JOURNAL OF COMPUTATIONAL PHYSICS 39, 22–45 (1981)

Application of Splitting-Up Method to the Numerical Treatment of Transport Equation. Analysis of the Transmission of Electrons through Thin Self-Supporting Metallic Targets

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Received July 23, 1979

This paper deals with the resolution of the transport equation describing the comportment of electrons during their transmission through metallic targets. The "splitting-up" resolution method is used for numerical treatment in the two cases presented here: partial differential equation and integro-differential equation corresponding to two different physical hypothesis for particles scattering. Discussion is included on the influence of mathematical parameters, and the difficulties connected to physical parameters are solved.

I. INTRODUCTION

Transmission and backscattering of electrons from metallic targets, as well as electron backscattering from bulk targets, have been widely studied, using models based upon Boltzmann's transport equation or upon statistical Monte Carlo methods.

However, direct solutions of these equations have up to now been obtained only for particular cases, related to small angle elastic diffusion [1–3] in the hypothesis of continuous slowing down.

Strickland and Bernstein [4] treat the Fokker–Planck equation and transfer equation numerically, neglecting energy effects, but taking into account the large angle scattering effects by means of a Rutherford scattering cross section.

Thus, they can only obtain angular and spatial distribution due to elastic scattering; moreover, they never examine the case of a monodirectional electron beam.

We use the same approach in regard to the elastic scattering term, but we take into account variations of the cross section with energy; the incident electron beam is monoenergetic and monodirectional, and the inelastic scattering is taken into account in the continuous slowing down approximation, i.e., there exists a unique relationship between energy loss and path length of the particle.

Boltzmann's transport equation may be formulated, either as a partial differential equation or an integro-differential equation. We propose in this paper a numerical

0021-9991/81/010022-24$02.00/0

method which allows us to solve such equations in a less limited manner than the earlier ones. This is a "splitting-up" method [5, 6], based upon finite differences, and it is presented in detail for the case of the small angle scattering equation. It is then generalized using an integro-differential equation, for which elastic scattering occurs for all possible angles.

Some results have been obtained for aluminum and compared with those of Rostaing [7].

II. Governing Equations

A. *Generalities*

When an electron beam strikes a metallic target and penetrates inside the material, it suffers elastic and inelastic scattering; when the number of collisions is sufficiently great, the phenomenon may be described by a transport equation [8].

The equations presented here have been written from the hypothesis of continuous slowing down; this is equivalent to supposing either that inelastic effects result only in an energy loss per unit length of path or that a unique range–energy relations exists.

In these conditions, the energy dispersion of electrons is due only to differences in path lengths, and angular deviations are due only to elastic collisions.

Thus, we can write

$$\frac{\partial f(s,u,x)}{\partial s} = -u\frac{\partial f(s,u,x)}{\partial x} + \frac{1}{|\mathbf{v}|}K_e(s,u,x)$$

where the path element $ds = |\mathbf{v}|\,dt$ and $u = \cos\theta$ is the angle of the particle velocity direction after a collision, with the inward normal. x is the depth measured normally from the surface and $K_e(s,u,x)$ relates all the elastic processes which induce variations of the particle density per unit of time.

If we denote by $\sigma_e(\Theta, s)$ the differential cross section for elastic scattering under an angle Θ (with $0 \leqslant \Theta \leqslant \pi$), and by $\sigma_{eT}(s)$ the total cross section, the equation may be written using the notations and indications of Fig. 1.

$$\frac{\partial f(s,u,x)}{\partial s} = -u\frac{\partial f(s,u,x)}{\partial x} + \frac{1}{\lambda_e(s)}\int_{-1}^{1}(f(s,u',x) - f(s,u,x))\,R(u,u')\,du'$$

with

$$\sigma_{eT}(s) = 2\pi\int_0^{\pi}\sigma_e(\Theta,s)\sin\Theta\,d\Theta,$$

$$R(u,u') = 2\int_0^{\pi}\frac{\sigma_e(\Theta,s)}{\sigma_{eT}(s)}\cdot d\phi \qquad \text{and} \qquad \int_{-1}^{1}R(u,u')\,du' = 1,$$

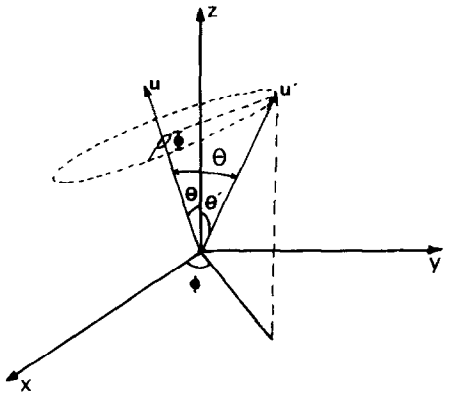

FIG. 1. Geometrical arrangement.

where $\lambda_e(s) = 1/n\sigma_{eT}(s)$ is the mean free path for elastic collisions and n is the number of scattering centers per volume unit.

Under these conditions, the equation may be written

$$\frac{\partial f(s,u,x)}{\partial s} = -u\frac{\partial f(s,u,x)}{\partial x} - \frac{f(s,u,x)}{\lambda_e(s)} + \frac{1}{\lambda_e(s)}\int_{-1}^{1} f(s,u',x)\cdot R(u,u')\,du'. \tag{1}$$

A simplified formulation of this equation, related to the case where the large angle scattering is neglected, has been widely used.

It is obtained from a Taylor's expansion of the integral term when u is near u' [3, 8]; this yields

$$\frac{\partial f(s,u,x)}{\partial s} = -u\frac{\partial f(s,u,x)}{\partial x} + \frac{1}{\Lambda(s)}\frac{\partial}{\partial u}\left((1-u^2)\frac{\partial f(s,u,x)}{\partial u}\right), \tag{2}$$

where $\Lambda(s)$ is the "transport mean free path" or "momentum transfert mean free path" defined by the expression proposed by Bethe, Rose, and Smith [8]

$$\frac{1}{\Lambda(s)} = \pi\cdot n\cdot\int_0^{\pi}\sin\Theta\,\sigma_e(\Theta,s)(1-\cos\Theta)\,d\Theta.$$

The results given by Eq. (2) could be obtained as particular case of the integro-differential equation [1] by introducing a maximum scattering angle Θ_c, in such a manner that for $\Theta \geqslant \Theta_c$, $\sigma_e(\Theta,s) = 0$.

Thus we have

$$\frac{\partial f(s,u,x)}{\partial s} = -u\frac{\partial f(s,u,x)}{\partial x} - \frac{f(s,u,x)}{\lambda'_e(s)} + \frac{1}{\lambda'_e(s)}\int_{-1}^{1} f(s,u',x)\cdot R(\Theta_c,u,u')\,du' \tag{3}$$

with

$$\frac{1}{\lambda'_e(s)} = n\sigma'_{eT}(s) = n\cdot 2\pi\int_0^{\Theta_c}\sigma_e(\Theta,s)\sin\Theta\,d\Theta,$$

$$R(\Theta_c,u,u') = 2\int_0^{\phi_{\text{Max}}}\left(\frac{\sigma_e(\Theta,s)}{\sigma'_{eT}(s)}\right)d\phi,$$

where ϕ_{Max} is a function of Θ_c, u, u'.

The analytical expressions of $R(u,u')$, $R(\Theta_c,u,u')$, and ϕ_{Max} are given in the appendix.

B. *Initial and Boundary Conditions of the Physical Problems*

Whichever equation is considered, we have the initial conditions

(a) $f(0,1,0) = 1/2\pi$,

(b) $f(0,u,0) = 0$ for $-1 \leqslant u < 1$,

(c) $f(0,u,x) = 0$ for $\forall x \neq 0$ and $-1 \leqslant u \leqslant 1$

and the boundary conditions

(d) $f(s,u,0) = 0$, $\forall u \geqslant 0$ and $\forall s > 0$,

(e) $f(s,u,R) = 0$, $\forall u$, $\forall s$,

where R is the range of the electrons in the metal under study for the energy in question. Condition (e) can be replaced for target of finite thickness X, by condition (f).

(f) $f(s,u,X) = 0$ for $\forall s$ and $u \leqslant 0$.

The geometry of the problem is given in the semi-infinite case and for a target of finite thickness in Figs. 2 and 3, respectively, where we have hatched the region where initial or boundary conditions are given.

C. *Elastic Scattering Cross Sections*

We use a Rutherford differential cross section with a screening parameter ξ which allows us to avoid divergence for diffusion angles equal to 0; in this way, the predominant character of the forward diffusions is maintained.

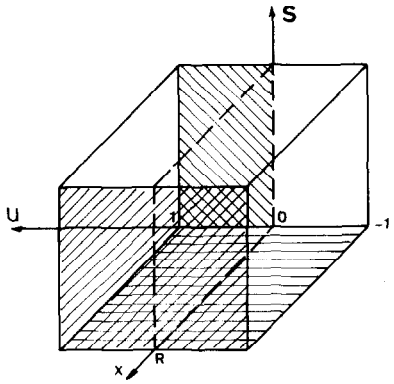

FIG. 2. Representation of initial and boundary conditions in the case of a semi-infinite target.

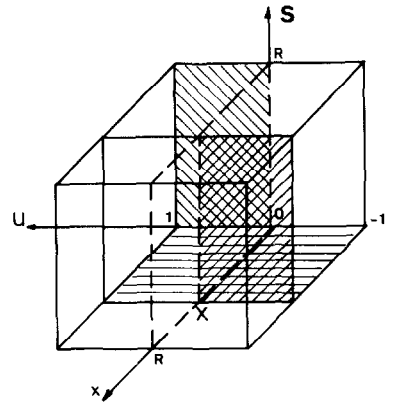

FIG. 3. Representation of initial and boundary conditions for a target of thickness X.

This form of differential cross section can be written

$$\sigma_e(E, \Theta) = \frac{Z^2 e^4}{4E^2 \Theta} \frac{1}{(1 - \cos \Theta + 2\xi)^2}$$

and the elastic mean free path is given by

$$\lambda_e(E) = \frac{4E^2}{n\pi Z^2 e^4} \xi(1 + \xi);$$

the values of ξ as a function of the energy are obtained by adjustment to the values of $\lambda_e(E)$ found in the literature.

II. Resolution Method

A. *Principle*

The principle of the "splitting-up" method used here could be briefly expressed in the following.

We have an equation of the form

$$\frac{\partial f(s, u, x)}{\partial s} = (A + B)f \tag{3a}$$

with, for the case of Eq. (2),

$$A = -u\frac{\partial}{\partial x} \qquad \text{and} \qquad B = \frac{1}{A(s)}\frac{\partial}{\partial u}\left((1-u^2)\frac{\partial}{\partial u}\right).$$

We discretize the s variable, writing $s = l \cdot \Delta s$, $l = 0, 1, \ldots$, and we use the simplified notation

$$f(l\,\Delta s, u, x) \equiv f^l(u, x) \equiv f^l.$$

The solution is computed successively for each value of $s = l\,\Delta s$, starting from initial condition given for $s = 0$, i.e., $l = 0$.

Equation (3a) could be written, after discretization of the derivative versus "s," and with the choice of an implicit scheme insuring the stability of computation:

$$\frac{f^{l+1} - f^l}{\Delta s} \simeq (A + B)f^{l+1}. \tag{3b}$$

The approximations made during the transcription from (3a) to (3b) concern the discretized form of the derivative and the discretized expression of the right-hand member of (3b) connected with the choice of an implicit computing scheme.

We can write (3b) in the form

$$f^l \simeq (I - (A + B)\,\Delta s)f^{l+1}. \tag{3c}$$

To overcome computing difficulties due to the form of the operator $(A + B)$, we take an approximate equation where the operators A and B appear separately; we have

$$\begin{aligned} I - (A + B)\,\Delta s &= (I - A \cdot \Delta s)(I - B \cdot \Delta s) - \Delta s^2 \cdot A \cdot B \\ &\simeq (I - A \cdot \Delta s)(I - B \cdot \Delta s) \end{aligned}$$

and we can write Eq. (3c) as

$$f^l \simeq (I - A \cdot \Delta s)(I - B \cdot \Delta s)f^{l+1}. \tag{3c'}$$

At each step in s, we can split problem (3b) into two parts:

(1) We solve an equation of the type

$$g^l \simeq (I - A \cdot \Delta s)\, g^{l+1} \tag{3d}$$

with

$$g^l \equiv f^l.$$

In this first step, the f^l are initial conditions or previously computed values of the solution, and the g^{l+1} are unknown. Equation (3d) could be written

$$\frac{g^{l+1} - g^l}{\Delta s} \simeq A \cdot g^{l+1}. \tag{3d'}$$

This equation is a discretized form of

$$\frac{\partial g(s, u, x)}{\partial s} = A \cdot g(s, u, x). \tag{3d''}$$

(2) In the second part of the resolution process we solve the equation

$$(I - B \cdot \Delta s)\, h^{l+1} \simeq h^l \tag{3e}$$

with

$$h^{l+1} \equiv f^{l+1} \qquad \text{and} \qquad h^l \equiv g^{l+1}.$$

In this second step the values of h^l are the values of g^{l+1} computed in the first step, the solution h^{l+1} of Eq. (3e) is the final solution f^{l+1} of Eq. (3c'), i.e., the solution of (3a) for $s = (l+1)\,\Delta s$.

We can write

$$\frac{h^{l+1} - h^l}{\Delta s} \simeq B \cdot h^{l+1} \tag{3e'}$$

which is a discretized form of

$$\frac{\partial h(s, u, x)}{\partial s} = Bh(s, u, x). \tag{3e''}$$

We can represent the process allowing the transition from $s = l\,\Delta s$ to $s = (l+1)\,\Delta s$, as follows

$$f^l \equiv g^l \xrightarrow{\text{1st step}} g^{l+1} \equiv h^l \xrightarrow{\text{2nd step}} h^{l+1} \equiv f^{l+1}.$$

Thus, at each step in s, we solve successively

$$\frac{\partial g(s,u,x)}{\partial s} = Ag(s,u,x) \qquad \text{then} \qquad \frac{\partial h(s,u,x)}{\partial s} = Bh(s,u,x)$$

in an approximate discretized form.

In this way, we can split a problem where operators A and B appear simultaneously in two simpler problems in which these two operators appear successively.

In the case of the equation treated here, the particularly simple form of the operator A allows us to obtain the exact solution of Eq. (3d″), in such a manner that it is possible in this case to use an explicit scheme which gives the same result. In the second step (Eq. (3e′) or (3e″)) we maintain an implicit computing scheme to ensure stability of the process.

The discretization gives

$$(1) \quad (g^{l+1} - g^l)/\Delta s \simeq A \cdot g^l$$

or

$$(I + A \cdot \Delta s)\, g^l \simeq g^{l+1} \qquad \text{with} \quad g^l \equiv f^l,$$

$$(2) \quad (h^{l+1} - h^l)/\Delta s \simeq B \cdot h^{l+1}$$

or

$$(I - B \cdot \Delta s)\, h^{l+1} \simeq h^l \qquad \text{with} \quad h^l \equiv g^{l+1} \text{ and } h^{l+1} \equiv f^{l+1}$$

which could be written

$$(I - B \cdot \Delta s) f^{l+1} \simeq (I + A \cdot \Delta s) f^l.$$

This gives

$$\frac{f^{l+1} - f^l}{\Delta s} \simeq A \cdot f^l + B \cdot f^{l+1}$$

$$\simeq (A + B) f^{l+1} - \underbrace{A \cdot \Delta s \left(\frac{f^{l+1} - f^l}{\Delta s} \right)}_{\text{term of error}}.$$

We obtain, in this way, Eq. (3b), with a "term of error" of the order of Δs. With this approximation, we can see that the proposed method allows us to obtain a solution of the initial equation (3a).

The main advantages of the "splitting-up" method lies in the fact that there is no restrictive condition concerning the choice of Δs with respect to the stability problem; furthermore, the method can be generalized without particular difficulties to the

integro-differential equation used here, which is particularly difficult with other methods as that proposed by Brown and Ogilvie [1], Bennett and Roth [2], or Rostaing *et al.* [7].

B. *Choice of the Increments and Discretization of Initial and Boundary Conditions*

The variables s, u, and x are divided into intervals Δs, Δu, and Δx with $\Delta u = 1/N$; we have

$s = l\,\Delta s$, therefore $0 \leqslant s \leqslant R$, i.e., $0 \leqslant l \leqslant l_M$ with $l_M = R/\Delta s$;

$u = 1 - n\,\Delta u$, therefore $-1 \leqslant u \leqslant 1$, i.e., $0 \leqslant n \leqslant 2N$;

$x = m\,\Delta x$, which gives for a target of finite thickness X, $0 \leqslant x \leqslant X$, i.e., $0 \leqslant m \leqslant M_X$ with $M_X = X/\Delta x$, and for a semi-infinite target, $0 \leqslant x \leqslant R$, i.e., $0 \leqslant m \leqslant M_R$ with $M_R = R/\Delta x$.

Using the method of "characteristics curves," we are led in evaluating the derivatives to use for x increments varying with the diffusion angles. The relation between s and x leads us to choose an increment $\Delta' x$ function of u, written as

$$\Delta' x = u\,\Delta s = (1 - n\,\Delta u)\,\Delta s = \Delta s\,\Delta u(N - n).$$

Thus, when $u = 1$, we have $\Delta' x = \Delta s$. This particular value of $\Delta' x$ will be the "increment" in x; we will denote this value as Δx.

This is a justification a posteriori of the remark of Bennett and Roth [2] who indicate that such a choice is necessary to obtain a "physically correct" solution.

The initial conditions (a), (b), and (c) can be condensed in the discretized form:

(a′) $f(0, n, m) = (1/2\pi)\,\delta(n, 0)\,\delta(m, 0)$ for $0 \leqslant n \leqslant 2N$ and $0 \leqslant m \leqslant M_X$ or M_R,

where δ is Kronecker's symbol.

The boundary conditions are

(d′) $f(l, n, 0) = 0$ for $0 \leqslant l \leqslant l_M$ and $0 \leqslant n \leqslant N$,

(e′) $f(l, n, M_R) = 0$ for $0 \leqslant l \leqslant l_M$ and $0 \leqslant n \leqslant 2N$.

This last condition is replaced in the case of a finite thickness target, by

(f′) $f(l, n, M_X) = 0$ for $0 < l \leqslant l_M$ and $N \leqslant n \leqslant 2N$.

C. *Resolution Method*

First step. One solves an equation of the type

$$\frac{\partial g(s, u, x)}{\partial s} = -u\,\frac{\partial g(s, u, x)}{\partial x} \tag{4}$$

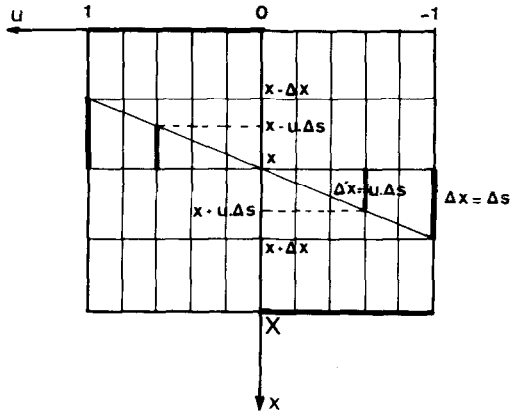

FIG. 4. Discretization versus u and x.

using boundary conditions (d′) and (f′) and the initial condition (a′). As previously mentioned, we use a discretization method which varies with the sign of u; this particular point is illustrated by Fig. 4.

(a) For $0 < u < 1$, i.e., $0 < n < N$.

Equation (4) is discretized in the following way:

$$\frac{\partial g(s,u,x)}{\partial s} = \frac{g(s+\Delta s,u,x) - g(s,u,x)}{\Delta s}$$

and

$$-u\frac{\partial g(s,u,x)}{\partial x} = -u\left(\frac{g(s,u,x) - g(s,u,x-u\,\Delta s)}{u\,\Delta s}\right),$$

whence

$$g(s+\Delta s,u,x) = g(s,u,x-u\,\Delta s) \qquad \text{if} \quad x-u\,\Delta s > 0$$

and

$$g(s+\Delta s,u,x) = 0 \qquad \text{if} \quad x-u\,\Delta s < 0.$$

With the grid defined for x, values such as $(x-u\,\Delta s)$ for $u \neq 1$ or $u \neq -1$ do not appertain to the grid and the corresponding values of the function are obtained by linear interpolation in x, starting from values on the grid; thus, we obtain

$$g(s+\Delta s,u,x) = (1-u)\,g(s,u,x) + ug(s,u,x-\Delta x)$$

or, with the discretization integers l, n, m,

$$g(l+1,n,m) = (n\cdot\Delta u)\,g(l,n,m) + (1-n\,\Delta u)\,g(l,n,m-1)$$

with the boundary condition (d′).

(b) For $-1 \leqslant u < 0$, i.e., $N < n \leqslant 2N$

in an identical manner, we obtain

$$g(s + \Delta s, u, x) = (1 + u)\, g(s, u, x) - u g(s, u, x + \Delta x);$$

thus, with the discretization integers l, n, m,

$$g(l + 1, n, m) = (2 - n\,\Delta u)\, g(l, n, m) - (1 - n\,\Delta u)\, g(l, n, m + 1)$$

with the boundary condition (f′)

(c) For $u = 0$, i.e., $n = N$, the second member of (4) is zero and the solution of discretized equation is

$$g(s + \Delta s, 0, x) = g(s, 0, x)$$

or, using the discretization integers,

$$g(l + 1, N, m) = g(l, N, m).$$

From the point of view of the notation, we have $g(l, n, m) \sim f^l$.

Second step. We must now solve an equation of the type

$$\frac{\partial h(s, u, x)}{\partial s} = \frac{1}{A(s)} \frac{\partial}{\partial u}\left((1 - u^2) \frac{\partial h(s, u, x)}{\partial u}\right). \tag{5}$$

This elliptical equation, which is degenerated at its limits, does not have boundary conditions; it may also be written as

$$\frac{\partial h(s, u, x)}{\partial s} = \frac{1}{A(s)}\left(-2u \frac{\partial h(s, u, x)}{\partial u} + (1 - u^2) \frac{\partial^2 h(s, u, x)}{\partial u^2}\right).$$

An implicit discretization versus s enable us to write

$$\frac{h(s + \Delta s, u, x) - h(s, u, x)}{\Delta s}$$

$$= \frac{1}{A(s)}\left(-2u \frac{\partial h(s + \Delta s, u, x)}{\partial u} + (1 - u^2) \frac{\partial^2 h(s + \Delta s, u, x)}{\partial u^2}\right)$$

with

$$h(s, u, x) \simeq g(s + \Delta s, u, x), \qquad \text{i.e.,} \quad h^l \equiv g^{l+1}$$

and

$$h(s + \Delta s, u, x) \simeq f(s + \Delta s, u, x), \qquad \text{i.e.,} \quad h^{l+1} \equiv f^{l+1}.$$

The discretization of angular derivatives leads to an equation of the type

$$\{B'\}\{h(s+\Delta s, u, x)\} = \{h(s, u, x)\},$$

where $\{B'\}$ is a matrix which depends, for a given value of s, only upon u and $\{h(s+\Delta s, u, x)\}$ is a solution vector.

Discretization Versus the Variable u

A centered discretization has been chosen for angular derivatives. However, for $u = 1$ and $u = -1$, the equation becomes simpler, and the remaining first derivative may be expressed by noncentered formulas, using a node on the boundary and another node inside the domain.

General case: $-1 < u < 1$ $(0 < n < 2N)$. With previously defined notations, the discretized equation may be written

$$h(l, n, m) = h(l+1, n, m) + \frac{\Delta s}{A(s)\cdot \Delta u}\left[B(n, n+1)\, h(l+1, n+1, m)\right.$$
$$\left. + B(n, n)\, h(l+1, n, m) + B(n, n-1)\, h(l+1, n-1, m)\right] \tag{6}$$

with

$$B(n, n+1) = n^2\,\Delta u + n\,\Delta u - 2n - 1,$$
$$B(n, n) = 4n - 2n^2\,\Delta u,$$
$$B(n, n-1) = n^2\,\Delta u - n\,\Delta u - 2n + 1.$$

Particular cases: $u = 1$ $(n = 0)$. Equation (6) becomes simpler and may be written, in its discretized form,

$$h(l, 0, m) = h(l+1, 0, m) + \frac{\Delta s}{A(s)\cdot \Delta u}$$
$$\cdot\,(B(0, 0)\, h(l+1, 0, m) + B(0, 1)\, h(l+1, 1, m)) \tag{7}$$

with

$$B(0, 0) = 2 \qquad \text{and} \qquad B(0, 1) = -2$$
$$:u = -1, \qquad \text{i.e.,} \quad n = 2N.$$

By analogy with the previous case this leads to

$$h(l, 2N, m) = h(l+1, 2N, m) + \frac{\Delta s}{A(s)\cdot \Delta u}\,(B(2N, 2N)\, h(l+1, 2N, m)$$
$$+ B(2N, 2N-1)\, h(l+1, 2N-1, m)) \tag{8}$$

with

$$B(2N, 2N) = 2 \qquad \text{and} \qquad B(2N, 2N-1) = -2.$$

Equations (6)–(8) could be written in the matrix form

$$\{h(l, i, m)\} = \underbrace{\left\{\{\mathbf{1}\} + \frac{\Delta s}{A(s) \cdot \Delta u}\{B\}\right\}}_{\{B'\}} \{h(l+1, i, m)\}, \tag{9}$$

where $\{h(l, i, m)\}$ and $\{h(l+1, i, m)\}$ are $2N+1$ dimension vectors and $\{\mathbf{1}\}$ and $\{B\}$ are square matrices of size $(2N+1)(2N+1)$.

Dependance Versus x

The solution vector $\{h(l+1, i, m)\}$ must be computed for every value of x in the discretized domain, i.e., $\forall m$.

Three cases must be considered

$$x \neq 0 \text{ and } x \neq X, \qquad \text{i.e.,} \quad m \neq 0 \text{ and } m \neq M_X,$$
$$x = 0, \qquad m = 0,$$
$$x = X, \qquad m = M_X,$$

General case: $x \neq 0$ *and* $x \neq X$. We obtain a tridiagonal system of size $(2N+1)(2N+1)$ which may be written

$$\begin{Bmatrix} h(l,0,m) \\ h(l,1,m) \\ \cdot \\ \cdot \\ \cdot \\ h(l,2N,m) \end{Bmatrix} = \begin{Bmatrix} B'_{0,0} B'_{0,1} & & & \\ B'_{1,0} B'_{1,1} B'_{1,2} & & & \\ & \ddots & & \\ & & B'_{2N-1,2N} & \\ & & B'_{2N,2N-1} B'_{2N,2N} \end{Bmatrix} \cdot \begin{Bmatrix} h(l+1,0,m) \\ h(l+1,1,m) \\ \cdot \\ \cdot \\ \cdot \\ h(l+1,2N,m) \end{Bmatrix}.$$

The solution is obtained by direct resolution of the system by Gauss' method for three-diagonal matrices.

Calculation on the input side: $x = 0 \rightarrow m = 0$. The calculation must be carried out for $-1 \leqslant u < 0$ because of boundary values which are null for $0 \leqslant u \leqslant 1$.

One can then write

$$\begin{Bmatrix} h(l,0,0) \\ h(l,1,0) \\ \\ h(l,N,0) \\ \\ h(l,2N,0) \end{Bmatrix} = \left\{ \begin{array}{c} \overset{N}{\downarrow} \\ \\ \\ \text{--------}1\ 0\ 0\ 0\ 0\ 0 \\ x\ x\ x \\ \text{coefficients} \\ \text{of } B' \\ x\ x\ x \\ x\ x \end{array} \right\} \cdot \begin{Bmatrix} h(l+1,0,0) \\ \\ \\ h(l+1,N,0) \\ \\ h(l+1,2N,0) \end{Bmatrix}.$$

Calculation on the output side: $x = X \to m = M_X$. Here, the calculation must be carried out for $0 < u \leqslant 1$ because of boundary values which are null for $-1 \leqslant u \leqslant 0$.

The following simplified matrix is used:

$$\begin{Bmatrix} h(l,0,M_X) \\ \\ \\ h(l,N,M_X) \end{Bmatrix} = \left\{ \begin{array}{c} \overset{N}{\downarrow} \\ x\ x \\ x \\ \text{coefficients} \\ \text{of } B' \\ x\ x\ x \\ 0\ 0\ 0\ 0\ 0\ 1 \end{array} \right\} \cdot \begin{Bmatrix} h(l+1,0,MX) \\ \\ \\ h(l+1,N,MX) \end{Bmatrix}.$$

D. *Continuity Condition*

Using the previously defined notation for operators in the transport equation, the continuity condition may be expressed, following Bethe, Rose, and Smith, by the relation

$$\int_{-1}^{1} B \cdot f \cdot du = 0. \tag{10}$$

The values of matrix $\{B\}$ elements as also linear interpolations in f imply that this condition is fulfilled, and it ensures the conservation of the particles number during the computation.

III. Generalization of the Computing Method in the Case of the Integro-Differential Equation (Eq. (1))

We present the resolution method in the case of a maximal scattering angle equal to π; this corresponds to the most realistic physical point of view. The use of a cutoff angle Θ_c is only an artefact allowing us to treat the small angle diffusion problem by simply introducing a supplementary parameter in a computation program.

So, our resolution method is valid whatever the value of the cutoff angle.

The diffusion equation may be written, using the notation previously indicated,

$$\frac{\partial f(s,u,x)}{\partial s} = -u\frac{\partial f(s,u,x)}{\partial x} - \frac{f(s,u,x)}{\lambda_e'(s)} + \frac{1}{\lambda_e'(s)}\int_{-1}^{1} f(s,u',x)\,R(u,u')\,du'. \tag{11}$$

In this case, initial conditions and boundary conditions are the same as in the case of small angle diffusion, and the equation may be written

$$\frac{\partial f(s,u,x)}{\partial s} = (A+B)\cdot f(s,u,x)$$

with

$$Af = -u\frac{\partial f}{\partial x}$$

and

$$Bf = \left(-\frac{1}{\lambda_e'(s)} + \frac{B''}{\lambda_e'(s)}\right) f = -\frac{f}{\lambda_e'(s)} + \frac{1}{\lambda_e'(s)}\int_{-1}^{1} f(s,u',x)\,R(u,u')\,du'.$$

The resolution method is identical to the one used in the case of small angle diffusion. Thus, only the type of discretization of B operator is developed.

A. *Discretization of B Operator*

In this discretization versus u, some difficulties arise, essentially due to the integral term. Indeed, the kernel $R(u,u')$ shows a marked characteristic of directivity for $u = u'$, related to the choice of a Rutherford differential cross section.

Furthermore, the number of nodes on the range of u must not be too great because it is in direct relationship to the size of a variable coefficient matrix, analogous to the $\{B'\}$ matrix of the previous section, which must be inverted at every step in s. Moreover, the method of integration must be chosen in such a manner that it describes the analytical properties of $R(u,u')$ with a numerical accuracy.

Indeed, we have, by definition,

$$\int_{-1}^{1} R(u, u')\, du' = 1, \qquad \forall u.$$

Under these conditions, if we chose the quadrature formula in such a manner that

$$B''h = \int_{-1}^{1} R(u, u')\, h(u')\, du' \simeq \sum_j B''_{ij} h(u_j),$$

where i is the grid index in u, j the grid index in u', and u_j the corresponding value of u', then, the elements B''_{ij} should respect the condition

$$\sum_j B''_{ij} = 1, \qquad \forall i. \tag{12}$$

To partially overcome this difficulty, we use the method proposed by Strickland *et al.* [4] and used again in [9], which can be resumed as follows:

(a) The grid in u is chosen with an increment of 0.2 or 0.1 and the integral is replaced by a finite sum of integrals, evaluated between the values of u belaying to the grid.

(b) $h(s, u', x)$ is linearly interpolated versus u.

(c) Then the coefficient B''_{ij} may be written, with $u_0 = -1$ and $u_{2N} = 1$,

$$B''(u_i, u_j) = B''_{i,j} = \int_{u_j}^{u_{j-1}} \left(\frac{u_{j-1} - u'}{\Delta u}\right) R(u_i, u')\, du' + \int_{u_{j+1}}^{u_j} \frac{u' - u_{j+1}}{\Delta u} R(u_i, u')\, du' \qquad \text{with} \quad 0 \leqslant j \leqslant 2N,\ 0 \leqslant i \leqslant 2N. \tag{13}$$

These integrals are computed by splitting each interval Δu into 10 zones. The calculation is carried out on each of these zones by an eight order Gauss method. Under these conditions, the properties of $R(u, u')$ are respected during the numerical integration.

B. *Discretized Form of the Equation*

This equation, which describes the second step of our method may be written in its discretized form versus u:

$$\frac{\partial h(s, u, x)}{\partial s} = -\frac{h(s, u, x)}{\lambda'_e(s)} + \frac{1}{\lambda'_e(s)} \sum_{j=0}^{2N} B''(u, u_j)\, h(s, u_j, x) \tag{14}$$

which gives, with an implicit discretization versus s,

$$h(l, n, m) = h(l+1, n, m) + \frac{\Delta s}{\lambda'_e(s)} \left(h(l+1, n, m) - \sum_{n'=0}^{2N} B''_{n,n'} h(l+1, n', m) \right)$$

or, with a matrix notation,

$$\{h(l, i, m)\} = \underbrace{\left\{ \{1\} + \frac{\Delta s}{\lambda'_e(s)} \{B\} \right\}}_{\{B'\}} \{h(l+1, i, m)\}, \qquad 0 \leqslant i \leqslant 2N, \tag{15}$$

with

$$\{B\} = \{1\} - \{B''\}$$

where matrix $\{B\}$ of size $(2N+1)(2N+1)$ is a full matrix.

Remark. Introducing a cutoff angle Θ_c different of π, we obtain a matrix which approaches a tridiagonal shape allowing us to recover the results given by small angle diffusion equation in Section II.

C. *x Dependence*

The x dependence is identical to that presented in Section I.

D. *Continuity Condition*

This condition must express the conservation of the particle number when the energy is varying. This condition, which has been written in its general form (10) for small angles, becomes

$$\int_{-1}^{1} f(s, u, x)\, du - \int_{-1}^{1} du \int_{-1}^{1} f(s, u', x)\, R(\Theta_c, u, u')\, du' = 0. \tag{16}$$

Now, in the discretization, a linear interpolation of f has been made between two values belaying to the grid. This necessarily implies that the first integral is computed by the trapeze method with an increment Δu, and, consequently, the integration versus u in the double integral is computed in the same way.

Under these conditions, the continuity condition can be written as a series of relations between coefficients B''_{ij}

$$\begin{aligned}
&\tfrac{1}{2}B''_{0,0} + B''_{1,0} + \cdots + B''_{2N-1,0} + \tfrac{1}{2}B''_{2N,0} = \tfrac{1}{2}, \\
&\tfrac{1}{2}B''_{0,1} + B''_{1,1} + \cdots + B''_{2N-1,1} + \tfrac{1}{2}B''_{2N,1} = 1, \\
&\vdots \\
&\tfrac{1}{2}B''_{0,2N} + B''_{1,2N} + \cdots + B''_{2N-1,2N} + \tfrac{1}{2}B''_{2N,2N} = \tfrac{1}{2}.
\end{aligned} \tag{17}$$

However, it is a priori evident that while elements of matrix $\{B''\}$ may be computed precisely, the continuity condition cannot be perfectly respected, since f is linearly interpolated. Indeed one can write

$$\int_{-1}^{1} f(s, u', x) \cdot R(\Theta_c, u, u')\, du' = K(s, u, x).$$

The function $K(s, u, x)$ has the same properties as $R(\Theta_c, u, u')$ from the point of view of directivity versus u. Under these conditions one can say that integration versus u is not correctly evaluated by the trapeze method starting from a reduced size grid in u and hence cannot be employed numerically.

Therefore the numerical values of the $B''(i,j)$ coefficients were slightly modified in order to ensure verification of relation (17), while maintaining the properties (12) of the kernel $R(\Theta_c, u, u')$; so, the form of angular distributions due to elastic scattering alone is maintained.

IV. Results and Discussion

We present here some results directly comparable with experimental results: energy distribution and transmission yield.

In order to obtain these results, f is expanded in spherical harmonics, whose components are F_0, F_1, F_2. Taking into account the relation between E and s, Bennett and Roth [2] give the following relations:

$$\frac{d\eta_R}{dE} = \frac{E \cdot F_1(E, 0)}{(\Delta u/2) \cdot \Delta s \cdot E_0(dE/ds)_{E_0}}, \qquad \eta_R = \int_0^{E_0} \frac{d\eta_R}{dE} \cdot dE,$$

$$\frac{d\eta_T}{dE} = \frac{E \cdot F_1(E, X)}{(\Delta u/2) \cdot \Delta s \cdot E_0(dE/ds)_{E_0}}, \qquad \eta_T = \int_0^{E_0} \frac{d\eta_T}{dE} \cdot dE.$$

A. *Physical Parameters*

Mean Free Path

The values of "transport" m.f.p. used in small angle scattering equations were deduced from values of differential cross sections computed by Cailler *et al.* [10] by the "phase shift" method. In the integro-differential equation, we use values of elastic scattering m.f.p. given by Ganachaud [11]. These values could be represented by the relation

$$\lambda_e\,(\text{cm}) = 6.048 \times 10^{-6} E^2 \cdot \xi(1 + \xi) \qquad \text{with} \quad E \text{ in keV}.$$

Law of Energy Loss

With a view to comparing our results with those of Rostaing [12], we use the range–energy relation

$$s = 335(E_0^{1.53} - E^{1.53}) \qquad \text{with} \quad s \text{ in Å and } E \text{ in keV.}$$

B. *Transmission and Backscattering Yields*

Results obtained with the small angle diffusion equation for some values of target thickness are shown in Table I; they are absolutely identical to Rostaing's values [3].

TABLE I

Theoretical (Small Angle Diffusion Equation) and Experimental Values of Transmission and Backscattering Yields for Al

Thickness X (Å)		200	500	1000
$E_p = 3$ keV	η_R	0.04	0.11	0.11
	η_T	0.91	0.59	0.11
	η_T expt.	0.86	0.57	0.08
$E_p = 2.5$ keV	η_R	0.065	0.12	
	η_T	0.84	0.4	
	η_T expt.	0.81	0.38	
$E_p = 2$ keV	η_R	0.095		
	η_T	0.73		
	η_T expt.	0.69		
$E_p = 1.5$ keV	η_R	0.12		
	η_T	0.49		
	η_T expt.	0.47		

We have used increments $\Delta s = 2$ Å and $\Delta u = 0.2$ in accordance with the choice of Bennett and Roth [2]. The verifications effected with $\Delta s = 5$ Å give results differing from the preceding ones by 1 or 2 %.

The results obtained with the integro-differential equation are shown in Table II. One can see that values of η_T corresponding to $\Theta_c = \pi/4$ and $\Theta_c = \pi$ "bracket" the results given by the small angle scattering equation.

These phenomena are shown in Fig. 5, where we mention the variations of η_R and η_T as functions of Θ_c for a target thickness of 1000 Å and an energy of 3 keV. In the same figure are also indicated values of η_R and η_T given by the small angle equation.

TABLE II

Theoretical (Integro-Differential Equation) and Experimental Values of Transmission and Backscattering Yields for Al

E_p (keV)	Thickness X (Å)		200	500	1000
3	$\Theta_c = \pi/4$	η_R	0.03	0.09	0.09
		η_T	0.92	0.65	0.18
	$\Theta_c = \pi$	η_R	0.075	0.165	0.16
		η_T	0.86	0.52	0.075
		η_T expt.	0.86	0.57	0.08
2.5	$\Theta_c = \pi/4$	η_R	0.04	0.085	
		η_T	0.88	0.5	
	$\Theta_c = \pi$	η_R	0.11	0.165	
		η_T	0.79	0.33	
		η_T expt.	0.81	0.38	
2	$\Theta_c = \pi/4$	η_R	0.065		
		η_T	0.8		
	$\Theta_c = \pi$	η_R	0.15		
		η_T	0.66		
		η_T expt.	0.69		
1.5	$\Theta_c = \pi/4$	η_R	0.075		
		η_T	0.62		
	$\Theta_c = \pi$	η_R	0.175		
		η_T	0.41		
		η_T expt.	0.47		

Note. Theoretical results are shown for two values of the limit diffusion angle Θ_c : $\Theta_c = \pi/4$ and $\Theta_c = \pi$.

Remarks. Tests realized with values of increment $\Delta u = 0.2$ and $\Delta u = 0.1$ show only small differences.

Tests upon Δs and Δu for the integro-differential equation give results analogous to those previously mentioned for the small angle scattering equation.

C. *Energy Distributions*

Energy distributions of electrons transmitted through 500-Å-thick targets, for some values of E_p, are shown in Fig. 6 in the case of the small angle scattering equation; they are identical with Rostaing's values. Analogous results obtained with the integro-differential equation can be seen in Fig. 7; they show that observations concerning transmission yield values are confirmed by the aspect of energy distribution curves.

However, these results disagree with experimental results [9, 12, 13]. The effect of the scattering limit angle Θ_c for a 1000-Å-thick target and an energy of 3 keV is shown in Fig. 8 and a comparison is made with results given by the small angle scattering equation. These results confirm those obtained for transmission yield η_T shown in Fig. 5.

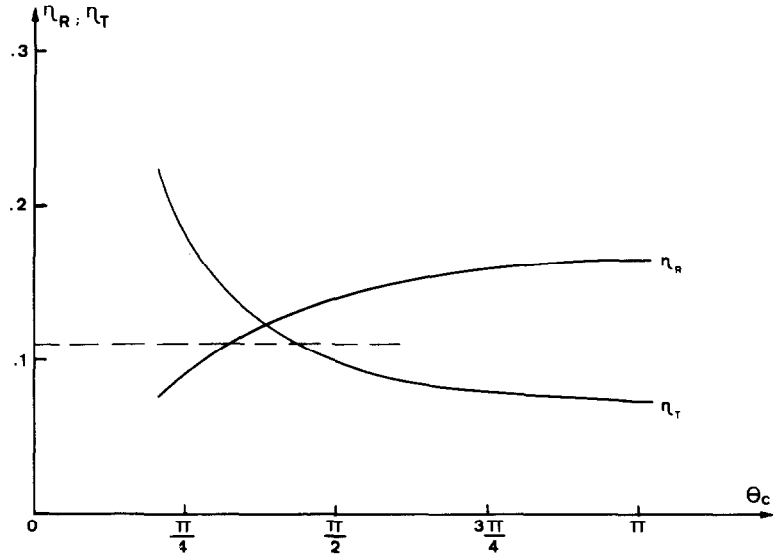

FIG. 5. Theoretical variations of η_R and η_T (integro-differential equation) as function of the limit diffusion angle Θ_c for 1000-Å-thick aluminum target and a primary energy 3 keV. The dotted line indicates the common value of η_R and η_T given in the same conditions by small angle diffusion equation.

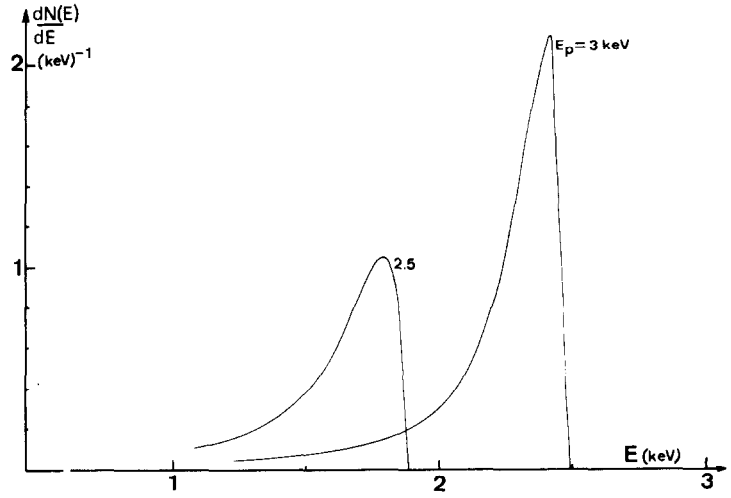

FIG. 6. Theoretical energy distributions of electrons transmitted through 500-Å-thick aluminum target for different values of primary energy (small angle diffusion equation).

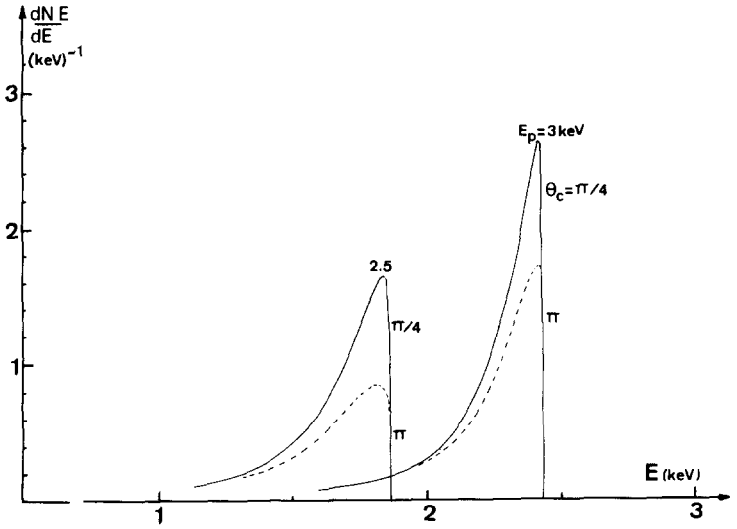

FIG. 7. Theoretical energy distribution of electrons transmitted through 500-Å-thick aluminum target for different values of primary energy E_p, and limit diffusion angle Θ_c (integro-differential equation).

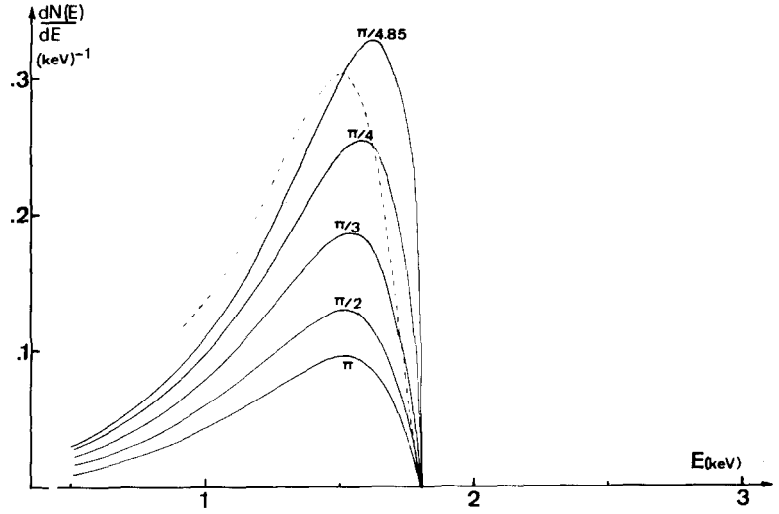

FIG. 8. Theoretical energy distribution of electrons transmitted through 1000-Å-thick aluminum target, for a primary energy of 3 keV and for different values of Θ_c (integro-differential equation). The dashed curve shows the analogous result given by small angle diffusion equation.

V. Conclusion

The numerical resolution method proposed here was initially developed for treatment of partial differential equations. Our method presents two advantages over the earlier ones [1–3]: on one hand if, with the same increments, computing time is identical to that of the other methods, it is possible to increase the size of increments and therefore to reduce computing time without stability problems; on the other hand, there is no difficulty in extending this method to integro-differential equation treatment.

Comparisons made between the different computing methods have shown that results obtained by the integro-differential equation make it possible by varying the cutoff angle Θ_c to find again the results given by the small angle scattering equation.

The most important problems encountered are connected with the directivity of the kernel $R(u, u')$ (or $R(\Theta_c, u, u')$) for $u = u'$; the discretization of these kernels is subject to difficulties in connection with the form of differential cross sections; these problems vanish for example when the energy is lowered and the directivity of the kernel is diminished. In the same way the problem of the "continuity condition" is not tied to the numerical treatment method, but essentially to the choice of physical parameters.

Appendix

The "function of diffusion" was established by Strickland [8] for $\Theta_c = \pi$. We have

$$R(u, u') = \frac{2\xi(1+\xi)(1+2\xi-uu')}{(u^2-u'^2+4\xi(1-uu')+4\xi^2)^{3/2}}$$

and for $0 < \Theta_c < \pi$, we have

$$R(\Theta_c, u, u') = \frac{2\xi(1+2\xi-u_c)}{\pi(1-u_c)} \frac{1}{(a^2-b^2)} \frac{b \cdot \sin \phi_M}{a - b\cos\phi_M} + \frac{2a}{\sqrt{a^2-b^2}} \operatorname{arctg} \frac{\sqrt{a^2-b^2}}{(a-b)} \frac{\operatorname{tg} \phi_M}{2}$$

with the azimuthal angle ϕ_M defined by

$$\phi_{\text{Max}} = 0 \quad \text{if} \quad |\theta - \theta'| \geqslant \Theta_c,$$

$$\phi_{\text{Max}} = \pi \quad \text{for} \quad \theta + \theta' \leqslant \Theta_c,\ 2\pi - (\theta + \theta') \leqslant \Theta_c, \text{ and } |\theta - \theta'| \leqslant \Theta_c \text{ with } u = 1 \text{ or } u = -1.$$

In all other cases

$$\phi_{\text{Max}} = \operatorname{Arccos} \frac{u_c - uu'}{\sqrt{1-u^2}\sqrt{1-u'^2}}$$

with

$$u_c = \cos \Theta_c,$$
$$a = 1 + 2\xi - uu',$$
$$b = \sqrt{(1-u^2)}\sqrt{(1-u'^2)}.$$

The expression of $R(\Theta_c, u, u')$ we have obtained (9) is different from that of Strickland, but all the expressions are the same for $\Theta_c = \pi$.

ACKNOWLEDGMENTS

The authors are grateful to Professor J. Cea of the Mathematical Department, for helpful discussions concerning the "splitting-up" method.

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