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PADÉ APPROXIMANT CALCULATIONS FOR NEUTRON ESCAPE PROBABILITY \*

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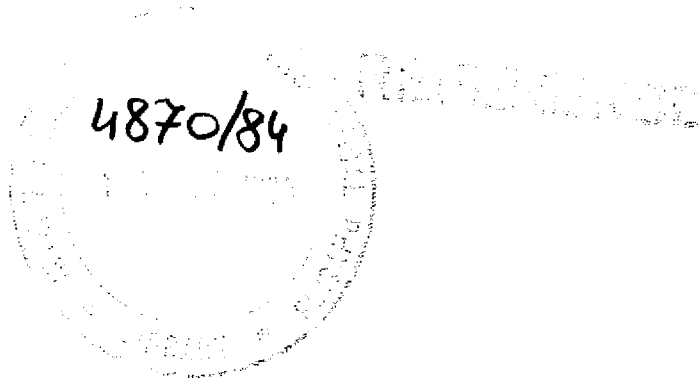
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ABSTRACT

The neutron escape probability from a non-multiplying slab containing internal source is defined in terms of a functional relation for the scattering function for the diffuse reflection problem. The Padé approximant technique is used to get numerical results which compare with exact results.

1. INTRODUCTION

Many physical quantities can be put in the functional form  $\langle S^+, \psi \rangle$  where  $\psi$  is the solution of the functional

$$\psi = S + \lambda K \psi,$$

where  $\psi$  and  $S$  are elements of a Hilbert space  $\mathcal{X}$ , and  $K = \mathcal{X} \rightarrow \mathcal{X}$  is a non-negative, but not necessarily hermitian operator. It has been shown that  $\langle S^+, \psi \rangle$  is an  $[N-1/N]$  Padé approximant (Baker 1975, 1981; El Wakil et al, 1979). Problems of this kind arise in particle transport theory, radiative transfer and rarified gas dynamics. One of the most interesting functionals to the first field is the wescape probability.

In this work a method is proposed to express the flux emerging from an inhomogeneous (homogeneous) media in terms of the emergent flux of the diffuse problem. The relation between the two problems is given and hence the escape probability can be defined in terms of the source function of the diffuse problem. The escape probability in this way is defined for arbitrary internal source. Numerical results are given for  $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$  Padé approximant and uniform isotropic source, which are compared with Pomraning and Badham results (1984).

2. BASIC EQUATIONS

Consider the particle transfer equation in a non-multiplying slab  $0 \leq x \leq a$  with internal source

$$\mu \frac{\partial}{\partial x} I(x, \mu) + I(x, \mu) = \frac{1}{2} \lambda(x) \int_{-1}^1 I(x, \mu') d\mu' + [1 - \lambda(x)] g(x) \quad (1)$$

subject to the boundary conditions

$$I(0, \mu) = 0, \quad \mu > 0 \quad (2)$$

$$I(a, \mu) = 0, \quad \mu > 0 \quad (3)$$

The integral equation for the source function

$$S(x) = \frac{1}{2} \lambda(x) \int_0^1 I(x, \mu') d\mu' + [1 - \lambda(x)] g(x) \quad (4)$$

is

$$S(x) = \frac{1}{2} \lambda(x) \int_0^a E_1(1-x-t) S(t) dt + [1 - \lambda(x)] g(x) \quad (5)$$

If the source function  $S(x)$  is found, the intensity emerging from

$$I(0, -\mu) = \int_0^a S(x) e^{-x/\mu} \frac{dx}{\mu}, \quad \mu > 0 \quad (6)$$

and

$$I(a, \mu) = \int_0^a S(x) e^{-(a-x)/\mu} \frac{dx}{\mu} \quad (7)$$

The escape probability is defined in terms of the emerging flux by

$$P = \frac{H(0) + H(a)}{2\pi \int_0^a (1-\lambda) g(x) dx} \quad (8)$$

where

$$H(0) = 2\pi \int_0^1 I(0, -\mu) \mu d\mu \quad (9)$$

and

$$H(a) = 2\pi \int_0^1 I(a, \mu) \mu d\mu \quad (10)$$

and by Eqs.(6) and (7)

$$H(0) = 2\pi \int_0^a S(x) E_2(x) dx \quad (11)$$

and

$$H(a) = 2\pi \int_0^a S(x) E_2(a-x) dx \quad (12)$$

Let us now try to find the relation between the emerging flux in the above problem and the diffused problem defined as

$$\mu \frac{\partial}{\partial x} \varphi(x, \mu) + \varphi(x, \mu) = \frac{1}{2} \lambda(x) \int_0^1 \varphi(x, \mu') d\mu' \quad (13)$$

Subject to the boundary conditions

$$\varphi(0, \mu) = 1 \quad (14)$$

$$\varphi(a, \mu) = 0 \quad (15)$$

In this case the source function  $\tilde{S}(x)$  is given by

$$\tilde{S}(x) = \frac{1}{2} \lambda(x) \int_0^1 \varphi(x, \mu') d\mu' = \frac{1}{2} \lambda(x) \theta(x) \quad (16)$$

which satisfies the equation

$$\tilde{S}(x) = \frac{1}{2} \lambda(x) \int_0^a E_1(1-x-t) \tilde{S}(t) dt + \frac{1}{2} \lambda(x) E_2(x) \quad (17)$$

The intensity of radiation emerging from the medium is given by

$$\varphi(0, -\mu) = \frac{e^{-a/\mu}}{\mu} + \int_0^a \tilde{S}(x) \frac{e^{-x/\mu}}{\mu} dx \quad (18)$$

and

$$\varphi(a, \mu) = \int_0^a \tilde{S}(x) \frac{e^{-(a-x)/\mu}}{\mu} dx \quad (19)$$

Multiplying Eq.(17) by  $\frac{S(x)}{\lambda(x)}$  using Eq.(5) one gets

$$H(0) = 4\pi \int_0^a \frac{\tilde{S}(x) [1 - \lambda(x)] g(x)}{\lambda(x)} dx \quad (20)$$

and

$$H(a) = 4\pi \int_0^a \frac{\tilde{S}(x) [1 - \lambda(x)] g(x)}{\lambda(x)} dx \quad (21)$$

Then the escape probability can now be written in terms of the source function of the diffused problem and the internal source as

$$P = \left[ \int_0^a \tilde{S}(x) [g(x) + g(a-x)] \frac{1 - \lambda(x)}{\lambda(x)} dx \right] \left[ \int_0^a g(x) [1 - \lambda(x)] dx \right]^{-1} \quad (22)$$

If we assume the internal source has the form

$$g(x) = 1 + \beta_1 x + \beta_2 x^2 + \dots + \beta_n x^n \quad (23)$$

then

$$H(0) = 2\pi [A_0 + \beta_1 A_1 + \beta_2 A_2 + \dots + \beta_n A_n] \quad (24)$$

and

$$H(a) = 2\pi [D_0 + \beta_1 D_1 + \beta_2 D_2 + \dots + \beta_n D_n] \quad (25)$$

where

$$A_n = \int_0^a \frac{\tilde{S}(x) [1 - \lambda(x)] x^n}{\lambda(x)} dx \quad (26)$$

and

$$D_n = \int_0^a \frac{\tilde{S}(x) [1 - \lambda(x)] (a-x)^n}{\lambda(x)} dx$$

$$= a^n A_0 - \binom{n}{1} a^{n-1} A_1 + \binom{n}{2} a^{n-2} A_2 + \dots + (-1)^n A_n \quad (27)$$

Hence the escape probability is completely defined in terms of the source function for diffuse problem and for polynomial internal source.

### 3. PARTICULAR CASE

Let us assume that  $g(x)$  is a uniformly isotropic source, i.e.  $g(x) = 1$ , hence

$$\frac{H(a)}{2\pi} = \frac{H(0)}{2\pi} = A_0 = 2 \int_0^a \theta(x) [1 - \lambda(x)] dx \quad (28)$$

where  $\theta(x)$  satisfies

$$\theta(x) = E_2(x) + \frac{1}{2} \int_0^a E_1(|x-t|) \lambda(t) \theta(t) dt \quad (29)$$

Integrating Eq.(11) over  $\mu \in [-1, 1]$  and  $\tau \in [0, a]$  one gets

$$2 \int_0^a [1 - \lambda] \theta(x) dx = 1 - 2 \int_0^1 \Phi(0, -\mu) \mu d\mu - 2 \int_0^1 \Phi(a, \mu) \mu d\mu$$

$$= 1 - R_d - T_d \quad (30)$$

where  $R_d$  and  $T_d$  are the diffuse reflection and transmission coefficients for the medium. Therefore

$$P = \frac{2(1 - R_d - T_d)}{\int_0^a [1 - \lambda(x)] dx} = \frac{2A_0}{\int_0^a [1 - \lambda(x)] dx} \quad (31)$$

In the next section we shall calculate the escape probability for constant internal source, and constant single albedo by the Padé approximant technique.

### 4. NUMERICAL CALCULATIONS AND RESULTS

For constant internal source and constant single scattering albedo Eqs.(28) and (29) become

$$A_0 = 2(1 - \lambda) \langle 1, \theta \rangle \quad (32)$$

$$\theta = E_2(x) + \frac{1}{2} \lambda \int_0^a E_1(|x-t|) \theta(t) dt \quad (33)$$

and

$$p = \frac{q}{2} \langle 1, \theta \rangle \quad (34)$$

where  $\langle 1, \theta \rangle$  can be calculated by the Padé approximant technique as follows. Rewrite Eq.(33) as

$$(1 - \frac{1}{2} \lambda k) \theta = E_2(x). \quad (35)$$

Operating by  $(1 - \frac{1}{2} \lambda k)^{-1}$  on both sides, hence

$$\theta(x) = (1 - \frac{1}{2} \lambda k)^{-1} E_2(x) \quad (36)$$

If we consider the Neumann series associated with Eq.(36), namely

$$\theta(x) = E_2(x) + \frac{1}{2} \lambda k E_2(x) + (\frac{1}{2} \lambda k)^2 E_2(x) + \dots \quad (37)$$

and take the inner product given by (37) with 1, we obtain a formal power series

$$h(\lambda) = \langle 1, \theta \rangle = \omega_0 + \frac{1}{2} \lambda \omega_1 + (\frac{1}{2} \lambda)^2 \omega_2 + \dots \quad (38)$$

where

$$\omega_n = \langle 1, K^n E_1(x) \rangle \quad (39)$$

This power series is proven to be equivalent to  $[N-1/N]$  Padé approximant (Baker 1975, 1981). For  $[\frac{0}{1}]$  Padé approximant, we have

$$\omega_0 = \int_0^a E_2(x) dx = \frac{1}{2} - E_3(a) \quad (40)$$

and

$$\begin{aligned} \omega_1 &= \int_0^a dx \int_0^a E_1(x-t) E_2(t) dt \\ &= 2\omega_0 - G_{22}(a) - G'_{22}(a) \end{aligned} \quad (41)$$

where  $G_{22}(a)$  and  $G'_{22}(a)$  are defined by

$$G_{nm}(a) = \int_0^a E_n(x) E_m(x) dx \quad (42)$$

and

$$G'_{nm}(a) = \int_0^a E_n(x) E_m(a-x) dx \quad (43)$$

and are tabulated by Chandrasekhar (1948) and Van de Hulst (1948). Numerical results are given in Table I and compared with Pomraning and Badham results (1984).

## 5. CONCLUSION

The particle escape probability is defined in terms of a functional relation for the scattering function for diffuse problem. This permits to calculate the escape probability in terms of any arbitrary internal source and for homogeneous and inhomogeneous medium. The calculations for  $[\frac{0}{1}]$  Padé approximant and uniform source gives quite good agreement. However for a large value of  $\lambda$  and  $a$ , it is necessary for best convergence to the exact result to consider higher order Padé approximant.

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REFERENCES

Baker, G.W. Jr. 1975, J. Math. Phys. 16, 813; 1981, Encyclopedia of Mathematics and its Applications, Vol.14 (Addison-Wesley, Mass.).

Chandrasekhar, S. 1948, Astrophys. J. 108, 92.

El Wakil, S.A., El Batanoni, F. and Saad, E.A. 1979, J. Phys. D 12, 1633.

Pomraning, G.C. and Badham, V.C. 1984, Nucl. Sci. Enging. 86, 63.

Van e Hulst, H.C. 1948, Astrophys. J. 107, 220.

Table I

Escape probability

$\lambda$	0.3		0.5		0.7		0.9	
	$\left(\frac{0}{1}\right)$	Exact	$\left(\frac{0}{1}\right)$	Exact	$\left(\frac{0}{1}\right)$	Exact	$\left(\frac{0}{1}\right)$	Exact
0.5	.6416	.6417	.7141	.7146	.8051	.8068	.9226	.9260
1.0	.4726	.4764	.5572	.5590	.6722	.6780	.8470	.8620
1.5	.3714	.3724	.4480	.4517	.5646	.5764	.7631	.8013
2.0	.3007	.3016	.3697	.3739	.4798	.4953	.6833	.7430
5.0	.1310	.1318	.1654	.1690	.2242	.2437	.3482	.4702

