\phi'_{i} = 2\pi w_{i} \tag{63f}$$

Consider Eqs. (63b-c). The first of these two equations shows that, as p_0 runs from 0 to 1, θ'_0 runs monotonically from 0 to

$$n[1 - (1 - \kappa_0)^{1/2}] = \psi_0,$$

where the equality follows upon substituting for κ_0 its definition in Eq. (63a). Eq. (63c) shows that for p_0 and hence also θ'_0 fixed, as q_0 runs from 0 to 1, v_0 runs monotonically from n/2 to

$$u[1/2 - (1 - \kappa_0 p_0)^{1/2}] = \theta'_0 - u/2,$$

where the equality follows upon substituting for $(1 - \kappa_0 p_0)^{1/2}$ from Eq. (63b). We conclude that Eqs. (63b–c) map the unit square in p_0q_0 -space onto the two-dimensional region in θ'_0v_0 -space defined by the integration limits on θ'_0 and v_0 in Eq. (60). Since θ'_0 is independent of q_0 , then the corresponding Jacobian of this subspace transformation is

$$\left|\frac{\partial(\theta'_0, v_0)}{\partial(p_0, q_0)}\right| = \left|\frac{\partial\theta'_0}{\partial p_0} \frac{\partial v_0}{\partial q_0}\right| = [n(1/2)(1 - \kappa_0 p_0)^{-1/2}(\kappa_0)][n(1 - \kappa_0 p_0)^{1/2}] = \kappa_0 n^2/2.$$

Turning next to Eqs. (63d–f), the first of these equations shows that, as p_i runs from 0 to 1, θ'_i , runs monotonically from n to 0. Eq. (63e) shows that for p_i and hence also θ'_i fixed, as q_i , runs from 0 to 1, v_i runs monotonically from n/2 to

$$n(1/2 - p_i^{1/2}) = \theta'_i - n/2,$$

where the equality follows upon substituting for $p_i^{1/2}$ from Eq. (63d). And finally, Eq. (63f) shows that, as w_i runs from 0 to 1, ϕ'_i runs monotonically from 0 to 2n. We conclude that Eqs. (63d-f) map the unit cube in $p_i q_i w_i$ -space onto the three-dimensional region in $\theta'_i v_i \phi'_i$ -space defined by the integration limits on θ'_i , v_i and ϕ'_i in Eq. (60). This mapping is one-to-one everywhere except on the plane defined by $p_i = 0$, which is mapped onto the line defined by $\theta'_i = n$ and $v_i = n/2$. But since that plane and line have zero volume, this lack of strict one-to-oneness has no effect on the three-dimensional integrals of interest to us here.

For i > 0 we note from Eqs. (63d-e) that θ'_{i} is independent of both q_{i} and w_{i} , while v_{i} is independent of w_{i} . It follows that the Jacobian of the transformation between $\theta'_{i}v_{i}\phi'_{i}$, space

and $p_i q_i w_i$ -space defined by Eqs. (63d-f) has zero entries everywhere on one side of the main diagonal. Therefore,

$$\left|\frac{\partial(\theta'_{i}, \mathbf{v}_{i}, \boldsymbol{\phi}'_{i})}{\partial(p_{i}, q_{i}, w_{i})}\right| = \left|\frac{\partial\theta'_{i}}{\partial p_{i}} \frac{\partial \mathbf{v}_{i}}{\partial q_{i}} \frac{\partial \boldsymbol{\phi}'_{i}}{\partial w_{i}}\right| = [\pi(1/2)p_{i}^{-1/2}][np_{i}^{1/2}][2n] = \pi^{3}$$

Finally, since there is no cross-coupling between integration variables with different index values, the Jacobian of the full transformation is just the product of the subspace Jacobians. Therefore,

$$\left|\frac{\frac{\partial(\theta'_{0}, \mathbf{v}_{0}, \theta'_{1}, \mathbf{v}_{1}, \phi'_{1}, \dots, \theta'_{n-2}, \mathbf{v}_{n-2}, \phi'_{n-2})}{\partial(p_{0}, q_{0}, p_{1}, q_{1}, \omega_{1}, \dots, p_{n-2}, q_{n-2}, \omega_{n-2})}\right| = \frac{\pi^{2} \kappa_{0}}{2} (\pi^{3})^{n-2} = \frac{1}{2} \pi^{3n-4} \kappa_{0}.$$
(64)

We conclude, then, that the integral in Eq. (60) transforms under Eqs. (63) to

$$P_{n}(t,0,0) = n^{3(n-1)} \kappa_{0} \beta_{s}^{n} c(ct)^{n-3} \exp(-\beta ct) \int_{0}^{1} dp_{0} \int_{0}^{1} dq_{0} \left\{ \prod_{i=1}^{n-2} \int_{0}^{1} dp_{i} \int_{0}^{1} dq_{i} \int_{0}^{1} dw_{i} \right\}$$

$$\times \left(\prod_{i=1}^{n-1} I(B_{i,2} > Vb/ct) \right) I(\cos\theta'_{0} > Vb/ct) \exp[\beta b(1 + \sec\theta'_{0})]$$

$$\times \left(\prod_{i=1}^{n} f(\theta_{i}) \right) \cos\theta'_{0} \left(\prod_{i=0}^{n-2} C_{i} \right) V^{-(n-2)}, \qquad (n \ge 2) \qquad (65)$$

In this our final expression for $P_n(t,0,0)$, it is understood that the product in braces is to be omitted in the case n = 2, and also that the integrand is to be evaluated in terms of the integration variables through the formulas listed in Eqs. (62) and (63) [see also Figs. 3 and 4].

Eqs. (63), (64) and (65) are quoted in Ref. 1 as Eqs. (47), (48) and (49), respectively.



FIGURE 1. Trajectory of an *n*-Scattered Photon. The photon leaves the origin O along the positive z-axis, scatters exactly *n* times in the cloud, and then returns to O at an angle ψ with the z-axis. The *i*th scattering, through polar angle θ_i and azimuthal angle ϕ_i , occurs at point S_i . The vector from S_i to S_{i+1} is denoted by $\mathbf{u}_i \equiv \mathbf{e}_i u_i$, where \mathbf{e}_i is a vector of unit length and $S_0 = S_{n+1} = 0$.



FIGURE 2. Geometric Interpretation of the Relations Among the Principle Variables in Eqs. (46) and (47) for (a) n=2, (b) n=3, and (c) n=4. The vector \mathbf{v}_i , with magnitude v_i and unit direction \mathbf{e}_i , represents the scaled path of the photon between the i^{th} and $(i+1)^{th}$ scatterings. The angles θ_i and ϕ_i are the polar and azimuthal angles of \mathbf{e}_i relative to the polar direction \mathbf{e}_{i-1} . The vector \overrightarrow{OS}_i for i=1,...,n-1 is designated \mathbf{B}_i ; the vector \overrightarrow{OS}_n is designated \mathbf{a} , and has unit length and polar angle ψ . The xyz-frame is defined so that $\mathbf{e}_0 = \mathbf{z}$ with \mathbf{a} lying in the xz-plane. Notice that the quantity V defined in Eq. (47f) is the perimeter of the (generally non-planar) figure $OS_1 \cdots S_n O$.



1.2.1

FIGURE 3. Geometric Interpretation of the Relations Among the Principle Variables in Eqs. (53), (60) and (62) for (a) n=2, (b) n=3 and (c) n=4. The angles θ_i' and ϕ_i' are the polar and azimuthal angles of $\mathbf{v}_i = \mathbf{v}_i \mathbf{e}_i$ relative to the polar direction $\mathbf{C}_i = \overline{\mathbf{S}_i \mathbf{S}_n}$ (i=1,...,n-2); the other quantities are as specified in Fig. 2. (The vectors $\mathbf{B}_i = \overrightarrow{\mathbf{OS}}_i$ are still present, but they are not shown here in order to avoid complicating the diagrams.) Note that \mathbf{a} and ψ in Fig. 2 have here been renamed \mathbf{C}_0 and θ_0' , respectively.



FIGURE 4. Geometric Interpretation of the Variable v_t Defined in Eq. (54). Together, Figs. 3 and 4 show geometrically the relations that obtain among the principle variables in Eq. (60) and (62).

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APPENDIX: COMPONENTS OF THE VECTORS e, IN THE xyz-FRAME

Let C be a vector with components C_x , C_y and C_z relative to some coordinate frame F with basis vectors x, y and z. Define frame F' as that frame whose basis vectors x', y' and z' satisfy $z' \propto C$ and $y' \propto z \times C$ [see Fig. A1]. Finally, let e be a unit vector having polar angle θ' and azimuthal angle ϕ' relative to frame F'. We want to calculate the components e_x , e_y and e_z of e relative to frame F in terms of the quantities C_x , C_y , C_z , θ' and ϕ' .

We begin by defining the auxiliary quantities c_x , c_y , c_z and c_{xy} by

$$c_x \equiv C_x/C, \ c_y \equiv C_y/C, \ c_z \approx C_z/C, \ c_{xy} \equiv (C_x^2 + C_y^2)^{1/2}/C.$$
 (A1)

Then the polar angle μ and azimuthal angle ξ of C in the F-frame are given by

$$\cos\mu = c_z, \qquad \sin\mu = c_{rv} \tag{A2a}$$

$$\cos\xi = c_x / c_{xy}, \quad \sin\xi = c_y / c_{xy}. \tag{A2b}$$

Fig. A1 shows how the angles μ and ξ determine the orientation of frame F' relative to frame F. From the geometry of that figure, we can see that the projections of the primed unit vectors onto the unprimed unit vectors are as follows:

$$\mathbf{x}' \cdot \mathbf{x} = \cos\mu \cos\xi = c_z c_x / c_{xy},$$

$$\mathbf{x}' \cdot \mathbf{y} = \cos\mu \sin\xi = c_z c_y / c_{xy},$$

$$\mathbf{x}' \cdot \mathbf{z} = -\sin\mu = -c_{xy};$$

$$\mathbf{y}' \cdot \mathbf{x} = -\sin\xi = -c_y / c_{xy},$$

$$\mathbf{y}' \cdot \mathbf{y} = \cos\xi = c_x / c_{xy},$$

$$\mathbf{y}' \cdot \mathbf{z} = 0;$$

$$\mathbf{z}' \cdot \mathbf{x} = \sin\mu \cos\xi = c_x,$$

$$\mathbf{z}' \cdot \mathbf{y} = \sin\mu \sin\xi = c_y,$$

$$\mathbf{x}' \cdot \mathbf{z} = \cos\mu = c_y.$$
(A3a)

Also, since θ' and ϕ' are defined as the polar and azimuthal angles of the unit vector **e** relative to frame F', then the projections of **e** on the primed unit vectors are

$$\mathbf{x'} \cdot \mathbf{e} = \sin\theta' \cos\phi',$$

$$\mathbf{y'} \cdot \mathbf{e} = \sin\theta' \sin\phi',$$

$$\mathbf{z'} \cdot \mathbf{e} = \cos\theta'.$$

(A4)





FIGURE A1. Relative Orientation of the xyz-Frame and the x'y'z'-Frame. The latter frame is defined by $z' \propto C$ and $y' \propto z \times C$. The angles μ and ξ are the polar and azimuthal angles of the vector C relative to the xyz-frame.

Now we observe that the x-component of e can be calculated as

$$e_{\mathbf{x}} = \mathbf{x} \cdot \mathbf{e} = [\mathbf{x}'(\mathbf{x}' \cdot \mathbf{x}) + \mathbf{y}'(\mathbf{y}' \cdot \mathbf{x}) + \mathbf{z}'(\mathbf{z}' \cdot \mathbf{x})] \cdot [\mathbf{x}'(\mathbf{x}' \cdot \mathbf{e}) + \mathbf{y}'(\mathbf{y}' \cdot \mathbf{e}) + \mathbf{z}'(\mathbf{z}' \cdot \mathbf{e})],$$

or

$$\boldsymbol{e}_{\boldsymbol{x}} = (\boldsymbol{x}' \cdot \boldsymbol{x})(\boldsymbol{x}' \cdot \boldsymbol{e}) + (\boldsymbol{y}' \cdot \boldsymbol{x})(\boldsymbol{y}' \cdot \boldsymbol{e}) + (\boldsymbol{z}' \cdot \boldsymbol{x})(\boldsymbol{z}' \cdot \boldsymbol{e}). \tag{A5a}$$

Similarly, the y- and z-components of e can be calculated as

$$e_{\mathbf{y}} = (\mathbf{x}' \cdot \mathbf{y})(\mathbf{x}' \cdot \mathbf{e}) + (\mathbf{y}' \cdot \mathbf{y})(\mathbf{y}' \cdot \mathbf{e}) + (\mathbf{z}' \cdot \mathbf{y})(\mathbf{z}' \cdot \mathbf{e}), \tag{A5b}$$

$$e_{z} = (\mathbf{x}' \cdot \mathbf{z})(\mathbf{x}' \cdot \mathbf{e}) + (\mathbf{y}' \cdot \mathbf{z})(\mathbf{y}' \cdot \mathbf{e}) + (\mathbf{z}' \cdot \mathbf{z})(\mathbf{z}' \cdot \mathbf{e}).$$
(A5c)

If we now substitute Eqs. (A3) and (A4) into Eqs. (A5), we find that the resulting equations for e_x , e_y and e_y can be written in matrix form as

$$\begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix} = \begin{bmatrix} c_z c_x / c_{xy} & -c_y / c_{xy} & c_x \\ c_z c_y / c_{xy} & c_x / c_{xy} & c_y \\ -c_{xy} & 0 & c_z \end{bmatrix} \begin{bmatrix} \sin\theta' \cos\phi' \\ \sin\theta' \sin\phi' \\ \cos\theta' \end{bmatrix}$$
(A6)

Together, Eqs. (A6) and (A1) give the F-frame components of e in terms of the F-frame components of C and the angles θ' and ϕ' . But notice that, if C should happen to coincide with z, then $c_x = c_y = c_{xy} = 0$, and the four quotient elements in the above 3×3 matrix become indeterminate. Since in that special case we will have z' = z, then we may as well take x' = x and y' = y. Therefore, if $c_{xy} = 0$ then we shall simply take the 3×3 matrix in Eq. (A6) to be the unit matrix (with 1's along the main diagonal and 0's elsewhere).

The foregoing result is actually used in two different ways in the text to calculate the xyzframe components of the unit vectors \mathbf{e}_i . The first way is in connection with Eqs. (5) and (6). There, \mathbf{e}_i (i = 1,...,n) is stipulated to have polar angle θ_i and azimuthal angle ϕ_i in the coordinate frame whose z-axis points along \mathbf{e}_{i-1} and whose y-axis points along $\mathbf{z} \times \mathbf{e}_{i-1}$. Therefore, if $e_{i,x}, e_{i,y}$ and $e_{i,x}$ are the components of \mathbf{e}_i in the xyz-frame, and if $e_{i,xy} \equiv (e_{i,x}^2 + e_{i,y}^2)^{1/2}$, then above result implies the recursion relation

$$\begin{bmatrix} e_{i,x} \\ e_{i,y} \\ e_{i,z} \end{bmatrix} = \begin{bmatrix} e_{i-1,z}e_{i-1,x}/e_{i-1,xy} & -e_{i-1,y}/e_{i-1,xy} & e_{i-1,x} \\ e_{i-1,z}e_{i-1,y}/e_{i-1,xy} & e_{i-1,x}/e_{i-1,xy} & e_{i-1,y} \\ -e_{i-1,xy} & 0 & e_{i-1,z} \end{bmatrix} \begin{bmatrix} \sin\theta_i \cos\phi_i \\ \sin\theta_i \sin\phi_i \\ \cos\theta_i \end{bmatrix}, (i=1,...,n)$$
(A7a)

where, from Eq. (5a),

$$P_{0,x} = 0, \quad e_{0,y} = 0, \quad e_{0,z} = 1,$$
 (A7b)

and where it is understood that, if $e_{i-1,xy} = 0$, then the 3×3 matrix in Eq. (A7a) is to be taken to be the unit matrix.

Eqs. (A7) show how the xyz-frame components of \mathbf{e}_i may be calculated from the xyz-frame components of \mathbf{e}_{i-1} and the angular variables θ_i and ϕ_i . These relations are required for a complete interpretation of the "early" formulas in our analysis [specifically, Eqs. (1) through (46)]. However, our final formulas for $P_n(t,0,0)$ for $n \ge 3$ [Eqs. (60) and (65)] have as their integration variables, not the angles θ_i and ϕ_i , but the angles θ'_i and ϕ'_i (i=1,...,n-2). These primed angles are defined [cf. Eqs. (52)] as the polar and azimuthal angles of \mathbf{e}_i in the frame whose z-axis points along \mathbf{C}_i and whose y-axis points along $\mathbf{z} \times \mathbf{C}_i$, where \mathbf{C}_i is the vector defined in Eq. (48). It follows from the foregoing analysis that, in Eqs. (62), the xyz-frame components of the vectors $\mathbf{e}_1,...,\mathbf{e}_{n-2}$ are to be calculated according to the following formula:

$$\begin{bmatrix} e_{i,x} \\ e_{i,y} \\ e_{i,z} \end{bmatrix} = \begin{bmatrix} c_{i,z}c_{i,x}/c_{i,xy} & -c_{i,y}/c_{i,xy} & c_{i,x} \\ c_{i,z}c_{i,y}/c_{i,xy} & c_{i,x}/c_{i,xy} & c_{i,y} \\ -c_{i,xy} & 0 & c_{i,z} \end{bmatrix} \begin{bmatrix} \sin\theta_i' \cos\phi_i' \\ \sin\theta_i' \sin\phi_i' \\ \cos\theta_i' \end{bmatrix}, \quad (i=1,...,n-2) \text{ (A8a)}$$

where

$$c_{i,x} \equiv C_{i,x}/C_i, \ c_{i,y} \equiv C_{i,y}/C_i, \ c_{i,z} \equiv C_{i,z}/C_i, \ c_{i,xy} \equiv (C_{i,x}^2 + C_{i,y}^2)^{1/2}/C_i,$$
 (A8b)

and where it is understood that if $c_{i,xy} = 0$ then the 3×3 matrix in Eq. (A8a) is to be taken to be the unit matrix.

Eqs. (A8) are quoted in Ref. 1 as Eqs. (46).

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