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# Technical Notes

## Collision Method in Spherical Geometry by Escape Probabilities

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ABSTRACT

*An integration method for the calculation of collision phenomena that overcomes the difficulties of the singularity of the kernel is applied in spherical geometry. Numerical results of a point source problem are given and compared with other methods.*

### INTRODUCTION

In Ref. 1 an integration method was presented that makes use, in collision problems, of the escape probabilities $P_f$ instead of the collision probabilities $P_c$. With this choice it is not necessary to calculate integrals over the function $P_c$ having the singularities of the kernel.

The function

$$N(r) = \int_0^r S(\rho)P_c^+(\rho,r)\,d\rho + \int_r^R S(\rho)P_c^-(\rho,r)\,d\rho \qquad (1)$$

can be calculated[1] by the expression

$$N(r) = N^+(r) + N^-(r) \quad , \qquad (2)$$

where

$$N^+(r) = S(r)\,P_f^+(r,r) - \frac{dj^+}{dr} \quad , \quad N^-(r) = S(r)\,P_f^-(r,r) + \frac{dj^-}{dr} \quad , \qquad (3)$$

$$j^+(r) = \int_0^r S(\rho)P_f^+(\rho,r)\,d\rho \quad , \quad j^-(r) = \int_r^R S(\rho)P_f^-(\rho,r)\,d\rho \quad , \qquad (4)$$

$$\frac{\partial P_f^+(\rho,r)}{\partial r} = -P_c^+(\rho,r) \quad , \quad \frac{\partial P_f^-(\rho,r)}{\partial r} = P_c^-(\rho,r) \quad . \qquad (5)$$

To apply the integration method conveniently it is necessary that the $P_f$ functions be easily calculated. In the following, the above method is applied in spherical geometry, and simple expressions for the corresponding escape probabilities are given.

### APPLICATION TO SPHERICAL GEOMETRY

Let us consider a homogeneous spherical system extended in the interval $(0,R)$. In this system let $S(\rho)$ be the function representing the source distribution per unit length. Let $P_c^+(\rho,r)dr$ $[P_c^-(\rho,r)dr]$ be the probability that a particle, born in a point $\rho < r$ $(\rho > r)$, suffers its next collision in the interval $(r, r + dr)$. Among all the particles coming from the system, let $N(r)dr$ be the number of particles that will suffer the next collision in the interval $(r, r + dr)$. Then the formal expression of $N(r)$ is

$$N(r) = N^+(r) + N^-(r) \quad , \qquad (6)$$

where

$$N^+(r) = \int_0^r S(\rho)P_c^+(\rho,r)\,d\rho \qquad (7)$$

$$N^-(r) = \int_r^R S(\rho)P_c^-(\rho,r)\,d\rho \quad . \qquad (8)$$

If the source is isotropic, the probability $P_c^+(\rho,r)$ for $\rho < r$ is given by the expression

$$P_c^+(\rho,r) = \frac{r}{2}\,\Sigma_t \int_0^\pi \frac{\sin\theta}{(r^2 - \rho^2\sin^2\theta)^{1/2}} \times \exp\{-\Sigma_t[\rho\cos\theta + (r^2 - \rho^2\sin^2\theta)^{1/2}]\}\,d\theta \quad , \qquad (9)$$

where $\Sigma_t$ is the total macroscopic cross section. The geometric clarification of $\theta$, $\rho$, and $r$ is shown in Fig. 1.

The probability $P_c^-(\rho,r)$ for $\rho > r$ is given by

$$P_c^-(\rho,r) = P_{c1}^-(\rho,r) + P_{c2}^-(\rho,r) \quad , \qquad (10)$$

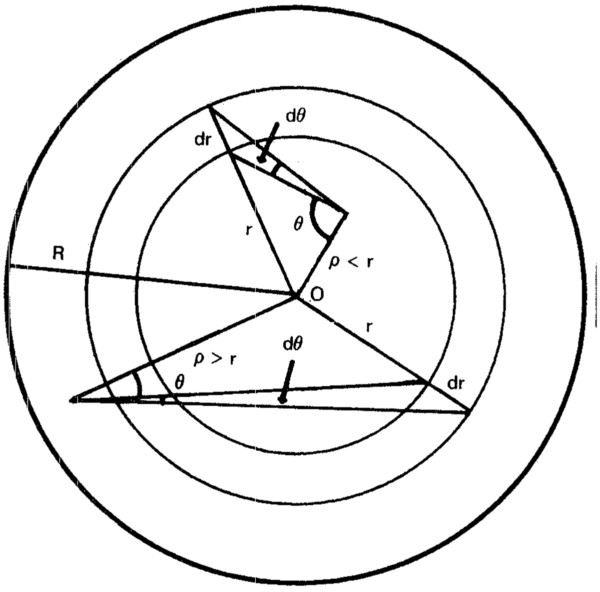


Fig. 1. Geometry for the formulation of the probabilities.

[1] G. BITELLI and A. TURRIN, *Nucl. Sci. Eng.*, **55**, 96 (1974).

where

$$P_{c1}^-(\rho,r) = \frac{r}{2}\Sigma_t \int_0^{\arcsin(r/\rho)} \frac{\sin\theta}{(r^2-\rho^2\sin^2\theta)^{1/2}} \times \exp\{-\Sigma_t[\rho\cos\theta - (r^2-\rho^2\sin^2\theta)^{1/2}]\}\,d\theta \quad (11)$$

$$P_{c2}^-(\rho,r) = \frac{r}{2}\Sigma_t \int_0^{\arcsin(r/\rho)} \frac{\sin\theta}{(r^2-\rho^2\sin^2\theta)^{1/2}} \times \exp\{-\Sigma_t[\rho\cos\theta + (r^2-\rho^2\sin^2\theta)^{1/2}]\}\,d\theta \;. \quad (12)$$

Let us consider the function $P_f^+$ and $P_f^-$ defined as follows:

$$P_f^+(\rho,r) = \int_0^\pi \frac{1}{2}\sin\theta\exp\{-\Sigma_t[\rho\cos\theta + (r^2-\rho^2\sin^2\theta)^{1/2}]\}\,d\theta \quad (13)$$

$$P_f^-(\rho,r) = P_{f1}^-(\rho,r) - P_{f2}^-(\rho,r) \;, \quad (14)$$

where

$$P_{f1}^-(\rho,r) = \int_0^{\arcsin(r/\rho)} \frac{1}{2}\sin\theta \times \exp\{-\Sigma_t[\rho\cos\theta - (r^2-\rho^2\sin^2\theta)^{1/2}]\}\,d\theta \quad (15)$$

$$P_{f2}^-(\rho,r) = \int_0^{\arcsin(r/\rho)} \frac{1}{2}\sin\theta \times \exp\{-\Sigma_t[\rho\cos\theta + (r^2-\rho^2\sin^2\theta)^{1/2}]\}\,d\theta \;. \quad (16)$$

The functions $P_f^+$ and $P_f^-$ represent escape probabilities. We can verify that the functions $P_c^+$, $P_c^-$, $P_f^+$, and $P_f^-$ satisfy Eqs. (5) and that the function $N(r)$ can be calculated by Eq. (2). Because $P_f^+(r,r) + P_f^-(r,r) = 1$, Eq. (2) becomes

$$N(r) = S(r) - \frac{d(j^+ - j^-)}{dr} \;, \quad (17)$$

where $j^+$ and $j^-$ are expressed by Eqs. (4).

The function $j^+$ represents the number of particles coming from the interval $(0,r)$ and passing through a sphere of radius $r$ without suffering collisions. Thus, either they have the next collision out of the above-mentioned sphere, or they escape from the system. The function $j^-$ represents the number of particles coming from the interval $(r,R)$ and suffering the next collision within the same sphere.

## ESCAPE PROBABILITIES IN TERMS OF EXPONENTIAL INTEGRALS

We can express the escape probabilities $P_f^+$ and $P_f^-$ in terms of the exponential integral function $E_2$. Substituting $x = \cos\theta$ into $P_f^+$, we obtain

$$2\,P_f^+ = \int_{-1}^{+1} \exp(-\Sigma_t s)\,dx \;, \quad (18)$$

where

$$s = \rho\left\{x + \left[\left(\frac{r}{\rho}\right)^2 - 1 + x^2\right]^{1/2}\right\} \quad (19)$$

for $(r/\rho) > 1$.

From Eq. (19) we get

$$dx = \left[\left(\frac{r}{\rho}\right)^2 - 1 + x^2\right]^{1/2}\frac{ds}{s} = \left(\frac{s}{\rho} - x\right)\frac{ds}{s}$$

and

$$x = \frac{1}{2}\frac{s}{\rho} - \frac{1}{2}\frac{\rho}{s}\left[\left(\frac{r}{\rho}\right)^2 - 1\right] \;.$$

Thus Eq. (18) becomes

$$2\,P_f^+ = \frac{1}{2}\int_{(r/\rho)-1}^{(r/\rho)+1} \exp(-\Sigma_t s)\,d\left(\frac{s}{\rho}\right) + \frac{1}{2}\left[\left(\frac{r}{\rho}\right)^2 - 1\right] \times \int_{(r/\rho)-1}^{(r/\rho)+1} \exp(-\Sigma_t s)\frac{d\left(\frac{s}{\rho}\right)}{\left(\frac{s}{\rho}\right)^2} \;. \quad (20)$$

Writing $\alpha_1 = \Sigma_t\rho$ and putting $\mu = s/\rho$, Eq. (20) above yields

$$2\,P_f^+ = \frac{1}{2}\int_{(r/\rho)-1}^{(r/\rho)+1} \exp(-\alpha_1\mu)\,d\mu + \frac{1}{2}\left[\left(\frac{r}{\rho}\right)^2 - 1\right] \times \int_{(r/\rho)-1}^{(r/\rho)+1} \exp(-\alpha_1\mu)\frac{d\mu}{\mu^2} \;. \quad (21)$$

To establish the second integral in Eq. (21) we write it as

$$\int_{(r/\rho)-1}^{(r/\rho)+1} \exp(-\alpha_1\mu)\frac{d\mu}{\mu^2} = \int_{(r/\rho)-1}^{\infty} \exp(-\alpha_1\mu)\frac{d\mu}{\mu^2} - \int_{(r/\rho)+1}^{\infty} \exp(-\alpha_1\mu)\frac{d\mu}{\mu^2}$$
$$= \frac{1}{\left(\frac{r}{\rho} - 1\right)}E_2\left[\alpha_1\left(\frac{r}{\rho} - 1\right)\right] - \frac{1}{\left(\frac{r}{\rho} + 1\right)}E_2\left[\alpha_1\left(\frac{r}{\rho} + 1\right)\right] \;,$$

where

$$E_n(z) = \int_1^\infty \frac{\exp(-zt)\,dt}{t^n}$$

is the $n$'th exponential integral function. Hence, if we put $\alpha_2 = \Sigma_t r$, we finally obtain

$$P_f^+ = \frac{1}{4\alpha_1}[\exp(\alpha_1 - \alpha_2) - \exp(-\alpha_1 - \alpha_2) + (\alpha_2 + \alpha_1)E_2(\alpha_2 - \alpha_1) - (\alpha_2 - \alpha_1)E_2(\alpha_2 + \alpha_1)] \;, \quad (22)$$

provided $\alpha_1 < \alpha_2$.

By a procedure similar to that above, the following results can be established:

$$P_{f1}^- = \frac{1}{4\alpha_1}\{\exp[-(\alpha_1^2 - \alpha_2^2)^{1/2}] - \exp(\alpha_2 - \alpha_1) - (\alpha_1^2 - \alpha_2^2)^{1/2} \times E_2(\alpha_1^2 - \alpha_2^2)^{1/2} + (\alpha_1 + \alpha_2)E_2(\alpha_1 - \alpha_2)\} \quad (23)$$

and

$$P_{f2}^- = \frac{1}{4\alpha_1}\{\exp[-(\alpha_1^2 - \alpha_2^2)^{1/2}] - \exp(-\alpha_1 - \alpha_2) - (\alpha_1^2 - \alpha_2^2)^{1/2} \times E_2(\alpha_1^2 - \alpha_2^2)^{1/2} + (\alpha_1 - \alpha_2)E_2(\alpha_1 + \alpha_2)\} \;, \quad (24)$$

provided $\alpha_1 > \alpha_2$. By substituting Eqs. (23) and (24) in Eq. (14), one gets

$$P_f^- = \frac{1}{4\alpha_1}[\exp(-\alpha_1 - \alpha_2) - \exp(\alpha_2 - \alpha_1) + (\alpha_1 + \alpha_2)E_2(\alpha_1 - \alpha_2) - (\alpha_1 - \alpha_2)E_2(\alpha_1 + \alpha_2)] \;. \quad (25)$$

## MULTIGROUP FORMULATION AND FLUXES OF A NEUTRON POINT SOURCE

Given the source $S_m^g(\rho)$ in the energy group $g$ of the $m$'th collision, the source of the $(m+1)$'th collision can be derived by the following expressions:

$$N^g_{(m+1)} = S^g_m - \frac{dj_m}{dr} \tag{26}$$

$$S^g_{(m+1)} = \sum_{k=1}^{G} \frac{\Sigma^{k\to g}}{\Sigma^k_t} N^k_{(m+1)} \quad , \tag{27}$$

where $\Sigma^{k\to g}/\Sigma^k_t$ is the number of particles that arise in energy group $g$ after the collision of one particle of energy $k$, and where $G$ is the number of energy groups.

The fluxes related to the sources of the $m$'th collision are given by

$$\Phi^g_m = \frac{N^g_{(m+1)}}{4\pi r^2 \Sigma^g_t} \quad . \tag{28}$$

In the above equations, the variable $r$ does not appear for the sake of simplicity.

As shown in Ref. 2, the solution of the Boltzmann equation with sources is given by

$$\Phi^g(r) = \Phi^g_0(r) + \Phi^g_1(r) + \ldots + \Phi^g_m(r) + \Phi^g_R(r) \quad ,$$

where $\Phi^g_0(r)$, $\Phi^g_1(r)$ ... $\Phi^g_m(r)$ are the fluxes of zeroth, first, ... $n$'th collision, and $\Phi^g_R(r)$ is a residual quantity.

It is possible to solve the problem by stopping the calculation at a collision such that $\Phi^g_R < \epsilon$, where $\epsilon$ is an arbitrarily small quantity. Otherwise, the residual flux $\Phi^g_R$ can be evaluated by other conventional methods such as diffusion and transport. If the initial source $S^g_0$ is a point source located at the center of the sphere, the expression for $N^g_1(r)$ is merely given by

$$N^g_1(r) = S^g_0 \, \Sigma^g_t \exp(-\Sigma^g_t r) \quad .$$

The first collision sources $S^g_1(r)$ and the zero collision fluxes $\Phi^g_0(r)$ can be calculated by Eqs. (27) and (28). To evaluate the quantities related to the successive collisions, we adopt the above-described collision method.

The energy group constants used in the calculations of a point source problem are reported in Table I. In Table II we give the results performed by the transport method ($S_8$ approximation) and by the present one. Collision calculations, performed by changing to some extent the number of mesh intervals, have given practically the same results.

In the transport calculation the system (radius = 20 cm) was subdivided in 80 mesh intervals with the source localized in the first mesh interval. Several authors (see, for example, Ref. 2) have stated that numerical errors are involved in transport calculations of point source problems. These errors arise in the point-by-point balances close to the source. However, we think that an adequate and high number of mesh intervals and angular subdivisions, introduced in the transport calculation, could give numerical results closer to those obtained in the present collision method.

The computer time required to obtain the results of the present method (64 mesh intervals and 49 collisions) is 16.90 sec on an IBM 370/165. The $P_f$ probabilities were calculated only at the beginning and were stored for all the iterations, and the time spent for it is small. Thus, an order of magnitude of calculation times for other cases can be deduced taking in account the fact that these times are approximately proportional to the number of energy groups, to the iteration number, and to the square of the mesh points number.

TABLE I

Macroscopic Cross Sections for the Point Source Problem

| Energy Group | $\Sigma_{total}$ ($cm^{-1}$) | $k \to k$ $\Sigma_{scattering}$ ($cm^{-1}$) | $k \to k+1$ $\Sigma_{scattering}$ ($cm^{-1}$) | Source (n/sec) |
|---|---|---|---|---|
| 1 | 0.23 | 0.119 | 0.0705 | 11.5 |
| 2 | 0.29 | 0.251 | --- | 6.52 |

TABLE II

Group Flux Ratios

| Radius (cm) | $\frac{\Phi^2(r)}{\Phi^1(r)}$ [a] | $\frac{\Phi^2(r)}{\Phi^1(r)}$ [b] |
|---|---|---|
| 1 | 0.935 | 0.981 |
| 2 | 1.323 | 1.355 |
| 3 | 1.719 | 1.714 |
| 4 | 2.121 | 2.099 |
| 5 | 2.530 | 2.494 |
| 6 | 2.950 | 2.897 |
| 7 | 3.382 | 3.309 |
| 8 | 3.828 | 3.730 |
| 9 | 4.286 | 4.161 |
| 10 | 4.757 | 4.601 |
| 11 | 5.235 | 5.047 |
| 12 | 5.724 | 5.496 |
| 13 | 6.211 | 5.940 |
| 14 | 6.688 | 6.372 |
| 15 | 7.138 | 6.775 |
| 16 | 7.537 | 7.126 |
| 17 | 7.847 | 7.390 |
| 18 | 8.005 | 7.508 |
| 19 | 7.880 | 7.348 |

[a]Point source problem: $S_N$ method with $N = 8$.
[b]Point source problem: collision method by escape probabilities ($m = 49$).

[2]E. E. PETROV and L. N. USACHEV, in *Theory and Methods of Nuclear Reactor Calculation*, p. 42, G. I. MARCHUK, Ed., Consultant Bureau, New York (1964).