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Application of the P_n-Method to the Calculation of the Angular Flux of Gamma Rays

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An application of the P_n-method to the transport of gamma rays is presented in the case where Compton-scattering is predominant. The geometry considered is a slab of medium bounded by vacuum. In this application the P_n-method is related to the Lagrange interpolation and the Gauss-quadrature rule. This is of practical importance for the choice of the boundary conditions and for the approximation of the angular flux, especially at the edges of the medium. In addition, the set of spatial differential equations becomes uncoupled, allowing explicit numerical solution. The solution of each differential equation is approximated by means of Hermite interpolation.

1. INTRODUCTION

To solve the Boltzmann transport equation describing the transport of neutrons or photons in a medium, three important principles are commonly used: (a) simulation by Monte-Carlo method, (b) discretisation of the angular flux of particles (S_n-method), and (c) expansion of the same flux in a series of spherical harmonics. Of the three principles the Monte-Carlo method has the most outstanding capability to handle an arbitrary configuration. In spite of this, another method may be preferred because of (pseudo-) statistical fluctuation of the result and long computing time. It can be easily shown that the computing time increases exponentially with medium thickness where constant variance of the result is pursued.

From the two other principles, the S_n-method [1] seems to be the easiest, but its advantages are doubtful for a highly anisotropic and incoherent scattering process. On the other hand, the expansion in spherical harmonics offers, by means of the addition theorema [2], an elegant approximation of the scattering integral operator. This is most obvious for the one-dimensional problem where the series of spherical harmonics reduces to a series of Legendre polynomials.

Based on the expansion of the angular flux in a series of Legendre polynomials, until recently, two methods have been used to compute the transport of photons where Compton-scattering is predominant [3, 4], viz., the moment method and the

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flux iteration technique. The moment method was used by Goldstein and Wilkins [3] to compute the scalar flux as a function of the distance from a source. This almost analytical method starts from an infinite series of functions of the spatial and angular coordinates. It has the severe limitation of assuming a homogeneous and infinite medium. The flux iteration technique, developed by Gopinath and Santhenam [4], is a semi-analytical method that is based on an integral form of the transport equation which is applicable to finite inhomogeneous slab. Its starting points are very comprehensible but it soon transforms into a set of non-uniform relations.

A third method called P_n-method has been developed for use in the neutron transport calculation [5–7]. In this method the boundary conditions are formulated in terms of a finite number of spherical harmonics. In case of slab geometry, this could be expressed in terms of the first $n + 1$ Legendre polynomials. The two most popular formulations of the boundary conditions are those of Marshak and Mark. Usually these conditions are presented as being somewhat artificial and arbitrary.

In this paper the P_n-method will be applied to the transport of photons for an infinite slab of medium where Compton-scattering is predominant. The P_n-form of the transport equation is transformed so that it allows interpretation in terms of the interpolation theory introducing the boundary condition of Mark in a natural way. This results in a set of uncoupled differential equations which are solved using the first spatial derivative at the nodes.

Attention is paid to the practical value of the approximation at the boundary.

2. Formulation of the Problem

The transport equation for the flux of photons, in the case of one-dimensional slab geometry and an external source (Fig. 1), can be written as

$$\mu \frac{dI}{dz} = -\sigma(\lambda) I + \int_{\lambda_0}^{\lambda} \int_{4\pi} f(\omega \cdot \omega', \lambda', \lambda) I(z, \mu', \lambda') \, d\omega' \, d\lambda' \tag{1}$$

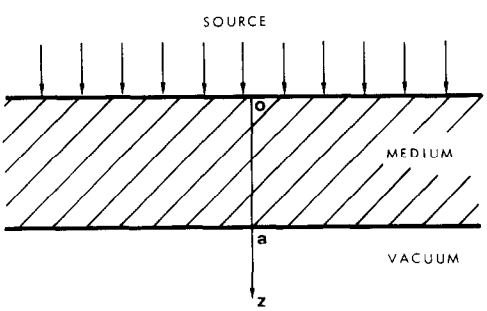

Fig. 1. Problem geometry.

where z is the depth coordinate, μ is the cosine of the direction of the photons relative to the z-axis, and λ is the wavelength in Compton units ($0.511/E$, E energy in MeV). The lowest wavelength λ_0 corresponds to the maximal energy present in the spectrum of the photon source. $\sigma(\lambda)$, the total attenuation coefficient, and $f(\omega \cdot \omega', \lambda', \lambda)$, the Compton-differential cross section, are defined in Appendix A.

$\omega \cdot \omega'$ is the cosine of the angle between the incident and scattered photon. $\omega \cdot \omega'$ is in relation with the azimuth and the cosine of the polar angle:

$$\omega \cdot \omega' = \mu\mu' + (1-\mu^2)^{1/2}\,(1-\mu'^2)^{1/2}\cos(\psi' - \psi). \tag{2}$$

The external source and the lack of backscattering from the vacuum implies the following boundary conditions:

$$I(o, \mu, \lambda) = \mathcal{J}(\mu, \lambda), \qquad \mu > 0 \tag{1a}$$

$$I(a, \mu, \lambda) = 0, \qquad \mu < 0 \tag{1b}$$

where $\mathcal{J}(\mu, \lambda)$ is a given function which describes the source. This function equals zero for $\mu \in [0, -1]$.

We can take advantage of the simplicity of the equation without scattering term by splitting the flux I into primary flux I_p and a secondary flux I_s:

$$I = I_p + I_s. \tag{3}$$

The primary flux I_p is the flux of non-scattered photons and the secondary flux I_s is the flux of at least once scattered photons.

So I_p is the solution of the problem

$$\mu \frac{dI_p}{dz} = -\sigma(\lambda) I_p \tag{4}$$

$$I_p(o, \mu, \lambda) = \mathcal{J}(\mu, \lambda) \tag{4a}$$

that is,

$$I_p(z, \mu, \lambda) = \mathcal{J}(\mu, \lambda)\exp\{-\sigma(\lambda) z/\mu\}. \tag{5}$$

Substitution of (3) and (4) into (1) produces for I_s the following problem:

$$\mu I_s = -\sigma(\lambda) I_s + \int_{\lambda_0}^{\lambda} \int_{4\pi} f(\omega \cdot \omega', \lambda', \lambda)\, I_s(z, \mu', \lambda')\, d\omega'\, d\lambda' + S_p \tag{6}$$

$$I_s(o, \mu, \lambda) = 0, \qquad \mu > 0 \tag{6a}$$

$$I_s(a, \mu, \lambda) = 0, \qquad \mu < 0 \tag{6b}$$

where the source term S_p accounts for the once scattered primary radiation:

$$S_p(z, \mu, \lambda) = \int_{\lambda_0}^{\lambda} \int_{4\pi} f(\omega \cdot \omega', \lambda', \lambda)\, I_p(z, \mu', \lambda')\, d\omega'\, d\lambda'. \tag{7}$$

Generally a split of the angular flux into primary and secondary flux will assure a better result for a source with a narrow angular spectrum, as in the present case where we deal with a highly anisotropic and incoherent scattering process. In the limiting case of a mono-directional source, in combination with a mono-energetic spectrum, this split allows evaluation of the scattering integral in a way as explained in the following section.

3. Application of the P_n-Method

In the P_n-method we search for an approximation of this problem, relative to the variable μ, in the space $\mathscr{P}^n$ of polynomials of degree n, in which we choose the basis $P^n = \{\sqrt{(2l+1)/2}\, P_l \mid l = 0, 1, \ldots, n\}$, where P_l is the lth polynomial of Legendre. Then the approximation $I^{(n)}$ of the flux is

$$I^{(n)}(z, \mu, \lambda) = \sum_{l=0}^{n} \sqrt{\frac{2l+1}{2}}\, I_l^{(n)}(z, \lambda)\, P_l(\mu). \tag{8}$$

Writing coefficients $I_l^{(n)}(z, \lambda)$ in a vector,

$$u(z, \lambda) = (I_0^{(n)}(z, \lambda)\; I_1^{(n)}(z, \lambda) \cdots I_n^{(n)}(z, \lambda))^T \tag{9}$$

and defining the vector $p(\mu)$ as

$$p(\mu) = \left(\sqrt{\frac{1}{2}}\, P_0(\mu)\, \sqrt{\frac{3}{2}}\, P_1(\mu) \cdots \sqrt{\frac{2n+1}{2}}\, P_n(\mu)\right)^T \tag{10}$$

Eq. (8) reduces to

$$I^{(n)}(z, \mu, \lambda) = u(z, \lambda)^T\, p(\mu). \tag{11}$$

With these notations the transport equation for the P_n-approximation is given by

$$M \frac{du_s}{dz} = -\sigma(\lambda)\, u_s + \int_{\lambda_0}^{\lambda} F(\lambda', \lambda)\, u_s(z, \lambda')\, d\lambda' + s_p(z, \lambda) \tag{12}$$

where $s_p(z, \lambda)$ is the vector of coefficients of $S_p(z, \mu, \lambda)$ and where M is the matrix

$$M = \begin{bmatrix} 0 & \frac{1}{\sqrt{3}} & 0 & \cdots & 0 \\ \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{3 \cdot 5}} & \cdots & 0 \\ 0 & \frac{2}{\sqrt{3 \cdot 5}} & 0 & & \vdots \\ \vdots & & & & \\ 0 & 0 & 0 & \frac{n}{\sqrt{(2n-1)(2n+1)}} & 0 \end{bmatrix}. \tag{13}$$

$F(\lambda', \lambda)$ is a diagonal matrix with diagonal elements $2\pi \sqrt{2/(2l+1)}\, f_l(\lambda', \lambda)$, where $f_l(\lambda', \lambda)$ is the lth coefficient in the serial expansion of the differential cross section for Compton-scattering. As described in Appendix B, f_l can be computed directly from relation (A.3) of Appendix A:

$$f_l(\lambda', \lambda) = \sqrt{\frac{2l+1}{2}} \frac{d\sigma}{d\omega}(\omega \cdot \omega', \lambda', \lambda)\Big|_{\omega \cdot \omega' = 1 + \lambda' - \lambda}. \tag{14}$$

The case of a mono-directional and mono-chromatic source is described by the distribution

$$\mathcal{J}(\mu, \lambda) = \delta(\mu - 1)\ \delta(\lambda - \lambda_0). \tag{15}$$

In combination with Compton-scattering it forms an anomaly for which the P_n-method must be applied with care. The flux of once scattered photons, $I_{p'}(z, \mu, \lambda)$, is the product of a function with the distribution $\delta(\mu - 1 - \lambda_0 + \lambda)$ and hence cannot be approximated in a functional sense. This is particularly important if we are not only concerned with integration of the flux on the whole μ-interval $[-1, +1]$, but also with integration on parts of this interval.

To overcome this difficulty we continue the splitting process and write

$$I_s = I_{p'} + I_{s'} \tag{16}$$

where $I_{s'}$ is the flux of the more than once scattered photons. Substituting (16) in

Eq. (6) we find for $I_{s'}$ a relation similar to (6) where the subscripts s and p are replaced by s′ and p′, respectively.

The flux $I_{p'}$ is given by

$$I_{p'}(z,\mu,\lambda) = f(\mu,\lambda_0,\lambda)\frac{1/\mu}{(\sigma(\lambda)/\mu)-\sigma(\lambda_0)}(e^{-\sigma(\lambda_0)z} - e^{-\sigma(\lambda)z/\mu}), \qquad \mu > 0 \tag{17a}$$

$$I_{p'}(z,\mu,\lambda) = f(\mu,\lambda_0,\lambda)\frac{1/\mu}{(\sigma(\lambda)/\mu)-\sigma(\lambda_0)}(e^{-\sigma(\lambda_0)z} - e^{-\sigma(\lambda)z/\mu} \times \exp\left\{\left(\frac{\sigma(\lambda)}{\mu}-\sigma(\lambda_0)\right)a\right\}), \qquad \mu < 0 \tag{17b}$$

where

$$f(\mu,\lambda_0,\lambda) = \delta(\mu-1-\lambda_0+\lambda)\frac{d\sigma}{d\omega}(\mu,\lambda_0,\lambda)\Big|_{\mu=1+\lambda_0-\lambda}. \tag{18}$$

Once done we can apply the P_n-method to $I_{s'}$ with ease, because the source term $S_{p'}$ is a normal function.

4. Approximation of the Integral

To approximate the integral $\int_{\lambda_0}^{\lambda} F(\lambda',\lambda)\,u_s(z,\lambda')\,d\lambda'$ we choose a set of points in the interval $[\lambda_0,\infty)$: $\{\lambda_1,\lambda_2,...,\lambda_m\}$, $\lambda_i > \lambda_j$ for $i > j$ and $\lambda_1 = \lambda_0$. Then Eq. (12) will be solved for $\lambda = \lambda_i$, $i = 1, 2, 3,..., m$, and the integral will be approximated by

$$\sum_{j=1}^{i} w_{ji} F(\lambda_j,\lambda_i)\,u_s(z,\lambda_j) \tag{19}$$

noting that for Compton-scattering $F(\lambda_j,\lambda_i) = 0$ if $\lambda_j - \lambda_i > 2$. The w_{ji}'s are weighting factors dependent on the integration rule. Substituting (19) in (12) we find for $i = 2, 3,..., m$ the approximation

$$M\frac{du_s}{dz}(z,\lambda_i) = -\sigma^*(\lambda_i)\,u_s(z,\lambda_i) + \sum_{j=1}^{i-1} w_{ji}F(\lambda_j,\lambda_i)\,u_s(z,\lambda_j) + s_p(z,\lambda_i) \tag{20}$$

where

$$\sigma^*(\lambda_i) = \sigma(\lambda_i) - w_{ii}\sigma_0. \tag{21}$$

σ_0 is the fraction of scattering to the same wavelength. It is clear from (20) that its solution can be computed iteratively relative to the variable λ. When $u_s(z,\lambda_j)$, $j = 1, 2,..., i-1$, are known from previous iterations the term $\sum_{j=1}^{i-1} w_{ji}F(\lambda_j,\lambda_i)\,u_s(z,\lambda_j)$ becomes part of the source term in (20).

5. Transformation of the P_n-Equation and Approximation of the Boundary Conditions

In this paragraph we will inspect some properties of the matrix M. Using these properties we will derive an orthonormal transformation on $\mathscr{S}^n$ in order to obtain a generalization of the method developed by Wick and Chandrasekhar for isotropic scattering [5], which is furthermore easier to calculate. Further we will introduce the approximation of the boundary conditions by the method of Mark. The first particularity of M is that its eigenvalues are the zeros of the Legendre polynomial P_{n+1}[5]. As a direct consequence M is singular for n even and regular for n odd. In fact M singular corresponds with the particular case of the transport equation where $\mu = 0$. We can, without loss of generality, only consider the cases where M is regular, i.e., n is odd.

Let n_1 be equal to $(n+1)/2$; we shall use the following set of indices in the next paragraphs:

$$\{n_1\} \equiv \{-n_1, -n_1+1, \ldots, -1, 1, 2, \ldots, n_1\}$$
$$\{n_1\}^- \equiv \{-n_1, -n_1+1, \ldots, -1\}$$
$$\{n_1\}^+ \equiv \{1, 2, \ldots, n_1\}.$$

The eigenvalues of M will be sorted such that $\mu_l > 0$ for $l \in \{n_1\}^+$ and $\mu_l < 0$ for $l \in \{n_1\}^-$.

The normalized eigenvector of M corresponding to the eigenvalue μ_l, noted ξ_l, is given using the definition (10) by

$$\xi_l = \frac{p(\mu_l)}{(p(\mu_l)^T p(\mu_l))^{1/2}}. \tag{22}$$

With the help of the $n+1$ eigenvectors of M we define a new set of polynomials, which are orthogonal in $\mathscr{L}^2[-1, +1]$:

$$\tilde{P}^n = \{\tilde{P}_l(\mu) \mid l \in \{n_1\}\} \tag{23}$$

where

$$\tilde{P}_l(\mu) = \frac{\xi_l^T p(\mu)}{(p(\mu)^T p(\mu))^{1/2}}. \tag{24}$$

In fact the polynomials $\tilde{P}_l$ are the Lagrange polynomials for the set of nodes given by the zeros of P_{n+1}. This follows directly from

$$\tilde{P}_i(\mu_j) = \delta_{ij} \tag{25}$$

which in turn follows from (22) and the definition of $\tilde{P}_l$. The quantities $(p(\mu_l)^T p(\mu_l))^{-1}$ are the coefficients of the integration rule of Gauss [5].

Now let Q be the matrix formed by the column-vectors ξ_l, $l \in \{n_l\}$. We rewrite Eq. (12) using the basis formed by these vectors in order to express the approximation of the flux as a combination of the polynomials of $\tilde{P}^n$.

Equivalent to (12) we obtain

$$\tilde{M} \frac{d\tilde{u}_s}{dz} = -\sigma(\lambda)\, \tilde{u}_s + \int_{\lambda_0}^{\lambda} \tilde{F}(\lambda', \lambda)\, \tilde{u}_s(z, \lambda')\, d\lambda' + \tilde{s}_p \tag{26}$$

where $\tilde{M}$ is the diagonal matrix with diagonal elements μ_l, $l \in \{n_1\}$, and

$$\tilde{F}(\lambda', \lambda) = Q^T F(\lambda', \lambda)\, Q \tag{27}$$

$$\tilde{u}_s(z, \lambda) = Q^T u_s(z, \lambda). \tag{28}$$

This form of the P_n-approximation can be understood as a Lagrange interpolation relative to a special set of nodes, while the P_n-approximation in its primitive form could be interpreted as a Fourier development in Legendre polynomials. Both forms can be used to find a solution of the equation. The differences are a manner of approximation of the boundary conditions and the ease in computing the solution.

For the interpolation, the method of Mark [6] using the given values of the flux at the nodes appears to be the most natural one, and will be used for the computation of the flux. The boundary conditions to (26) become

$$\tilde{u}_{s_l}(o) = 0, \qquad l \in \{n_1\}^+ \tag{26a}$$

$$\tilde{u}_{s_l}(a) = 0, \qquad l \in \{n_1\}^-. \tag{26b}$$

A natural way for the primitive form of the P_n-approximation should be to search a minimalization in the $\mathscr{L}^2$-norm, i.e., by replacing the boundary conditions by

$$\min \left\{ \int_0^1 [u_s(o, \lambda)^T p(\mu)]^2\, d\mu + \int_{-1}^0 [u_s(a, \lambda)^T p(\mu)]^2\, d\mu \right\}. \tag{29}$$

This was done in a test case; the results were not significantly different. This agrees with the good $\mathscr{L}^2$-convergence of the Lagrange interpolation relative to the zeros of a Jacobi polynomial [8] (for example, if we consider the class of bounded and Riemann integrable functions).

For the sake of simplicity we further use "u" instead of "$\tilde{u}$."

6. Evaluation of the Result at the Boundary of the Medium

At the boundary of the medium one must approximate a discontinuous function (discontinuity for $\mu = 0$) with a polynomial, which is an intrinsic difficulty in using

the P_n-method. To avoid this Yvon (see [7]) has used two sets of polynomials (double P_n-method) which are orthogonal on the intervals $[-1, 0]$ and $[0, +1]$, respectively. In this case the boundary conditions are exactly fulfilled and the discontinuity for $\mu = 0$ does not influence the approximation.

It will now be shown that the simple P_n-method can also be effectively used.

Using the P_n-method with the boundary conditions of Mark is equivalent to using the Gauss-rule for integration on the whole μ-interval. As a general rule, the integration procedure behaves much better than corresponding interpolation. In the case of the Gauss-rule Erdös and Turán [8] have shown that even in the case where the corresponding Lagrange interpolation diverges at some points, his integration converges to the true value of the integral. For these reasons (disregarding the errors due to other approximation), we can assume that the flux will be computed correctly at the nodes μ_l, $l \in \{n_1\}$. In the case where we are interested in point values or in the result of integration on sub-interval of $[-1, +1]$, we can, as a practical solution, connect the value at the nodes μ_1 by some simpler interpolation.

To test this statement the function

$$\mathscr{S}(\mu) = \begin{cases} 0, & \mu < 0 \\ \mu, & \mu \geqslant 0 \end{cases}$$

was used to represent the angular distribution of a monochromatic source of 5.11 Compton units, i.e., (4a) was taken as

$$I(o, \mu, \lambda) = \mathscr{S}(\mu)\, \delta(\lambda - 5.11)$$

and the once scattered flux was computed at the boundary of a slab of 2 cm water. The P_n-method was used to approximate the flux as a function of μ, but the solution of the differential equation was computed exactly. Figure 2 shows the full P_n-approximation for $\lambda = 5.51$, and $n = 9$ and $n = 13$. As can be seen the increase of n

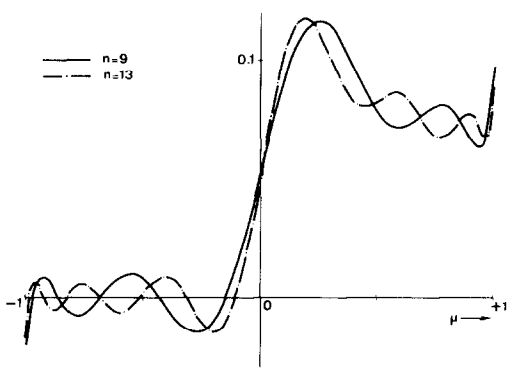

FIG. 2. P_n-approximation of once scattered flux of photons, at a wavelength 5.51 Compton-unit, in case of the test-source $\mathscr{S}(\mu)\, \delta(\lambda - 5.11)$.

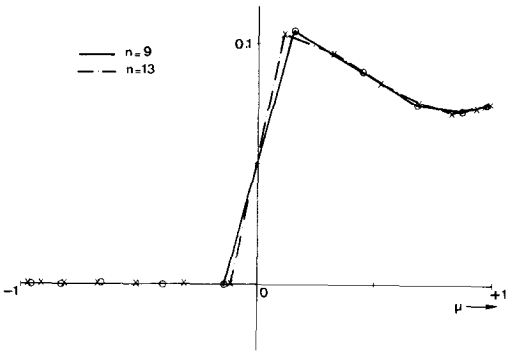

FIG. 3. Linear interpolation between the value of the P_n-approximations at the zeros of P_{n+1} (○, $n = 9$; ×, $n = 13$). Wavelength and source are the same as for Fig. 2.

does not really give an improvement. In Fig. 3 the value at the nodes μ_l is plotted and connected by lines. The linear interpolation between the points μ_l for $n = 9$ turned out to be a sufficient good approximation.

7. Numerical Solution of the Differential Equation

Using the approximation of Section 4 in the case of Eq. (26) with the boundary conditions of Mark, we are faced with the following problem ($i = 2, 3, \ldots, m$):

$$\tilde{M}\frac{du_s}{dz}(z, \lambda_i) = -\sigma^*(\lambda_i)\, u_s(z, \lambda_i) + \sum_{j=1}^{i-1} w_{ji}\tilde{F}(\lambda_j, \lambda_i)\, u_s(z, \lambda_j) + s_p(z, \lambda_i) \tag{30}$$

$$u_{s_l}(o, \lambda_i) = 0, \qquad l \in \{n_1\}^+ \tag{30a}$$

$$u_{s_l}(a, \lambda_i) = 0, \qquad l \in \{n_1\}^-, \tag{30b}$$

In simplified form:

$$\mu_l \frac{du_l}{dz}(z) = -\alpha u_l(z) + s_l(z), \qquad l \in \{n_1\} \tag{31}$$

$$u_l(o) = 0, \qquad l \in \{n_1\}^+ \tag{31a}$$

$$u_l(a) = 0, \qquad l \in \{n_1\}^-. \tag{31b}$$

For $l \in \{n_1\}^+$, the solution of (2) is given by the convolution product

$$u_l(z) = \frac{1}{\mu_l}\int_0^z s_l(z')\, e^{-\alpha(z-z')/\mu_l}\, dz' \tag{32a}$$

and for $l \in \{n_1\}^-$ by

$$u_l(z) = -\frac{1}{\mu_l} \int_z^a s_l(z')\, e^{-\alpha(z-z')/\mu_l}\, dz'. \tag{32b}$$

Call $g(z, z')$ the vector with elements

$$g_l(z, z') = s_l(z')\, e^{-\alpha(z-z')/\mu_l}, \qquad l \in \{n_1\} \tag{33}$$

and let $\{z_0, z_1, ..., z_p\}$ be a set of discrete points of $[0, a]$, where $z_0 = 0$ and $z_p = a$.

In order to compute an approximate solution of (31) the relations (32a) and (32b) were approximated by

$$u_l(z_k) = \frac{1}{\mu_l} \sum_{k'=0}^{k} \left[w_{kk'}^{(1)}\, g_l(z_k, z_{k'}) + w_{kk'}^{(2)} \frac{\partial g_l}{\partial z_{k'}}(z_k, z_{k'}) \right], \qquad l \in \{n_1\}^+ \tag{34a}$$

$$u_l(z_k) = -\frac{1}{\mu_l} \sum_{k'=k}^{p} \left[w_{k'k}^{(3)}\, g_l(z_k, z_{k'}) + w_{k'k}^{(4)} \frac{\partial g_l}{\partial z_{k'}}(z_k, z_{k'}) \right], \qquad l \in \{n_1\}^- \tag{34b}$$

where the $w_{kk'}^{(j)}$, $j = 1, 2, 3, 4$, were found by using cubic Hermite interpolation of the g_l's.

Use of the Hermite interpolation is possible because after each i-iteration not only $u_s(z, \lambda_i)$ is known but also $(du_s/dz)(z, \lambda_i)$ by substituting $u_{s_l}(z, \lambda_i)$ into Eq. (30).

The Hermite interpolation $\tilde{g}_l$ of g_l in the subinterval $[z_{k-1}, z_k]$ is given by

$$\begin{aligned} \tilde{g}_l(z, z') = {} & g_l(z, z_{k-1})(t-1)^2 (1+2t) + g_l(z, z_k)\, t^2(3-2t) \\ & + h_k \left[\frac{\partial g_l}{\partial z_{k-1}}(z, z_{k-1})\, t(t-1)^2 + \frac{\partial g_l}{\partial z_k}(z, z_k)\, t^2(t-1) \right] \end{aligned} \tag{35}$$

where

$$t = \frac{z - z_{k-1}}{z_k - z_{k-1}} = \frac{z - z_{k-1}}{h_k}. \tag{36}$$

The values of the weight factor $w_{kk'}^{(j)}$ are found by integration of (35) on the interval $[z_{k-1}, z_k]$.

Substituting these values into (34a) and (34b) and using the relations

$$\exp\{-\alpha(z_k - z_{k'})/\mu_l\} = \exp\{-\alpha h_k/\mu_l\} \exp\{-\alpha(z_{k-1} - z_{k'})/\mu_l\} \tag{37a}$$

$$\exp\{-\alpha(z_k - z_{k'})/\mu_l\} = \exp\{\alpha h_k/\mu_l\} \exp\{-\alpha(z_{k+1} - z_{k'})/\mu_l\} \tag{37b}$$

we get for the u_l's the following iterative relations:

$$u_l(z_k) = u_l(z_{k-1})\, e^{-\alpha h_k/\mu_l} + \frac{1}{2}\frac{h_k}{\mu_l}\left\{\left[s_l(z_{k-1})\left(1+\frac{1}{6}\frac{h_k}{\mu_l}\alpha\right)+\frac{h_k}{6}s_l'(z_{k-l})\right] e^{-\alpha h_k/\mu_l}\right.$$

$$\left. + s_l(z^k)\left(1-\frac{1}{6}\frac{h_k}{\mu_l}\alpha\right)-\frac{h_k}{6}s_l'(z_k)\right\}, \qquad l\in\{n_1\}^+ \tag{38a}$$

$$u_l(z_k) = u_l(z_{k+1})\, e^{\alpha h_{k+1}/\mu_l} - \frac{1}{2}\frac{h_{k+1}}{\mu_l}\left\{\left[s_l(z_{k+1})\left(1-\frac{1}{6}\frac{h_{k+1}}{\mu_l}\alpha\right)-\frac{h_{k+1}}{6}s_l'(z_{k+1})\right]\right.$$

$$\left.\times e^{\alpha h_k/\mu_l} + s_l(z_k)\left(1+\frac{1}{6}\frac{h_k}{\mu_l}\alpha\right)+\frac{h_k}{6}s_l'(z_k)\right\} \tag{38b}$$

(s' denotes ds/dz). The boundary conditions are

$$u_l(z_0) = 0, \qquad l\in\{n_1\}^+ \tag{39a}$$

$$u_l(z_p) = 0, \qquad l\in\{n_1\}^-. \tag{39b}$$

Clearly this method is consistent with the differential equation and stable for $\alpha > 0$. Its order, defined as local truncation error, is given by integrating the local interpolation error. This is, in the case of a constant stepsize h, $O(h^5)$.

8. Computer Implementation

Based on the formulation presented in the preceding paragraphs, a FORTRAN program has been written and implemented on a PDP 11/44 computer.

This program is able to compute the secondary flux produced by a mono-directional, mono-chromatic source, as well as produced by a mono-chromatic source with a broad angular spectrum. The parameters governing the convergence are input to the program.

From preliminary tests it was found that in our case $n = 9$ gave satisfactory results, and is used in most calculations.

In a first version the approximation of the convolution integral (see Section 6) was performed by means of linear interpolations and in a second version by means of the cubic Hermite interpolation; the two versions have a step size which is constant on the interval $[o, a]$. Calculations showed that in the case of Hermite interpolation a step size of 5 to 7 times the step size of the linear approximation was enough to obtain the same accuracy.

The wavelength increment used in calculating the scattering integral is also taken as a constant in such a way that the wavelength interval in Compton units $[0, 2]$ is divided into an integer number of subintervals, so taking advantage that $F(\lambda_j, \lambda_i)$ equals zero when $\lambda_j - \lambda_i > 2$. An increment value less than 0.1 Compton units does not give a significant improvement, while for integrated quantities as build-up factors and depth-doses an increment of 0.2 Compton units gave results which agree within 3% with the value obtained with an increment value of 0.1.

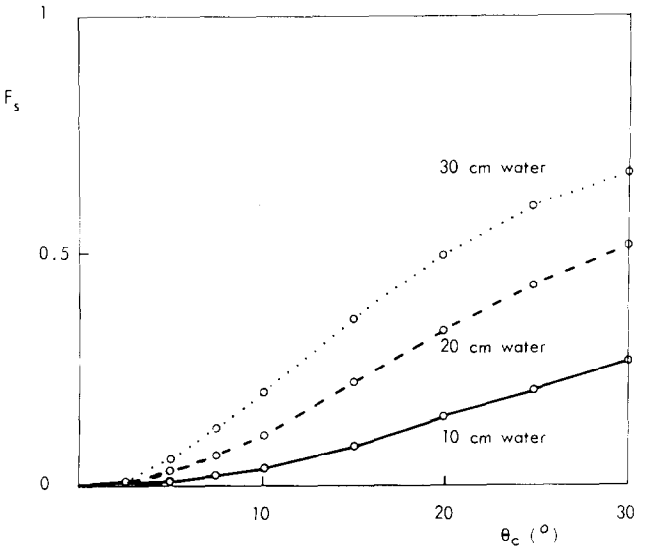

FIG. 4. Contribution of the scattered photons to the detector signal as function of the half collimator aperture θ_c. F_s is the ratio of the energy delivered by the secondary photons to the total detected energy. A mono-chromatic source of 100 keV is considered incident on a water medium with thickness 10, 20, and 30 cm.

The necessary maximal wavelength λ_m, for use in the computations, depends on the type of material, the material thickness, and also on the quantities to be computed from the angular fluxes: build-up factor, spectra, depth-doses, etc.

The program has been mainly used to study the influence of collimation on the amount of detected scattered radiation from the irradiated medium. Figure 4 gives some examples of the results. $F_s(\theta_c)$ is defined as the ratio of the detected scatter to the total intensity for a half-aperture angle θ_c,

$$F_s(\theta_c) = \frac{\bar{I}_s(\theta_c)}{\bar{I}_p(\theta_c) + \bar{I}_s(\theta_c)} \tag{40}$$

where $\bar{I}_s(\theta_c)$ and $\bar{I}_p(\theta_c)$ are given by the following simplified model of detection:

$$\bar{I}_{s,p}(\theta_c) = \int_0^{E_0} 2\pi \int_0^{\theta_c} EI_{s,p}(a, \theta, E) \sin\theta \, d\theta \, dE. \tag{41}$$

a is the thickness of the medium between the source and the detector and E_0 is the initial energy corresponding to λ_0. For these calculations, the step size in the z-direction was equal to 1 cm, which is about 0.17 mean-free-path of the initial energy. λ_m was equal to $\lambda_0 + 10$ and the wavelength increment equal to 0.1 Compton unit.

Figure 5 shows results of calculations in comparison to phantom measurements for the purpose of radiotherapy. The correction taking beam divergence into account

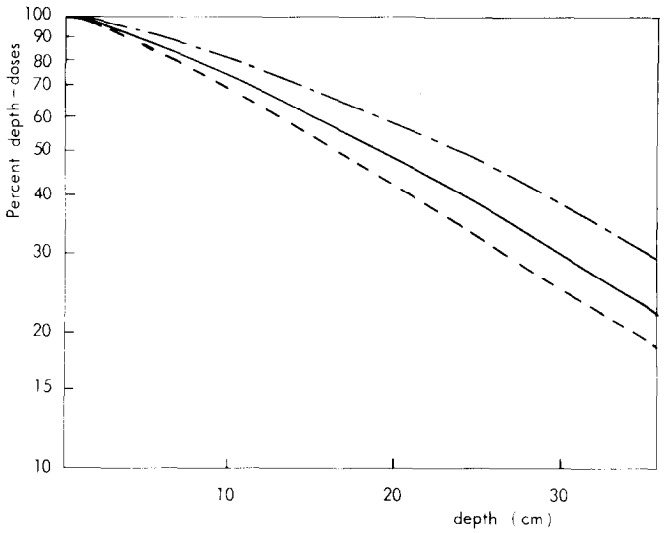

FIG. 5. Comparison between computed and measured doses in water for a Cobalt source ($E \sim 1.25$ MeV). (– · –) Calculation for an infinite parallel beam. (——) Calculation for an infinite beam with correction for divergence (see text). (– – –) Measured 50×50-cm^2 beam, with a source to surface distance of 150 cm.

consists of multiplying the primary flux of the mono-chromatic, mono-directional source by the factor $z^2/(b+z)^2$, i.e.,

$$I_p(z, \mu, \lambda) = \left(\frac{z}{b+z}\right)^2 \delta(\mu - 1)\, \delta(\lambda - \lambda_0)\, e^{-\sigma(\lambda_0) z} \tag{42}$$

where b is the source to water surface distance. These calculations were made for a thickness of 40 cm water and with a step size of 1 cm, which is about 0.06 mean-free-path of the initial energy. λ_m was equal to $\lambda_0 + 12$ and the wavelength increment equal to 0.1 Compton units. The difference between the measurements and the calculation is due to the imperfection of the divergence correction and to the finite field defined by the radiotherapy treatment unit.

9. CONCLUSION

The P_n-method in case of a slab geometry with azimuthal symmetry has primarily to be interpreted as a polynomial approximation relative to the angular variable μ. The first $n+1$ Legendre polynomials form a suitable basis to approximate the scattering operator, but it is useful to change it for the basis formed by the Lagrange polynomials defined by the zeros of P_{n+1}.

This change of basis and some considerations from the approximation theory show that the boundary conditions of Mark are well suited and well defined to the P_n-

method. Furthermore an interpretation of the approximation is obtained which can be used for practical calculation at the boundaries of the medium.

Another advantage of the new basis is that it gives a set of uncoupled differential equations, whose solutions are given by convolution products. To approximate these convolution products cubic Hermite interpolation is used.

Appendix A

Media as considered in medical physics consist of elements with atomic numbers up to 20 (calcium). For the media and in the energy range from a few keV up to 2 to 3 MeV the attenuation and scattering of photons traversing materials are described by three processes [9]: photo-electric effect, Compton-scattering (incoherent), and Raleigh-scattering (coherent).

Tables of cross sections for these processes are given in [10] and more recently for 0.1 KeV to 1 MeV in [11].

The photo-electric effect can be considered as pure absorption. Compton-scattering is a combination of scattering and energy dissipation, while Raleigh-scattering is pure coherent scattering. The differential cross section per electron for Compton-scattering, for the theoretical case of free electrons, is given by the Klein–Nishina relation [9]

$$\frac{d\sigma_c}{d\omega} = \frac{r_0^2}{2}\left(\frac{\lambda'}{\lambda}\right)\left(\frac{\lambda'}{\lambda} + \frac{\lambda}{\lambda'} + (\lambda - \lambda')(\lambda - \lambda' - 2)\right) \quad \frac{\text{cm}^2}{\text{electron}} \tag{A.1}$$

where λ', the wavelength of the incident photon, and λ, the wavelength of the scattered photon, fulfill the Compton-relation (Fig. 6)

$$\lambda - \lambda' = 1 - \cos\theta. \tag{A.2}$$

Since the electron cannot be considered as free, this differential cross section must be corrected for the binding energy of the electron to the nucleus. However, for energies

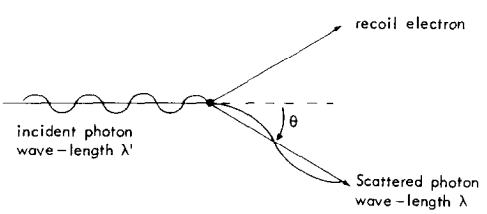

FIG. 6. Compton-scattering of a photon by an atomic electron.

above 50 keV this correction is largely compensated by Raleigh-scattering. In this case the differential cross section per centimeter is given by

$$f(\cos\theta,\ \lambda',\ \lambda) = n_e \frac{d\sigma_c}{d\omega}\,\delta(\cos\theta - 1 - \lambda' + \lambda) \tag{A.3}$$

where n_e is the electron density of the material.

Appendix B

The expansion of a δ-distribution [12] (usually called δ-function) will be discussed, because it is of practical importance to make the difference between distribution and function in the application of the P_n-method for the combination: mono-chromatic, mono-directional source, and Compton-scattering.

The $\mathscr{L}_2$-space in the case of a δ-distribution is meaningless and hence one must take care in expanding a δ-distribution in a series of Legendre polynomials. This problem is handled as follows: Let f be a function on $[-1, +1]$, x_0 a point of $[-1, +1]$, and define the operator $\mathscr{Q}$ as

$$\mathscr{Q}f = \int_{-1}^{+1} \delta(x - x_0)\, f(x)\, dx = f(x_0). \tag{B.1}$$

The formal expansion of $\delta(x - x_0)$ in a series of Legendre polynomials is given by

$$\delta(x - x_0) \sim \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(x_0)\, P_l(x). \tag{B.2}$$

Define now the operator $\mathscr{Q}^{(n)}$ replacing $\delta(x_0)$ by the partial sum

$$\sum_{l=0}^{n} \frac{2l+1}{2} P_l(x_0)\, P_l(x)$$

into Eq. (B.1):

$$\mathscr{Q}^{(n)}f = \sum_{l=0}^{n} \frac{2l+1}{2} \int_{-1}^{+1} P_l(x)\, f(x)\, dx\, P_l(x_0). \tag{B.3}$$

The right part of (B.3) is the partial sum of the expansion of $f(x)$ in a series of Legendre polynomials. Thus $\mathscr{Q}^{(n)}f$ will converge to $\mathscr{Q}f$ if and only if this expansion converges in the point x_0.

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