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MULTIGROUP DIFFUSION THEORY FORMULATION OF THE CALCULATION OF THE MEAN SQUARE SLOWING DOWN DISTANCE IN AN INFINITE MEDIUM

by

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ABSTRACT

Simple expressions for the mean square distance from a point fission source for slowing down past a given energy and for the mean square distance of neutrons that belong to a given energy group are derived within the framework of multigroup diffusion theory. The expressions may be applied to systems having arbitrary group transfer cross sections.

I. INTRODUCTION

Multigroup diffusion theory is one of the commonly used approximations to the exact transport theory. In particular, for complicated, reflected reactors having hydrogenous constituents, the multigroup approach is a feasible one (particularly with the aid of modern digital computers), whereas, for example, continuous slowing down theory is not applicable. The main difficulty encountered in utilizing the multigroup diffusion theory is that of the selection of the proper group parameters (cross sections). Owing to inadequacies in the basic experimental information about cross sections as well as, for example, averaging techniques used, any multigroup set of cross sections is necessarily uncertain to a greater or lesser extent. It is desirable therefore as a check to use the derived cross sections to calculate certain macroscopic quantities which are measurable experimentally.

One such quantity is the mean square distance for slowing down of fast neutrons. For the case of a point source of fast neutrons, one-sixth of this quantity is sometimes known as the "age" of the neutrons. Owing to the relationship of the "age" to the fast leakage from the system, it is important to compare the result calculated using the assumed multigroup cross sections with the experimentally measured quantity.

The present paper describes the calculation of the mean square slowing down distance for the case of multigroup diffusion theory with arbitrary group transfer cross sections.

II. THEORY

Let $P_\infty(E, \underline{r}, \underline{r}')$ be the infinite medium, point fission source kernel which gives the slowing down density at energy E and position $\underline{r}$ due to a unit point fission source at position $\underline{r}'$. Then for a distributed fission source $S(\underline{r}')$, the slowing down density $Q_E(\underline{r})$ at energy E and position $\underline{r}$ is given by

$$Q_E(\underline{r}) = \int_{\underline{r}'} S(\underline{r}')\, P_\infty(E, \underline{r}, \underline{r}')\, d\,\underline{r}' \quad . \tag{1}$$

We shall consider an infinite medium which is homogeneous and isotropic. In this case, $P_\infty(E, \underline{r}, \underline{r}')$ will depend spatially only upon the separation $|\underline{r} - \underline{r}'| = r$. In addition, if the source satisfies the wave equation

$$\nabla^2 S(\underline{r}) + B^2 S(\underline{r}) = 0 \quad , \tag{2}$$

one can show (Ref. 1) that

$$Q_E(\underline{r}) = S(\underline{r})\, \overline{P}_\infty(E, B^2) \quad , \tag{3}$$

where $\overline{P}_\infty(E, B^2)$ is the three-dimensional Fourier transform of $P_\infty(E, r)$. Denoting the ratio of slowing down density $Q_E(\underline{r})$ to source $S(\underline{r})$ by $q_E(B^2)$,

$$q_E(B^2) \equiv \overline{P}_\infty(E, B^2) = q_E(0)\left[1 - \frac{1}{6} B^2\, \overline{r^2_E} + O\cdot B^4 - \ldots\right] \quad . \tag{4}$$

The quantity $\overline{r^2_E}$ is the mean square distance from a point source for slowing down past energy E.[1*]

Alternatively, let $K_\infty(E, r)$ be the infinite medium point fission source kernel which gives the flux of neutrons per unit energy at energy E and position $\underline{r}$ due to a unit point fission source at position $\underline{r}'$ (where again $r = |\underline{r} - \underline{r}'|$). Then, denoting the ratio of flux $\Phi(E, \underline{r})$ to source $S(\underline{r})$ by $\phi(E, B^2)$, where again $S(\underline{r})$ satisfies Eq. (2), one can write (Ref. 2)

$$\phi(E, B^2) \equiv \overline{K}_\infty(E, B^2) = \phi(E,0)\left[1 - \frac{1}{6} B^2\, \overline{r^2}(E) + O\cdot B^4 - \ldots\right] \quad . \tag{5}$$

The quantity $\overline{r^2}(E)$ is the mean square distance from a point source of neutrons which have the energy E.[2] Also $\overline{r^2}(E)$ will be larger than $\overline{r^2_E}$.[3]

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*See end of paper for footnotes.

In the limit of vanishingly small B^2, Eq. (4) may be written as

$$\frac{\overline{r^2_E}}{6} = \lim_{B^2 \to 0} \frac{1}{B^2} \left[1 - \frac{q_E (B^2)}{q_E (0)} \right] \quad . \tag{6}$$

Similarly, Eq. (5) may be written

$$\frac{\overline{r^2} (E)}{6} = \lim_{B^2 \to 0} \frac{1}{B^2} \left[1 - \frac{\phi(E, B^2)}{\phi(E, 0)} \right] \quad . \tag{7}$$

Equations (6) and (7) may be used to evaluate neutron "age" by obtaining $q_E(B^2)$ or $\phi(E, B^2)$ for various B^2 and extrapolating (perhaps graphically) to the case of $B^2 = 0$. The difficulty with such a procedure is that as B^2 approaches zero, it is difficult to retain enough significant figures so that round-off errors do not impair the accuracy of the calculation.

In the present paper, Eqs. (6) and (7) are evaluated in closed form using multigroup diffusion theory so that the limiting process is replaced by a single analytic expression which can easily be evaluated on a desk calculator.

We shall assume that the multigroup diffusion theory equation for the group i flux, $\Phi_i (\underline{r})$, due to the fission source $S(\underline{r})$ can be written[4] as

$$D_i \nabla^2 \Phi_i(\underline{r}) - (\Sigma_{c_i} + \Sigma_{rem_i}) \Phi_i(\underline{r}) + \sum_{\lambda=1}^{i-1} \Sigma_{\lambda \to i} \Phi_\lambda(\underline{r}) + \beta_i S(\underline{r}) = 0 \quad . \tag{8}$$

In Eq. (8) and subsequently, the index on the flux and on the various cross sections refers to an energy group of finite width, the group cross sections being appropriately averaged values. Thus if the group i has the energy limits E_{iL} and E_{iH},

$$\Phi_i (\underline{r}) = \int_{E_{iL}}^{E_{iH}} \Phi(E, \underline{r}) \, dE \quad . \tag{9}$$

Similarly, the β_i give the integral of the fission spectrum over the group i (the sum of all the β_i is normalized to unity). The removal cross section, Σ_{rem_i}, is given explicitly by

$$\Sigma_{rem_i} = \sum_{\lambda=1}^{N-i} \Sigma_{i \to i + \lambda} \quad , \tag{10}$$

where N is the number of groups. The Σ_{c_i} will include the fission cross section if the medium contains fissionable material.

The fundamental mode solution[5] of Eq. (8) is given by the group fluxes ϕ_i, where

$$\phi_i(B^2) = \frac{\beta_i + \sum_{\lambda=1}^{i-1} \Sigma_{\lambda \to i} \, \phi_\lambda(B^2)}{D_i B^2 + \Sigma_{c_i} + \Sigma_{rem_i}} \quad . \tag{11}$$

III. MEAN SQUARE DISTANCE OF NEUTRONS SLOWING DOWN PAST ENERGY E_{jL}

In the framework of the multigroup formalism stated above, we have for the slowing down density at the lower energy limit E_{jL} of group j[6]

$$q_{jL}(B^2) = \sum_{i=1}^{j} \left[\beta_i - \Sigma_{c_i} \phi_i(B^2) - D_i B^2 \phi_i(B^2) \right] \quad . \tag{12}$$

Equation (12) is not surprising, since the neutrons slowing down past energy E_{jL} must be just all of the originating source neutrons less those which are captured and leak out for all energies above E_{jL}.

For the case $B^2 = 0$, Eq. (12) reduces to

$$q_{jL}(0) = \sum_{i=1}^{j} \left[\beta_i - \Sigma_{c_i} \phi_i(0) \right] \quad . \tag{13}$$

Equations (12) and (13) can be substituted into Eq. (6). The result is

$$\frac{\overline{r^2_{jL}}}{6} = \lim_{B^2 \to 0} \frac{\sum_{i=1}^{j} \left[D_i \phi_i(B^2) + \Sigma_{c_i} \dfrac{\phi_i(B^2) - \phi_i(0)}{B^2} \right]}{\sum_{i=1}^{j} \left[\beta_i - \Sigma_{c_i} \phi_i(0) \right]} \quad .$$

From the definition of the derivative (or by using L' Hôpital's rule) we have finally

$$\frac{\overline{r^2_{jL}}}{6} = \frac{\sum_{i=1}^{j} \left[D_i \ \phi_i(0) + \Sigma_{c_i} \ \phi_i'(0) \right]}{\sum_{i=1}^{j} \left[\beta_i - \Sigma_{c_i} \ \phi_i(0) \right]} \quad , \tag{14}$$

where

$$\phi_i'(0) \equiv \left. \frac{d\ \phi_i\ (B^2)}{dB^2} \right|_{B^2 = 0} \quad . \tag{15}$$

From Eq. (11),

$$\phi_i'(0) = \frac{-D_i \ \phi_i(0) + \sum_{\lambda=1}^{i-1} \Sigma_{\lambda \to i} \ \phi_i'(0)}{\Sigma_{c_i} + \Sigma_{rem_i}} \quad . \tag{16}$$

The form of Eqs. (11) and (16) are very similar; the source term β_i in Eq. (11) is replaced by the term $-D_i \phi_i(0)$ in Eq. (16). Hence, after obtaining the $\phi_i(0)$ using Eq. (11) with $B^2 = 0$ (beginning with group 1 and proceeding to successively lower groups as usual), one can obtain the $\phi_i'(0)$ computationally in the same manner.

IV. MEAN SQUARE SLOWING DOWN DISTANCE OF NEUTRONS BELONGING TO GROUP j

From Eq. (7), we have

$$\frac{\overline{r^2}(E)}{6} = - \frac{\phi'(E, 0)}{\phi(E, 0)} \quad , \tag{17}$$

where

$$\phi'(E, 0) \equiv \left. \frac{d\phi(E, B^2)}{dB^2} \right|_{B^2 = 0} \quad . \tag{18}$$

Now we have by definition

$$\phi_j(0) = \int_{E_{jL}}^{E_{jH}} \phi(E, 0)\, dE \tag{19}$$

and

$$\phi_j'(0) = \int_{E_{jL}}^{E_{jH}} \phi'(E, 0)\, dE \quad . \tag{20}$$

Then if we define the mean square distance, from the source, of neutrons belonging to the group j by

$$\bar{r}^2(j) = \frac{\int_{E_{jL}}^{E_{jH}} \bar{r}^2(E)\, \phi(E, 0)\, dE}{\int_{E_{jL}}^{E_{jH}} \phi(E, 0)\, dE} \quad , \tag{21}$$

we have finally[7]

$$\frac{\bar{r}^2(j)}{6} = - \frac{\phi_j'(0)}{\phi_j(0)} \quad . \tag{22}$$

The ordinary age theory approach is not able to cope with a situation in which neutrons may lose a large amount of energy per collision. On the other hand, the solutions as given in Eqs. (14) or (22) with (11) and (16) may be applied to a system having arbitrary transfer cross sections. In particular, the present approach may be applied to the light elements where age theory is not applicable.

V. NUMERICAL EXAMPLE

In order to illustrate the method described above, the mean square slowing down lengths have been calculated for a 12-group representation above 0.4 ev of normal density H_2O. The assumed macroscopic cross sections are given in Table I. All neutrons below group 12 belong to a single "thermal group." (The zeros in the transfer cross sections are due to the arbitrary decision to hold only four-decimal-point accuracy for those cross sections.)

Table I

MACROSCOPIC MULTIGROUP H_2O CROSS SECTIONS (cm^{-1})

j	Group Lower Energy, E_L	Σ_c	$3\Sigma_{tr}$	$\Sigma_{j \to j+1}$	$\Sigma_{j \to j+2}$	$\Sigma_{j \to j+3}$	$\Sigma_{j \to j+4}$	$\Sigma_{j \to j+5}$
1	1.353 Mev	0.001	0.3085	0.0665	0.0230	0.0084	0.0031	0.0011
2	0.4979 Mev	0	0.6714	0.1356	0.0458	0.0168	0.0062	0.0023
3	0.1832 Mev	0	1.0425	0.2248	0.0767	0.0283	0.0104	0.0038
4	0.0674 Mev	0	1.1381	0.3323	0.1180	0.0434	0.0159	0.0059
5	0.0248 Mev	0	1.4013	0.4385	0.1567	0.0574	0.0212	0.0069
6	0.00912 Mev	0	1.5615	0.5035	0.1798	0.0663	0.0216	0.0165
7	0.00335 Mev	0.0001	1.6742	0.5412	0.1938	0.0631	0.0482	0.0014
8	0.001234 Mev	0.0001	1.7009	0.5486	0.1737	0.1327	0.0038	0.0003
9	454 ev	0.00016	1.7009	0.4877	0.3608	0.0104	0.00074	
10	200 ev	0.00020	1.7009	0.9028	0.0255	0.0018		
11	6 ev	0.00070	1.7343	0.3489	0.0246			
12	0.4 ev	0.00300	1.7677	0.4906				

j	Group Lower Energy, E_L	$\Sigma_{j \to j+6}$	$\Sigma_{j \to j+7}$	$\Sigma_{j \to j+8}$	$\Sigma_{j \to j+9}$	$\Sigma_{j \to j+10}$	$\Sigma_{j \to j+11}$	$\Sigma_{j \to j+12}$
1	1.353 Mev	0.0004	0.0002	0.0001	0	0	0	0
2	0.4979 Mev	0.0008	0.0003	0.0001	0.0001	0	0	
3	0.1832 Mev	0.0014	0.0005	0.0003	0	0		
4	0.0674 Mev	0.0019	0.0015	0	0			
5	0.0248 Mev	0.0053	0.0002	0				
6	0.00912 Mev	0.0005	0					
7	0.00335 Mev	0.0001						

n = 0.0334×10^{24} molecules/cc.

Table II gives the ϕ_j and ϕ_j' calculated using Eqs. (11) and then (16). Equations (14) and (22) with $j = 12$ ($E_L = 0.4$ ev) yield, respectively, $\overline{r^2}_{0.4\ ev} = 184.92\ cm^2$ and $\overline{r^2}(12) = 186.72\ cm^2$.

Table II

CALCULATED VALUES FOR ϕ_j AND ϕ_j'

j	ϕ_j	ϕ_j'
1	5.5395	-172.9888
2	3.2182	- 78.3507
3	1.8914	- 47.4216
4	1.2413	- 32.3619
5	0.9251	- 24.6339
6	0.8040	- 21.7630
7	0.7464	- 20.5340
8	0.7358	- 20.5594
9	0.7359	- 20.8819
10	0.6032	- 17.3479
11	2.5780	- 77.3933
12	1.8779	- 58.4422

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APPENDIX

The slowing down density at energy E_{jL} is, by definition,

$$q_{jL}(B^2) = \sum_{i=1}^{j} \sum_{\lambda=1}^{N-j} \Sigma_{i \to j+\lambda} \, \phi_i(B^2) \quad , \tag{A1}$$

where the $\phi_i(B^2)$ are obtained using Eq. (11). $q_{jL}(0)$ is given by Eq. (A1) using $\phi_i(0)$ which, in turn, is obtained from Eq. (11) for the case of zero B^2. Eq. (A1) can be rewritten as

$$q_{jL}(B^2) = \sum_{i=1}^{j} \left[\Sigma_{rem_i} - \sum_{\lambda=1}^{j-i} \Sigma_{i \to i+\lambda} \right] \phi_i(B^2) \quad ; \tag{A2}$$

and using Eq. (11), we have

$$q_{jL}(B^2) = \sum_{i=1}^{j} \left[\beta_i - \Sigma_{c_i} \phi_i(B^2) - D_i B^2 \phi_i(B^2) + \sum_{\lambda=1}^{i-1} \Sigma_{\lambda \to i} \phi_\lambda(B^2) \right.$$

$$\left. - \sum_{\lambda=1}^{j-i} \Sigma_{i \to i+\lambda} \phi_i(B^2) \right] \quad . \tag{A3}$$

Then, owing to the following not altogether obvious identity

$$\sum_{i=1}^{j} \sum_{\lambda=1}^{i-1} \Sigma_{\lambda \to i} \phi_\lambda(B^2) = \sum_{i=1}^{j} \sum_{\lambda=1}^{j-i} \Sigma_{i \to i+\lambda} \phi_i(B^2) \quad ,$$

we have finally the previous Eq. (12)

$$q_{jL}(B^2) = \sum_{i=1}^{j} \left[\beta_i - \Sigma_{c_i} \phi_i(B^2) - D_i B^2 \phi_i(B^2) \right] \quad . \tag{A4}$$

FOOTNOTES

1. If $P_\infty(E, E_s, r)$ is the infinite medium slowing down kernel which gives the neutrons slowing down past energy E at $\underline{r}$ due to a unit point source of energy E_s at position $\underline{r}'$, where $r = |\underline{r} - \underline{r}'|$, then

$$P_\infty(E,r) = \int_0^\infty f(E_s) P_\infty(E, E_s, r)\, dE_s \quad ,$$

where $f(E_s)$ is the fission spectrum. If one does not admit energy upscattering, the integral is zero for $E_s < E$. Explicitly, $\overline{r^2}_E$ is given as

$$\overline{r^2}_E = \frac{\int_0^\infty \int_0^\infty 4\pi r^4 P_\infty(E, E_s, r) f(E_s) dr\, dE_s}{\int_0^\infty \int_0^\infty 4\pi r^2 P_\infty(E, E_s, r) f(E_s) dr\, dE_s} \quad ,$$

where the denominator is just $q_E(0)$.

2. Comments similar to those in footnote 1 apply now if the P's are replaced by the K's, if $\overline{r^2}_E$ is replaced by $\overline{r^2}(E)$, and if $q_E(0)$ is replaced by $\phi(E,0)$. When E coincides with the source energy, the flux will include a component due to the virgin source neutrons. This component is responsible for the so-called first flight correction.

3. For example, in the common "age theory" expression, $\overline{r^2}(E)$ is larger than $\overline{r^2}_E$ owing to the so-called last flight correction. Experimentally, one normally measures $\overline{r^2}(E)$.

4. The subsequent development will be limited to the case in which the neutron energy can only be degraded (or unchanged); that is, we shall not consider energy upscattering.

5. The source, slowing down density and all of the group fluxes are taken to have the same spatial distribution where

$$\Phi_i(\underline{r}) = \phi_i \cdot S(\underline{r}) \text{ and } \nabla^2 S(\underline{r}) + B^2 S(\underline{r}) = 0 \quad .$$

6. Equation (12) is formally derived in the Appendix.

7. Equation (22) is the multigroup analogue of Marshak's $\frac{1}{2}\phi_0^{(2)}/\phi_0^{(0)}$ (Ref. 3); Hurwitz and Zweifel state it also as

$$\frac{1}{2} \lim_{k \to 0} \frac{\delta^2}{\delta k^2} n_0(k,u) \Big/ \lim_{k \to 0} N_0(k,u)$$

(see Ref. 4). Note that since $\overline{r^2}(j)$ refers to a group of finite width, for very wide groups, $\overline{r^2}(j)$ could conceivably become less than $\overline{r^2}_{jL}$.