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An Adjoint Monte Carlo Treatment of the Equations of Radiative Transfer for Polarized Light*

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The equation of radiative transfer for a Stokes' intensity vector is used to define a four-vector Green's function. The physical quantities of interest are represented by a response vector which is found by integrating the product of a suitable response matrix and the Stokes' intensity vector over phase space. Equations adjoint to those for the Stokes' intensity vector and for the Green's function vector are given. The response vector is then expressed in terms of the adjoint vector Green's function. A Monte Carlo sampling procedure is given for the adjoint Green's function vector equation. When the adjoint source vector is given by a Dirac delta function in phase space, the response vector is the Stokes' intensity vector and the "backward Monte Carlo method" of Collins and Wells (Report RRA-T74, Radiation Research Associates, Inc.) obtains.

1. INTRODUCTION

The speed and versatility of the modern digital computer have enabled the solution of a variety of radiative transfer problems. A calculation tool, which is often used for solving these problems, is random sampling with the Monte Carlo method. The flexibility of Monte Carlo allows the solution of three-dimensional geometries, the treatment of complicated interaction phenomena, and the use of otherwise difficult boundary conditions.

The Monte Carlo method has been utilized to include polarization effects by Kastner [2], Cashwell [3], Collins and Wells [1], Sandford and Pauls [4], Collins *et al.* [5], Mikhaylov and Nazaraliyev [6], and by a number of other investigators. The statistical errors in such calculations become large when information is required in a small portion of phase space. A pertinent example is the determination of Stokes' intensities in a given direction at a receiver position. The paper by Collins *et al.* [5] presents a "backward" Monte Carlo technique that overcomes this difficulty. In this calculational method, the four Stokes' parameters, I_ℓ, I_r, U, V, that characterize the radiation at a receiver position were evaluated by a backward simulation of the radiation flight paths from the receiver to the source.

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The "backward" method is actually a Monte Carlo simulation of the equations that are adjoint to the four coupled transport equations for the Stokes' parameters, and a description of the Monte Carlo calculation in the adjoint framework would seem to have the advantage of mathematical clarity. This formulation also provides a basis for algorithms that will simulate polarization effects in either the direct or adjoint mode.

In this paper, we derive the equations adjoint to the four coupled transport equations for the Stokes' parameters. A reciprocity relationship is obtained between a Green's function four-vector and an adjoint Green's function four-vector. This is similar to reciprocity in neutron transport [7] except that we obtain reciprocity between two four-vectors. The reciprocity relation enables a physical interpretation of the similarities and differences between Monte Carlo simulations of the direct and adjoint equations. The adjoint simulation is described in detail.

2. Statement of the Direct Problem

The vector transport equation for the Stokes' parameters, as derived by Chandrasekhar [8], is

$$\vec{\imath} \cdot \vec{\nabla} \vec{I}(\vec{r}, \mu, \phi) + \kappa\rho(\vec{r})\, \vec{I}(\vec{r}, \mu, \phi) - \frac{\kappa\rho(\vec{r})}{4\pi} \int_{-1}^{1} \int_{0}^{2\pi} \mathbf{P}(\mu, \phi; \mu', \phi')\, \vec{I}(\vec{r}, \mu', \phi')\, d\mu'\, d\phi' = \vec{S}(\vec{r}, \mu, \phi), \tag{1}$$

where $\vec{I}$ is the intensity vector with the four components (I_ℓ, I_r, U, V), $\mathbf{P}$ is a four by four matrix, κ is the mass absorption coefficient, ρ is the density of the material, $\vec{S}$ is an extraneous source vector, $\vec{r}$ is the position vector, and $\vec{\imath}$ is a unit photon propagation (flight) vector defined by the cosine of the polar angle, $\mu = \cos\theta$; and ϕ, the azimuth angle. The notation will subsequently be simplified by allowing R to denote both the space position and the direction of flight; i.e., $R \to \vec{r}, \mu, \phi$; or equivalently, $R \to \vec{r}, \vec{\imath}$.

The purpose of the calculation is assumed to be the computation of a response vector denoted by $\vec{F}$. The definition of a response vector as

$$\vec{F} = \int \mathbf{A}(R)\, \vec{I}(R)\, dR, \tag{2}$$

will become apparent when we later consider the adjoint equation. In Eq. (2), $\mathbf{A}(R)$ is a diagonal response matrix, the elements of which depend upon the quantity of interest. For example, if the A_{11} element of the matrix was defined as

$$A_{11} = \delta(R - R_0), \tag{3}$$

then the first element of the vector $\vec{F}$ would represent the parallel intensity component,

$I_\ell(R_0)$. The delta function notation in Eq. (3) is understood to symbolize a product of Dirac delta functions in space and direction:

$$\delta(R - R_0) = \delta(x - x_0)\,\delta(y - y_0)\,\delta(z - z_0)\,\delta(\mu - \mu_0)\,\delta(\phi - \phi_0). \tag{4}$$

A Green's function will be defined for the direct vector transport equation in order to later introduce reciprocity. To compact the notation, an operator L is defined for Eq. (1) such that

$$L\vec{I}(R) = \vec{S}(R). \tag{5}$$

A Green's function vector, $\vec{G}$, is then required to satisfy the equation

$$L\vec{G}(R; R') = \delta(R - R')\,\vec{S}(R'), \tag{6}$$

where each of the four elements of the vector $\vec{S}$ is multiplied by the delta function. The principle of superposition allows the intensity vector to be expressed as

$$\vec{I}(R) = \int \vec{G}(R; R')\,dR', \tag{7}$$

provided that the vector $\vec{G}$ satisfies the same boundary conditions as the vector $\vec{I}$.

The expression for the intensity in Eq. (7) may be utilized in Eq. (2) to express the response vector as

$$\vec{F} = \iint \mathbf{A}(R)\,\vec{G}(R; R')\,dR'\,dR. \tag{8}$$

3. Derivation of the Adjoint Vector Equation

A vector equation for the adjoint intensity vector, $\vec{I}^\dagger$, is obtained by finding an operator, $L^\dagger$, such that

$$\int \tilde{\vec{I}}^\dagger(R)\,L\vec{I}(R)\,dR - \int \tilde{\vec{I}}(R)\,L^\dagger\vec{I}^\dagger(R)\,dR = 0, \tag{9}$$

where each tilde mark denotes a transpose. A satisfactory $L^\dagger$ is postulated such that its operation on $\vec{I}^\dagger$ gives

$$L^\dagger\vec{I}^\dagger(R) = -\vec{i}\cdot\vec{\nabla}\vec{I}^\dagger(R) + \kappa\rho(\vec{r})\,\vec{I}^\dagger(R) - \frac{\kappa\rho(\vec{r})}{4\pi}\int \tilde{\mathbf{P}}(\vec{i}'; \vec{i})\,\vec{I}^\dagger(\vec{r}, \vec{i}')\,d\vec{i}' = \vec{S}^\dagger(R), \tag{10}$$

where the adjoint source four-vector, $\vec{S}^\dagger$, will be discussed later. The boundary conditions for $\vec{I}^\dagger$ are chosen to be consistent with those for $\vec{I}$ and are such that the

bilinear concomitant [7] is zero term by term; i.e., on the outer surface of the system:

$$\tilde{I}(R) = \vec{O} \qquad \text{for } \vec{i} \text{ inward} \tag{11}$$

and

$$\tilde{I}^{\dagger}(R) = \vec{O} \qquad \text{for } \vec{i} \text{ outward,} \tag{12}$$

where $\vec{O}$ is a vector whose elements are zero.

The proof, that Eq. (9) is satisfied by the operators $L^{\dagger}$ of Eq. (10) and L of Eq. (5), may be given term by term. We first multiply Eq. (5) on the left by $\tilde{\tilde{I}}^{\dagger}(R)\, dR$, multiply Eq. (10) on the left by $\tilde{\tilde{I}}(R)\, dR$, extract the difference of the resulting two equations, and integrate this difference over all of phase space. The resluting leakage, attenuation, and scattering terms are considered separately:

Leakage Term

This term consists of a sum of individual terms of the form

$$\int [I_j^{\dagger}(R)\, \vec{i} \cdot \vec{\nabla}\, I_j(R) + I_j(R)\, \vec{i} \cdot \vec{\nabla}\, I_j(R)]\, dR, \tag{13}$$

where j denotes the jth element of the vector. From the vector differentiation sum rule, this is simply

$$\int \vec{\nabla} \cdot \{\vec{i}\, I_j^{\dagger}(R)\, I_j(R)\}\, dR. \tag{14}$$

The divergence theorem may be utilized to change to a surface integral, which vanishes due to the boundary conditions of Eqs. (11) and (12).

Attenuation Term

This term consists of a sum of individual terms of the form

$$\int [I_j^{\dagger}(R)\, \kappa\rho(\vec{r})\, I_j(R) - I_j(R)\, \kappa\rho(\vec{r})\, I_j^{\dagger}(R)]\, dR. \tag{15}$$

Each such term is clearly identically zero since the scalar integrand is zero.

Scattering Term

The scattering term may be written as

$$\frac{1}{4\pi} \iiint \kappa\rho(\vec{r}) \{\tilde{\tilde{I}}^{\dagger}(\vec{r}, \vec{i})\, \mathbf{P}(\vec{i}; \vec{i}')\, \tilde{I}(\vec{r}, \vec{i}') - \tilde{I}(\vec{r}, \vec{i}')\, \tilde{\mathbf{P}}(\vec{i}; \vec{i}')\, \tilde{I}^{\dagger}(\vec{r}, \vec{i})\, d\vec{i}'\, d\vec{i}\, d\vec{r}, \tag{16}$$

where the integration variables $\vec{i}$ have been inverted with $\vec{i}'$ in the $\tilde{\vec{I}}\tilde{\mathbf{P}}\vec{I}^{\dagger}$ term. The integrand is zero due to the matrix identity

$$\tilde{\vec{I}}\tilde{\mathbf{P}}\vec{I}^{\dagger} = \tilde{\vec{I}}^{\dagger}\mathbf{P}\vec{I}. \tag{17}$$

This proof that the operators L and $L^{\dagger}$ satisfy Eq. (9) may be utilized to obtain a reciprocity relationship.

4. Reciprocity

The adjoint Green's function vector is required to satisfy the equation

$$L^{\dagger}\vec{G}^{\dagger}(R; R'') = \delta(R - R'')\,\vec{S}^{\dagger}(R''). \tag{18}$$

It is also required to satisfy the same boundary conditions as $\vec{I}^{\dagger}$. The adjoint source vector, $\vec{S}^{\dagger}$, is as yet unspecified.

A reciprocity relation is obtained by multiplying Eq. (6) on the left by $\tilde{\vec{G}}^{\dagger}(R; R'')\,dR$, multiplying Eq. (18) on the left by $G(R; R')\,dR$, extracting the difference of the resulting two equations, and integrating this difference over all of phase space. The application of Eq. (9) for the Green's function vectors, rather than for the intensity vectors, removes all terms involving L and $L^{\dagger}$. The two terms remaining give the reciprocity relation

$$\tilde{\vec{G}}(R; R')\,\vec{S}^{\dagger}(R) = \tilde{\vec{G}}^{\dagger}(R'; R)\,\vec{S}(R'). \tag{19}$$

The above proof could just as easily be repeated for each individual component of the vector. The result of such an operation is that

$$G(R; R')_j\,S^{\dagger}(R)_j = G^{\dagger}(R'; R)_j\,S(R')_j \qquad (j = 1, 2, 3, 4). \tag{20}$$

The adjoint source vector has not been specified so we are free to choose its components. In order to relate an adjoint simulation to the response vector, we need to express the response vector of Eq. (8) in terms of the adjoint Green's function vector; i.e., express $\mathbf{A}(R)\,\vec{G}(R; R')$ as some function of $\vec{G}^{\dagger}$. This is accomplished by requiring that $\vec{S}^{\dagger}(R)$ satisfy the relation

$$\vec{S}^{\dagger}(R) = \mathbf{A}(R)\begin{pmatrix}1\\1\\1\\1\end{pmatrix}, \tag{21}$$

where $\mathbf{A}(R)$ is the response matrix that was utilized in Eq. (8). Similarly, a diagonal

matrix **B** is defined such that its diagonal components are equal to the components of $\vec{S}$,

$$\vec{S}(R') = \mathbf{B}(R') \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}. \tag{22}$$

These definitions and the reciprocity relationships of Eq. (20) yield the vector equality

$$\mathbf{A}(R)\, \vec{G}(R; R') = \mathbf{B}(R')\, G^{\dagger}(R'; R). \tag{23}$$

Equation (22) may finally be utilized in Eq. (8) to express the response vector in terms of the adjoint Green's function vector as

$$\vec{F} = \iint \mathbf{B}(R)\, \vec{G}^{\dagger}(R'; R)\, dR\, dR'. \tag{24}$$

The response vector, $\vec{F}$, in Eq. (24) may clearly be computed by obtaining a numerical solution of the adjoint Green's function vector equation (18).

5. Sampling the Adjoint Equation

A. *General Considerations*

The adjoint Green's function vector equation (18) has a slightly different form than the direct Green's function vector equation (6). We are interested in sampling from Eq. (18) so it would be pertinent to first transform it into an equation that has the identical form of the direct equation, since we already know how to sample from such an equation. This type of an approach has been found useful for sampling from the adjoint neutron transport equation [9, 10].

The primary difference between Eqs. (18) and (6) is the sign of the leakage term. Therefore, the direction coordinate is reflected in Eq. (18) and a new vector $\vec{g}^{\dagger}$ is defined as

$$\vec{g}^{\dagger}(\vec{r}, \vec{i}; \vec{r}'', \vec{i}'') = \vec{G}^{\dagger}(\vec{r}, -\vec{i}; \vec{r}'', -\vec{i}''). \tag{25}$$

Then Eq. (18) may be written as

$$\begin{aligned} &\vec{i} \cdot \vec{\nabla} \vec{g}^{\dagger}(R; R'') + \kappa\rho(\vec{r})\, \vec{g}^{\dagger}(R; R'') \\ &\qquad - \frac{\kappa\rho(\vec{r})}{4\pi} \int \bar{\mathbf{P}}(-\vec{i}'; -\vec{i})\, \vec{g}^{\dagger}(\vec{r}, \vec{i}'; R'')\, d\vec{i}' \\ &\qquad = \delta(\vec{r} - \vec{r}'')\, \delta(-\vec{i} - \vec{i}'')\, \vec{S}^{\dagger}(R''). \end{aligned} \tag{26}$$

Equation (26) has the identical form of the vector transport equation (6). The transformed vector, $\vec{g}^{\dagger}$, also satisfies the same boundary condition on the outer

surface as $G^{\dagger}$, i.e., no incoming current. Therefore, the sampling of the transformed adjoint equation (26) parallels a sampling of the direct vector equation with an altered scattering kernel and a reflection of the direction of flight coordinates in the extraneous source term. The scattering kernel matrix has been transposed, the direction of flight in the kernel has been reflected, and the primed and unprimed direction of flight variables in the kernel have interchanged roles for the sampling.

Equation (26) has been obtained by Collins and Wells [1] by making coordinate transformations to the direct vector equation. This approach, termed the "backward" Monte Carlo method, is valid for *coherent* scattering problems because the time invariance of the Maxwell's equation yields the reciprocity relation [11]:

$$\tilde{\mathbf{P}}(-\vec{i}'; -\vec{i}) = \mathbf{P}(\vec{i}; \vec{i}').$$

The sampling of the adjoint equation (26) may therefore be viewed entirely from the standpoint of reciprocity (coordinate transformation) where particles originate at the detector and scatter according to a reciprocal phase matrix.

B. *Sampling a New Direction at a Scattering Collision*

The postcollision direction of flight coordinates, $\vec{i}(\mu, \phi)$, given the precollision direction of flight coordinates, $\vec{i}'(\mu', \phi')$, may be sampled with any density function that is greater than zero for all values of μ and ϕ. The particle vector weight is altered at each collision in such a manner as to yield unbiased results for the particular density function that is utilized. A reasonable choice of a density function is one that is proportional to the total postcollision adjoint intensity. This density function may be written as

$$f(\vec{i}; \vec{i}') = \frac{\vec{X}\tilde{\mathbf{P}}(-\vec{i}'; -\vec{i})\ \vec{W}(\vec{r}, \vec{i}')}{4\pi \vec{X}\ \vec{W}(\vec{r}, \vec{i}')}, \tag{27}$$

where in the Monte Carlo calculation $\vec{W}(\vec{r}, \vec{i}')$ is a vector containing the four weights in the adjoint sampling upon entering the collision, and $\vec{X}$ is the row vector

$$\vec{X} = (1\ 1\ 0\ 0). \tag{28}$$

For the special case of Rayleigh scattering, the density function of Eq. (27) is almost the same as the corresponding density function that occurs for sampling from the direct vector equation. In the Appendix we discuss Boson scattering from spherical centers and compare the direct and adjoint density functions. Schemes are presented for sampling from these density functions.

The four weights after the collision are obtained as

$$\vec{W}(\vec{r}, \vec{i}) = \frac{\tilde{\mathbf{P}}(-\vec{i}'; -\vec{i})\ \vec{W}(\vec{r}, \vec{i}')}{4\pi f(\vec{i}; \vec{i}')}, \tag{29}$$

where the $\vec{i}(\mu, \phi)$ in Eq. (29) is the final propagation direction vector selected at the

collision using the density function f. It should be emphasized that the density function f need not be chosen to satisfy Eq. (27). The weight vector modification given by Eq. (29) will produce unbiased results for any choice of the density function as long as f is greater than zero for any choice of $\vec{i}(\mu, \phi)$. For complicated interactions, a useful simplification is to set f to the corresponding density function that is obtained by ignoring polarization effects. Then a one-dimensional table is all that is required for sampling $\vec{i}(\mu, \phi)$ in an isotropic media.

C. *Sampling Initial Source Particle Coordinates*

The relation of Eq. (25), between the transformed adjoint Green's function vector and the adjoint Green's function vector, may be utilized to express the response vector of Eq. (24) as

$$\vec{F} = \iint \mathbf{B}(\vec{r}, \vec{i})\, \vec{g}^{\dagger}(\vec{r}, -\vec{i}; \vec{r}', -\vec{i}')\, d\vec{r}\, d\vec{i}\, d\vec{r}'\, d\vec{i}'. \tag{30}$$

Since the source term for $\vec{g}^{\dagger}$ depends upon the receiver, the integrand in Eq. (30) is nonzero only if the primed variables correspond to the receiver position in phase space. Hence, the initial spatial position in the adjoint simulation may be selected randomly within the spatial volume of the receiver, and the direction of flight may also be selected randomly within the solid angle of propagation incident on the receiver. This direction of flight is then reflected, due to the reflection in direction that occurs in the adjoint source term of Eq. (26), and the initial four-vector weight is given by

$$\vec{W} = \vec{S}^{\dagger}(\vec{r}'', -\vec{i}'') \int_{V_R} dR, \tag{31}$$

where $\vec{r}''$ was the initial position selected and $-\vec{i}''(\mu'', \phi'')$ is the initial direction vector selected prior to reflection. The integration in Eq. (31) is defined to be over the phase space volume of the receiver. The initial vector weight, $\vec{W}$, of Eq. (31) yields the correct expectation values in a volume element dR about R since these are

$$E(\vec{W}) \text{ in } dR'' \text{ about } R'' = \begin{pmatrix} \text{Probability of selecting} \\ \text{initial coordinates} \\ \text{in } dR'' \text{ about } R'' \end{pmatrix} \times \begin{pmatrix} \text{Particle weight,} \\ \text{given coordinates} \\ \text{in } dR'' \text{ about } R'' \end{pmatrix},$$

which is

$$E(\vec{W}) = \left(\frac{dR''}{\int_{V_R} dR}\right)\left(\vec{S}^{\dagger}(\vec{r}'', -\vec{i}'') \int_{V_R} dR\right),$$

or

$$E(\vec{W}) = \vec{S}^{\dagger}(\vec{r}'', -\vec{i}'')\, dR''. \tag{32}$$

This is in agreement with the source term of Eq. (26) and the observation that there are no factors other than $\vec{g}^{\dagger}$ in Eq. (30) that depend upon the primed variables.

A situation of particular interest occurs when each element of $\vec{S}^{\dagger}$ is a product of Dirac delta functions in both position and direction of propagation. The response vector, $\vec{F}$, then represents the intensity vector at a space point for a fixed direction of propagation (the Stokes' intensities at a detector). If $\vec{S}^{\dagger}$ is given by

$$\vec{S}^{\dagger}(\vec{r}'', \mu'', \phi'') = \delta(\vec{r}'' - \vec{r}')\,\delta(\vec{\imath}'' - \vec{\imath}')\begin{pmatrix}1\\1\\1\\1\end{pmatrix}, \tag{33}$$

the appropriate limit of Eq. (31) may be taken for square waves increasing in heights and decreasing in widths so as to approach Dirac delta functions, resulting in initial coordinates for the Monte Carlo of $(\vec{r}', -\vec{\imath}')$ and the initial weight vector:

$$\vec{W} = \begin{pmatrix}1\\1\\1\\1\end{pmatrix}, \tag{34}$$

which are the initial source particles employed by Collins and Wells [1].

D. *Estimation*

A collision estimator will be considered for the scoring. An unbiased estimate of $\vec{g}^{\dagger}(R; R'')\,\kappa\rho(\vec{r})\,dR$ is given by

$$\vec{g}^{\dagger}(R; R'')\,\kappa\rho(\vec{r})\,dR = \sum_{i} \vec{W}_i \tag{35}$$

where $\vec{W}_i$ is the weight vector at the ith collision and the summation is over all collisions that occur in dR about R. The weight vector, $\vec{W}_i$, is obtained from the initial weight vector given by Eq. (31) and the product of the changes in this weight vector at each collision as given by Eq. (29). Then from Eqs. (30) and (35), the contribution to the functional four-vector at each collision point, R, is given by

$$[1/\kappa\rho(\vec{r})]\,\mathbf{B}(\vec{r}, -\vec{\imath})\;\vec{W}, \tag{36}$$

where $\vec{W}$ is the vector weight at the collision point and $\mathbf{B}$ is defined by Eq. (22). The matrix $\mathbf{B}$ is a diagonal matrix whose diagonal components are the components of the photon source vector, $\vec{S}$. The source $\vec{S}$ could be an extraneous source or, alternatively, it is sometimes convenient to define [5] $\vec{S}$ as the source due to photons emerging from their first collision after being emitted by the extraneous source. In this latter case, the functional $\vec{F}$ will not include any contribution from these photons that are emitted by the extraneous source and that subsequently reach the receiver before suffering a collision. If this first flight contribution is also to be included, it must be added to the Monte Carlo results [4]. This first flight contribution may often be computed numerically, but it can also be computed with the Monte Carlo method if necessary.

6. Numerical Results

To numerically compare the adjoint and direct Monte Carlo methods we consider the plane-parallel, Rayleigh-scattering, conservative, emitting atmosphere with uniform distribution of sources. This problem is solved exactly in Horak [14] and his analytic solution has been numerically evaluated by Sandford and Pauls [4]. We compare adjoint and direct method results from our test program with analytic evaluations provided us by Pauls.

The test problem follows from Eq. (1) when

$$\vec{\imath} \cdot \vec{\nabla} = \mu(d/d\imath), \qquad \kappa\rho \, d\imath = d\tau, \qquad d\omega = d\mu' \, d\rho',$$

and

$$\vec{S} = \kappa\rho\epsilon_0 \vec{I}_0 ,$$

where μ is the emergent angle cosine, τ is the optical depth, ϵ_0 is the source constant, and $\vec{I}_0$ is the unpolarized unit intensity vector. Equation (1) becomes

$$\mu \frac{d\vec{I}}{d\tau} = \vec{I} - \frac{1}{4\pi} \oint \mathbf{P}(\omega) \, \vec{I}(\tau, \omega) \, d\omega - \epsilon_0 \vec{I}_0 . \tag{37}$$

The formal solution of (37) with zero incident intensity at $\tau = \tau_1$ is:

$$\vec{I}(0, \mu) = \int_0^{\tau_1} e^{-(\tau/\mu)} \frac{d\tau}{\mu} \oint \mathbf{P}(\omega) \, \vec{I}(\tau, \omega) \frac{d\omega}{4\pi} - \epsilon_0 \vec{I}_0 \int_0^{\tau_1} e^{-(\tau/\mu)} \frac{d\tau}{\mu} . \tag{38}$$

which may be written as

$$I(0, \mu) = I(0, \mu)_{\text{diffuse}} + I(0, \mu)_{\text{direct}} , \tag{39}$$

to define a diffuse intensity component containing only scattered photons. The diffuse component consists of the summation of intensities $I_n(0, \mu)$ from each scattering order:

$$\vec{I}(0, \mu)_{\text{diffuse}} = \sum_{n=1}^{\infty} \vec{I}_n(0, \mu). \tag{40}$$

Referring to Fig. 1, we write the analytic expression for the first-order ($n = 1$) intensity:

$$\vec{I}_1(0, \mu) = \int_0^{\tau_1} e^{-(\tau/\mu)} \frac{d\tau}{\mu} \oint \mathbf{P}(\omega) \frac{d\omega}{4\pi} \int_0^{\tau} e^{-(\tau - t)/\mu'} \epsilon_0 \vec{I}_0 \, dt. \tag{41}$$

where $\mu' = \cos(\pi - \theta)$. Repeated random sampling of (41) to obtain successive scattering orders effects a Monte Carlo solution for the diffuse intensity.

The direct Monte Carlo integration of (41) consists of sampling the integration variable τ and t from exponential distributions, and initializing a source particle at optical depth t with the flight direction cosine μ' sampled from the isotropic distri-

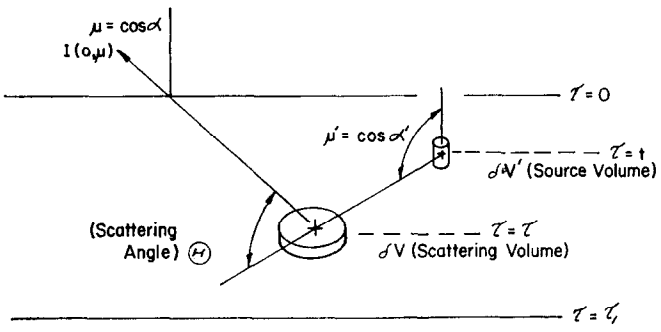

FIG. 1. Plane parallel single scattering geometry.

bution. The initial particle vector is $\epsilon_0 \vec{I}_0$ times bias factors that may be needed for the sampling scheme used. Estimates of the single-scattered intensity are made for each emergent cosine μ by multiplying the particle vector weight by the phase matrix for the angle $\omega(\tau, t, \mu, \mu')$ and a scalar scoring factor:

$$(1/\mu)\, e^{-(\tau/\mu)} \mathbf{P}(\omega)\, \vec{W}_n\,. \tag{42}$$

Subsequent scattering orders are estimated by sampling a value for θ (Fig. 1) and a new τ value for the depth of the next collision. These are sampled from the phase matrix and exponential density functions as required by (38). The particle is propagated to the next collision by application of rotation matrices to the vector weight, and estimates of the intensity scattered to the emergent cosines (μ-values) are again made. This process is repeated for N collisions of M independent particles, and the emergent intensity estimate is:

$$\vec{I}(0, \mu)_{\text{diffuse}} \cong \frac{1}{M} \sum_{m=1}^{M} \sum_{n=1}^{N} \vec{I}_n{}^m(0, \mu). \tag{43}$$

As discussed in Section 5, the adjoint method randomly samples the reciprocal intensity. Thus, the statistical particle originates at the detector with unit vector weight $\vec{I}_0$ and enters the atmosphere with direction cosine $-\mu$. The collision depth τ (Eq. (41) is sampled from the exponential distribution and the direction cosine μ' to the source point is sampled isotropically. The source is scored at each collision by sampling t from density dt and evaluating the scalar $\epsilon_0 e^{-(\tau - t)/\mu'}$. The scattered intensity in the emergent direction cosine μ is estimated with

$$\epsilon_0 e^{-((\tau - t)/\mu')}\, \mathbf{P}(\omega)\, \vec{W}_n\,, \tag{44}$$

where $\vec{W}_n$ is the particle weight vector at the nth collision. The particle is propagated to the next collision by sampling θ and τ from the phase and exponential density functions and by performing the proper rotations. The estimate for the intensity scattered to emergent cosine μ from the new collision is made by again scoring the source and evaluating the estimator (44). All scattering orders estimated for a single

statistical particle contribute to the same emergent cosine μ. By computing N collisions of M particles the estimate (43) is obtained.

The direct method uses the source distribution to initialize the statistical particle weights. These move randomly through the atmosphere and provide estimates of intensity scattered to all the desired emergent angles at each collision. The adjoint method uses the emergent angle distribution to initialize source particles of unit weight. These also move randomly through the atmosphere and at each collision one scores the source to provide estimates of the intensity scattered to their initial entrance direction.

Figure 2 shows solutions obtained by direct and adjoint Monte Carlo for an atmosphere of thickness $\tau_1 = 0.2$. Both methods agree well with the exact solution for this thin case, using 25,000 particles and 7 scattering orders. Figure 3 shows solutions for a thickness $\tau_1 = 2.0$, using 125,000 particles and 7 scattering orders.

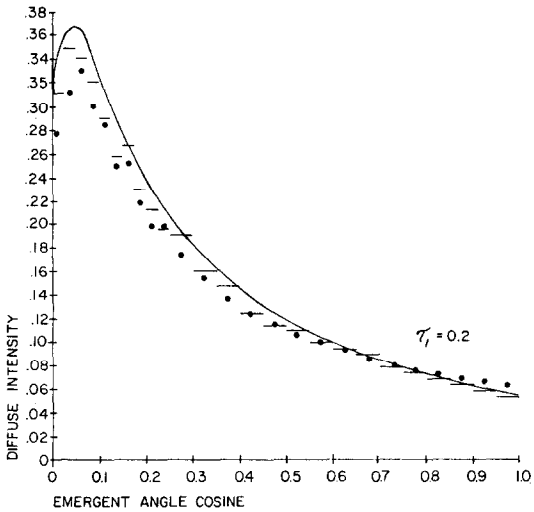

FIG. 2. Adjoint (bars) and direct (open circles) Monte Carlo solutions of diffuse intensity for $\tau_1 = 0.2$. The solid curve is the exact result.

The direct method is noticeably deficient at small μ because, when viewed at this angle, the atmosphere appears optically much thicker. The adjoint method compensates this by injecting particles at small angles and thereby obtaining better sampling of the small contributions from collisions at large distances. The direct estimator (42) is dominated by $1/\mu$ at small μ. The adjoint method is distinctly advantageous for computing the limb darkening of astrophysical bodies, where smaller values are needed.

Figure 4 shows the case $\tau_1 = 1.0$, calculated with 25,000 particles and 7 collisions. The first and second scattering orders computed with the adjoint and direct methods are also shown. The error of the direct method is largely due to poor first collision

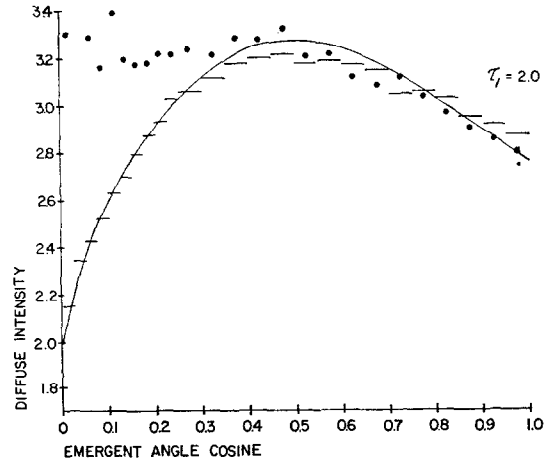

FIG. 3. Adjoint (bars) and direct (open circles) Monte Carlo solutions of diffuse intensity for $\tau_1 = 2.0$.

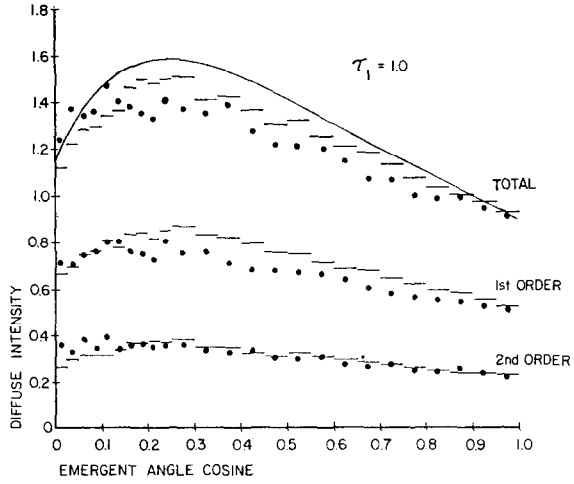

FIG. 4. Adjoint (bars) and direct (open circles) Monte Carlo solutions of diffuse intensity for $\tau_1 = 1.0$. First and second scattering orders are also shown.

estimates, but for $0 \leqslant \mu = = 0.1$ the second-order intensity is also important to the total. The error of the adjoint method is distributed evenly through all scattering orders and a better adjoint result can be obtained by using more particles. It appears difficult to obtain good agreement by the direct method, even with more particles. The adjoint result shown is sufficiently smooth to allow determination of the μ-value at the intensity maximum, but the direct solution gives a curve with no well-defined peak value. While the variance in the direct method can perhaps be improved, the adjoint method appears attractive for optically thick problems ($\tau_1 \geqslant 1.0$).

APPENDIX: Boson Scattering from Spherical Centers

I. *Introduction*

At a scattering event we employ the geometry shown in Fig. 5, where $\vec{I}'$ is the Stokes' four-vector characterizing the plane electromagnetic wave incident on the scattering center with wavevector $\vec{K}'$; and $\vec{I}$ is the Stokes' vector characterizing the plane wave scattered with wavevector $\vec{K}$.

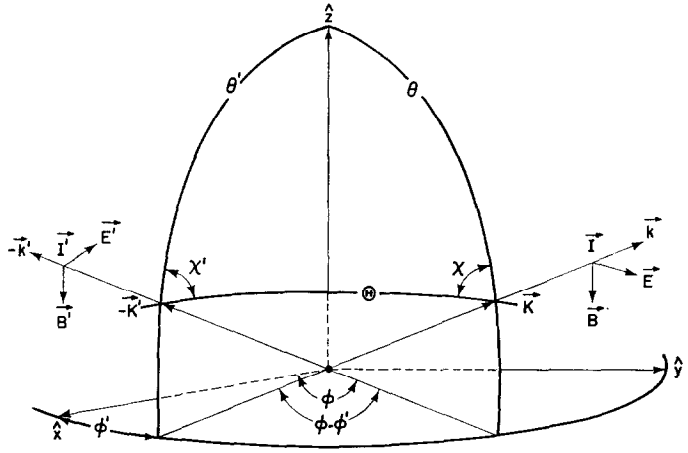

FIG. 5. Coordinates for single scattering by a particle at the origin.

The Stokes' vector, $\vec{I}'$, is assumed to characterize the incident wave with reference to the incident meridian plane whose unit normal vector is

$$\vec{N}' = (\vec{K}' \times \hat{z})/\sin\theta', \tag{A-1}$$

where the unit propagation vector (Fig. 5) is

$$\vec{K}' = -\cos\phi' \sin\theta' \hat{x} - \sin\phi' \sin\theta' \hat{y} - \cos\theta' \hat{z}. \tag{A-2}$$

The scattered Stokes' vector, $\vec{I}$, is referenced to the meridian plane whose unit normal vector is

$$\vec{N} = (\vec{K} \times \hat{z})/\sin\theta, \tag{A-3}$$

where the unit propagation vector (Fig. 5) is

$$\vec{K} = \cos\phi \sin\theta \hat{x} + \sin\phi \sin\theta \hat{y} + \cos\theta \hat{z}. \tag{A-4}$$

The physics involved in the interaction of the incident wave and the matter is usually described with reference to the scattering plane whose unit normal vector is

$$\vec{N}_s = (\vec{K}' \times \vec{K})/\sin(\Theta), \tag{A-5}$$

where Θ is the scattering angle defined by

$$\tan(\Theta) = |\vec{K}' \times \vec{K}|/(\vec{K}' \cdot \vec{K}). \tag{A-6}$$

II. *Rotation Matrices*

To change the reference plane of a Stokes' four-vector, one operates on the vector with a 16-element matrix [8]. Thus, the incident Stokes' vector referenced to the scattering plane is

$$\vec{I}'' = \mathbf{L}(\chi') \cdot \vec{I}', \tag{A-7}$$

where χ' is the angle between the old and new reference planes (Fig. 5) defined by

$$\tan(\chi') = |\vec{N}' \times \vec{N}_s|/(\vec{N}' \cdot \vec{N}_s), \tag{A-8}$$

and the rotation matrix [8] is:

$$\mathbf{L}(\chi') = \begin{bmatrix} \cos^2\chi' & \sin^2\chi' & \frac{1}{2}\sin 2\chi' & 0 \\ \sin^2\chi' & \cos^2\chi' & -\frac{1}{2}\sin 2\chi' & 0 \\ -\sin 2\chi' & \sin 2\chi' & \cos 2\chi' & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{A-9}$$

if the components of $\vec{I}'$ are: I_ℓ', the intensity parallel to the reference plane; I_s', the intensity perpendicular to the reference plane:

$$U' = (I_\ell' - I_s') \tan 2\alpha',$$

and

$$V' = (I_\ell' - I_s') \tan 2\beta' \sec 2\alpha',$$

where α' is the angle of polarization and β' is the eccentric angle. We therefore obtain for Eq. (A-7):

$$\vec{I}'' = \begin{bmatrix} (I_\ell' \cos^2\chi' + I_s' \sin^2\chi' + (U'/2)\sin 2\chi') \\ (I_\ell' \sin^2\chi' + I_s' \cos^2\chi' - (U'/2)\sin 2\chi') \\ (-I_\ell' \sin 2\chi' + I_s' \sin 2\chi' + U' \cos 2\chi') \\ V' \end{bmatrix}. \tag{A-10}$$

III. *Scattering Interaction*

For a scattering center possessing spherical symmetry, the interaction is described [12] by a scattering matrix of the form

$$\mathbf{S}(\Theta) = \begin{bmatrix} \sigma_1(\Theta) & 0 & 0 & 0 \\ 0 & \sigma_2(\Theta) & 0 & 0 \\ 0 & 0 & \sigma_3(\Theta) & -\sigma_4(\Theta) \\ 0 & 0 & \sigma_4(\Theta) & \sigma_3(\Theta) \end{bmatrix}, \tag{A-11}$$

which is normalized by the relation

$$\tfrac{1}{2}\int_0^{\pi} \sin(\Theta)[\sigma_1(\Theta) + \sigma_2(\Theta)]\, d\Theta = 1.0. \tag{A-12}$$

The scattered Stokes' vector referenced to the scattering plane is given by

$$\vec{I}''' = \mathbf{S}(\Theta) \cdot \vec{I}'', \tag{A-13}$$

which expands as:

$$\vec{I}''' = \begin{bmatrix} (I_\ell'\sigma_1 \cos^2\chi' + I_t'\sigma_1 \sin^2\chi' + (U'\sigma_1/2)\sin 2\chi') \\ (I_\ell'\sigma_2 \sin^2\chi' + I_t'\sigma_2 \cos^2\chi' - (U'\sigma_2/2)\sin 2\chi') \\ (-I_\ell'\sigma_3 \sin 2\chi' + I_t'\sigma_3 \sin 2\chi' + U'\sigma_3 \cos 2\chi' + V'\sigma_4) \\ (I_\ell'\sigma_4 \sin 2\chi' - I_t'\sigma_4 \sin 2\chi' - U'\sigma_4 \cos 2\chi' + V'\sigma_3) \end{bmatrix}. \tag{A-14}$$

This Stokes' vector must be rotated through the angle χ to reference it to the scattering meridian (Fig. 5). The rotation angle is defined by

$$\tan\chi = |\vec{N}_s \times \vec{N}|/(\vec{N}_s \cdot \vec{N}). \tag{A-15}$$

We therefore obtain

$$\vec{I} = \mathbf{L}(\chi) \cdot \vec{I}''', \tag{A-16}$$

the expansion of which is shown in Fig. 6. The scattered Stokes' vector may be written as

$$\vec{I} = \mathbf{P}(\chi', \Theta, \chi) \cdot \vec{I}', \tag{A-17}$$

where

$$\mathbf{P} = \mathbf{L}(\chi) \cdot \mathbf{S}(\Theta) \cdot \mathbf{L}(\chi'), \tag{A-18}$$

is the phase matrix appearing in the equation of radiative transfer [Eq. (1)]. The variables (χ, Θ, χ') are clearly related to $\mu' = \cos\theta'$, $\mu = \cos\theta$, ϕ, and ϕ' by Eqs. (A-6), (A-7), and (A-15); so that

$$\mathbf{P} = \mathbf{P}(\mu, \phi; \mu', \phi') = \mathbf{P}(\vec{i}, \vec{i}').$$

IV. *Random Sampling*

The direct density function for sampling (μ, ϕ) is:

$$d = \frac{\tilde{\vec{X}} \cdot \mathbf{P}(\mu, \phi; \mu', \phi') \cdot \vec{W}(\vec{r}; \mu', \phi')}{4\pi \tilde{\vec{X}} \cdot \vec{W}(\vec{r}; \mu', \phi')}, \tag{A-19}$$

where $\vec{W}$, the weight vector entering the collision, is identified with the incident Stokes' intensities:

$$\vec{W} \equiv \vec{I}',$$

and

$$\vec{X} = (1\ 1\ 0\ 0).$$

$$
\begin{aligned}
I_\ell = \{ & I'_\ell \left(\sigma_1 \cos^2\chi' \cos^2\chi + \sigma_2 \sin^2\chi' \sin^2\chi - \frac{\sigma_3}{2} \sin 2\chi' \sin 2\chi\right) \\
& + I'_r \left(\sigma_1 \sin^2\chi' \cos^2\chi + \sigma_2 \cos^2\chi' \sin^2\chi + \frac{\sigma_3}{2} \sin 2\chi' \sin 2\chi\right) \\
& - \frac{U'}{2} \left(\sigma_1 \sin 2\chi' \cos^2\chi - \sigma_2 \sin 2\chi' \sin^2\chi + \sigma_3 \cos 2\chi' \sin 2\chi\right)\}
\end{aligned}
$$

$$
\begin{aligned}
I_r = \{ & I'_\ell \left(\sigma_1 \cos^2\chi' \sin^2\chi + \sigma_2 \sin^2\chi' \cos^2\chi + \frac{\sigma_3}{2} \sin 2\chi' \sin 2\chi\right) \\
& + I'_r \left(\sigma_1 \sin^2\chi' \sin^2\chi + \sigma_2 \cos^2\chi' \cos^2\chi - \frac{\sigma_3}{2} \sin 2\chi' \sin 2\chi\right) \\
& - \frac{U'}{2} \left(\sigma_1 \sin 2\chi' \sin^2\chi' - \sigma_2 \sin 2\chi' \cos^2\chi - \sigma_3 \cos 2\chi' \sin 2\chi\right)\}
\end{aligned}
$$

$$
\begin{aligned}
U = \{ & I'_\ell \left(\sigma_1 \cos^2\chi' \sin 2\chi - \sigma_2 \sin^2\chi' \sin 2\chi + \sigma_3 \sin 2\chi' \cos 2\chi\right) \\
& + I'_r \left(\sigma_1 \sin^2\chi' \sin 2\chi - \sigma_2 \cos^2\chi' \sin 2\chi - \sigma_3 \sin 2\chi' \cos 2\chi\right) \\
& - \frac{U'}{2} \left[(\sigma_1 + \sigma_2) \sin 2\chi' \sin 2\chi - \sigma_3 \cos 2\chi' \cos 2\chi\right]\}
\end{aligned}
$$

$$
V = \{I'_r \sigma_4 \sin 2\chi' - I'_\ell \sigma_4 \sin 2\chi' - U' \sigma_4 \cos 2\chi' + V' \sigma_3\}
$$

FIG. 6. Stokes' parameters for light scattered by the geometry shown in Fig. 1.

Expanding Eq. (A-19) using Eq. (A-17) and the relations in Fig. 6, we obtain:

$$
\begin{aligned}
d = \left(\frac{1}{4\pi(I_\ell' + I_r')}\right) \cdot \Big\{ & I_\ell'(\sigma_1 \cos^2\chi' + \sigma_2 \sin^2\chi') \\
& + I_r'(\sigma_1 \sin^2\chi' + \sigma_2 \cos^2\chi') + \frac{U'}{2} \sin 2\chi'(\sigma_1 - \sigma_2)\Big\}.
\end{aligned} \tag{A-20}
$$

This equation shows that one may sample the angles (χ', Θ) as equivalent to sampling (μ, ϕ).

The density function for adjoint sampling is [Eq. (27)]:

$$
f = \frac{\vec{X} \cdot \tilde{\mathbf{P}}(-\vec{\imath}'; -\vec{\imath}) \cdot \vec{W}(\vec{r}; \vec{\imath}')}{4\pi \vec{X} \cdot \vec{W}(\vec{r}; \vec{\imath}')}.
$$

We write the adjoint phase matrix with the aid of Eq. (A-18):

$$
\tilde{\mathbf{P}} = \tilde{\mathbf{L}}(\chi') \cdot \tilde{\mathbf{S}}(\Theta) \cdot \tilde{\mathbf{L}}(\chi). \tag{A-21}
$$

Inspection of Eq. (A-11) reveals:

$$
\tilde{\mathbf{S}}(\Theta) = \tilde{\mathbf{S}}[-\sigma_4(\Theta)]. \tag{A-22}
$$

Thus we obtain

$$\tilde{\mathbf{P}}(\vec{i}, \vec{i}) = \tilde{\mathbf{L}}(\chi') \cdot \mathbf{S}(-\sigma_4) \cdot \tilde{\mathbf{L}}(\chi). \tag{A-23}$$

Inspection of Fig. 5 or analysis with Eqs. (A-6), (A-7), and (A-15) shows that the angles χ', Θ, and χ are invariant under the reciprocity introduced by $\vec{i} \to -\vec{i}$ and $\vec{i}' \to -\vec{i}'$. Thence, we obtain for the adjoint density function:

$$f = \left(\frac{1}{4\pi(I_\ell' + I_r')}\right)\{I_\ell'(\sigma_1 \cos^2 \chi + \sigma_2 \sin^2 \chi) + I_r'(\sigma_1 \sin^2 \chi + \sigma_2 \cos^2 \chi) - U \sin 2\chi(\sigma_1 - \sigma_2)\}, \tag{A-24}$$

which shows that one may sample the angles (χ, Θ) as equivalent to sampling (μ, ϕ). The adjoint and direct density functions are seen to have similar functional form when they are expressed in terms of rotation and scattering angles. The transformations to (μ, ϕ) of the random variables (χ, Θ) or (χ', Θ) produce different distributions than those given by Eqs. (A-20) and (A-24). The sign reversal of $\sigma_4(\Theta)$ in the adjoint scattering matrix [Eq. (A-22)] indicates that the scattered adjoint weight vector [Eq. (29)] has the opposite helicity of a direct beam. These properties of the adjoint density function are due to the invariance of Maxwell's equations under time reversal. We emphasize that they hold only in the special case of coherent scattering from spherical particles.

V. *Rejection Sampling*

We may sample the density functions d or f by defining the marginal density functions $h_{f,d}(\Theta)$; and $q_{f,d}(\chi, \Theta)$, the corresponding conditional density functions for χ. The following definitions result [13]:

$$h_f(\Theta) = \int_0^{2\pi} f(\chi, \Theta)\, d\chi; \qquad h_d(\Theta) = \int_0^{2\pi} d(\chi', \Theta)\, d\chi'; \tag{A-25}$$

and

$$q_f(\chi, \Theta) = f(\chi, \Theta)/h_f(\Theta); \qquad q_d(\chi, \Theta) = d(\chi, \Theta)/h_d(\Theta). \tag{A-26}$$

Integrating Eq. (A-25) yields the same result for both marginal density functions:

$$h_{f,d}(\Theta) = \tfrac{1}{4}[\sigma_1(\Theta) + \sigma_2(\Theta)],$$

and

$$q_{f,d}(\chi, \Theta) = \left[\frac{1}{2\pi(I_\ell' + I_r')}\right] \times \left\{\frac{2}{(\sigma_1 + \sigma_2)}\left[I_\ell'(\sigma_1 \cos^2 \chi + \sigma_2 \sin^2 \chi) + I_r'(\sigma_1 \sin^2 \chi + \sigma_2 \cos^2 \chi) + \left(\frac{3s}{2} - 1\right) U' \times (\sigma_1 - \sigma_2) \sin 2\chi\right]\right\}, \tag{A-27}$$

where $s = 0$ for q_f and $s = 1$ for q_d. In the case of unpolarized incident light ($I_\ell' = I_r' = 1$; $U' = 0$) we obtain

$$q_{f,d}(\chi, \Theta) = 1/2\pi \qquad \text{(unpolarized light)},$$

which indicates χ is uniform on $(0, 2\pi)$. The conditional density functions may be sampled with the rejection scheme given in Fig. 7.

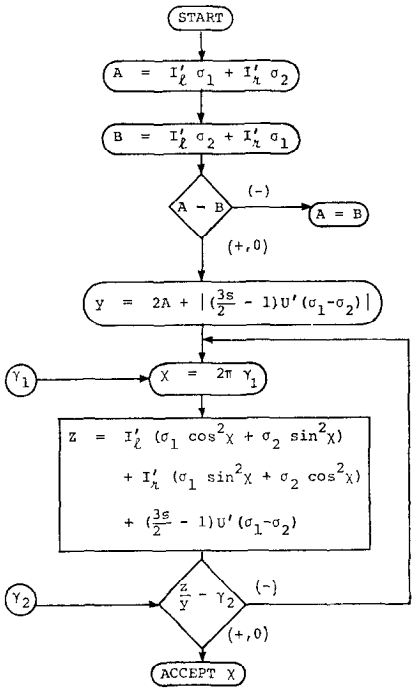

FIG. 7. Rejection scheme for sampling the conditional density functions given by Eq. (A-27).

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