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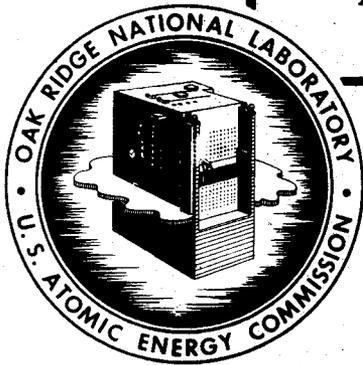
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**CRITICALITY CALCULATIONS
FOR HYDROGEN
MODERATED REACTORS
FROM MICROSCOPIC
DATA**

By

**Mathew Shapiro
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CRITICALITY CALCULATIONS FOR HYDROGEN MODERATED REACTORS
FROM MICROSCOPIC DATA

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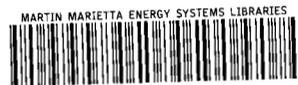
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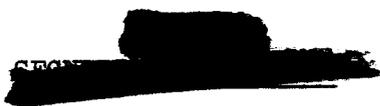


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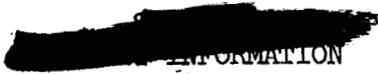


Abstract

The probability for a fission neutron to escape fast leakage from bare, hydrogen moderated reactors is calculated by a method utilizing only the microscopic cross section of the materials. These results can be employed to determine the effectiveness of other substances in preventing fast neutron leakage. These calculations are carried out for aluminum and iron.

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INFORMATION

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1. Introduction. A major difficulty in determining the critical mass of a hydrogen moderated reactor is the calculation of the fraction of neutrons which become thermal or epi-thermal. The discrete nature of the slowing down process, arising from the fact that a neutron can lose all of its energy in a single collision with a hydrogen atom, rules out any straight forward application of Fermi age theory. An additional complication arises from the fact that the scattering cross section of hydrogen varies strongly with energy. If the moderator is water one can circumvent these difficulties by making use of the measured slowing down distributions in water (1). Utilizing these measurements it is possible to estimate the critical mass of water moderated, reflected reactors whose reflectors are composed of water of the same properties as that in the core. This approach is of limited usefulness because it provides no natural extension to water mixtures without further experimentation, or to bare reactors of interesting sizes because of the sensitivity of the buckling to the extrapolation distance, which is itself in doubt because of the rapid variation of the transport mean free path of water with energy.

If there were available a method for computing the probability of a neutron's escaping fast leakage while slowing down in plain water, bare assemblies which depended only on the microscopic cross section data for water, then it could be hoped that it would yield credible results for, say, water-metal mixtures if the microscopic data for the metal were available.

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2. Summary of Results. A method for calculating the probability that a fission neutron will escape fast leakage from a hydrogen moderated, bare reactor is given below. It is based on the use of diffusion theory and an energy dependent extrapolation distance. When compared with critical experiments, the method is found to underestimate the reactivity by 10 to 20 percent depending on the pile size.

A variational technique for estimating the effect of the slowing down of neutrons by a heavy moderator is developed in the appendix.

When the method is applied to aluminum-water and iron-water mixtures it shows that, for the purpose of preventing fast leakage, volume for volume aluminum is equivalent to water of density ≈ 0.3 ; the equivalent density for iron is ≈ 0.5 . The result for aluminum is in good agreement with measured mean square slowing down lengths. No such measurements with fission neutrons for iron-water systems are known to us.

3. Derivation of the Probability of Escaping Fast Leakage.

If we assume that diffusion theory is valid for hydrogen moderators, then for monoenergetic neutrons we can write

$$\nabla^2 \phi = -k^2 \phi.$$

In a multigroup calculation we can then write for the number of neutrons lost from each energy group due to leakage, absorption and slowing down

$$-D\nabla^2 \phi + \sum_{\epsilon} \phi + \sum_{SH} \phi = (DK^2 + \sum_a + \sum_{SH}) \phi.$$

If we assume that scattering of neutrons by hydrogen in the center of mass system is spherically symmetric, so that neutrons of energy E' are scattered uniformly into the energy interval from 0 to E' , we find for the number of neutrons slowed down by hydrogen to energy E

$$\int_E^{\infty} \phi(E'') \sum_{SH}(E'') \frac{dE''}{E''} .$$

These assumptions lead to the equation derived in TAB-53 for the slowing down of neutrons in homogeneous media in the presence of a heavy moderator.

$$(1) \quad (\sum_{SH} + DK^2 + \sum_a)\phi - \frac{\partial}{\partial u}(\xi \sum_S \phi) = .$$

$$e^u \int_u^{\infty} \phi(u') \sum_{SH}(u') e^{-u'} du' + g(u)$$

where: $\phi(u)du$ = neutron flux in the logarithmic energy interval u to $u+du$.

- \sum_{SH} = macroscopic scattering cross section of hydrogen
- \sum_a = macroscopic absorption cross section of all materials
- \sum_S = macroscopic scattering cross section of the heavy moderator.
- ξ = average logarithmic energy loss in a collision with the heavy moderator.
- K^2 = the buckling of the assembly

$$D = \text{diffusion coefficient} = \frac{1}{3\Sigma_{\text{tr}}}$$

Σ_{tr} = macroscopic transport cross section of moderator

$g(u)$ = fission source spectrum, normalized so that

$$\int_0^{\infty} g(u) du = 1.$$

$$u = \text{logarithmic energy} = \log_e \frac{E}{E(\text{thermal})}$$

Equation (1) with $\xi = 0$ has been solved by Wigner (without the source term). The case of the monochromatic source has been treated by Young⁽⁷⁾. For the sake of completeness we carry out the solution again here.

The first term on the left of equation (1) is the number of neutrons per second which leave the interval between u and $u+du$ for all reasons except slowing down by the heavy moderator. The second term on the left is the net number of neutrons leaving this same interval due to moderation by the heavy element. The integral on the right side of equation (1) is the number of neutrons per second slowed down into the logarithmic interval du by hydrogen.

The buckling, K^2 , is a function of the dimensions of the extrapolated pile boundary. Because the transport cross section of hydrogen is a strong function of the energy, there is no unique extrapolation distance. Following a suggestion by E. Greuling, we have taken the extrapolation length, and hence

the buckling, to be energy dependent. We used for the extrapolation length

$$\frac{2}{3} \lambda_{tr} = 2D .$$

For the moment we shall ignore the moderation of the heavy element by placing $\xi = 0$. However, the scattering by this element is taken into account through the diffusion coefficient, D .

For convenience we introduce instead of the flux, the collision density defined as

$$n(u) = (\sum_a + DK^2 + \sum_{SH})\phi(u)$$

and the probability of a hydrogen collision

$$B = \frac{\sum_{SH}}{\sum_a + DK^2 + \sum_{SH}}$$

Then equation (1) becomes

$$(2) \quad n(u) = e^u \int_u^\infty B(u') e^{-u'} n(u') du' + g(u)$$

The differential equation for $n(u)$ is readily found to be:

$$(2') \quad \frac{d}{du} (n-g) = (1-B)n - g$$

with the boundary condition $n(\infty) = 0$.

Since $(1-B)ndu$ represents the number of neutrons/sec in the interval u to $u+du$ which leak out of the reactor or are

absorbed, the equation for the slowing down density is

$$(3) \quad \frac{dq}{du} = (1-B)n - g \quad q(\infty) = 0.$$

Since q and $n-g$ satisfy the same differential equation and boundary condition, they are identical.

We can now rewrite equation (2') in terms of q to obtain

$$(3') \quad \frac{dq}{du} - (1-B)q = -Bg \quad q(\infty) = 0.$$

this equation has the solution

$$(4) \quad q(u) = e^{-\int_u^{u_0} (1-B)du'} \int_u^{u_0} B e^{\int_{u'}^{u_0} (1-B)du''} g(u') du'$$

$u_0 = \log_e \frac{E_0}{E_{th}}$. E_0 is the maximum energy with which a neutron is produced in the fission process.

In equations (3) and (4) one notices that the neutron source $g(u)$ appears multiplied by B , the probability that a neutron will collide with a hydrogen atom. Thus the effective source for the slowing down function is the once-collided neutrons. Since \sum_{SH} falls to quite low values at high energies, this effective source can be appreciably less than the actual source of fission neutrons.

If the neutron source is monoenergetic with energy E_S so that $g(u) = \delta(u-u_S)$, then (4) becomes

$$(4') \quad q(u) = B(u_S) e^{-\int_u^{u_S} (1-B)du'}$$

We see this agrees with Young's result (reference 7, equ. 24) since $B(u_s)$ is the number of neutrons from a unit source which are scattered to lower energies, corresponding to his quantity S .

In the event that $\sum_a \ll DK^2 \ll \sum_{SH}$ a comparison with Fermi age theory can be made. Under these conditions

$$1-B \cong \frac{DK^2}{\sum_{SH} \left(1 + \frac{DK^2}{\sum_{SH}}\right)} \cong \frac{DK^2}{\sum_{SH}} \left(1 - \frac{DK^2}{\sum_{SH}}\right)$$

Then*

$$\begin{aligned} q(u) &= B(u_s) \exp \left[- \int_u^{u_s} \frac{DK^2}{\sum_{SH}} \left(1 - \frac{DK^2}{\sum_{SH}}\right) du' \right] \\ &= B(u_s) \exp \left[- \int_u^{u_s} \frac{K^2}{3 \sum_{tr} \sum_{SH}} \left(1 - \frac{DK^2}{\sum_{SH}}\right) du' \right] \end{aligned}$$

Fermi age theory with a first flight correction yields

$$q = B(u_s) \exp \left[- \int_u^{u_s} \frac{K^2}{3 \xi \sum_{tr} \sum_S} du' \right] \quad \text{If we recall}$$

that ξ for hydrogen equals unity, then the results are formally the same except for the departure of the factor $\left(1 - \frac{DK^2}{\sum_{SH}}\right)$ from unity and for the fact that K^2 is here taken as energy dependent.

Utilizing the cross section for hydrogen given in reference 4 and the fission spectrum given in reference 5, we have calculated

*A similar result has been obtained by D. Selengut in NEPA-1484, except that his result does not include the factor $B(u_s)$.

$q(o)$, the probability of a fission neutron becoming thermal for several water moderated systems. The oxygen data used is believed to be the best compilation of data existing at this time.*

Table I

The Probability of Escaping Fast Leakage in Full Density Water Systems

Geometry	Dimensions (cm)		$q(o)$
	radius	height	
Sphere	36	-	.820
	28	-	.741
	18.8	-	.572
Cylinder	18.9	41.4	.618**
	25.3	20.4	.539
	11.4	29.1	.401

The quantity $q(o)$ depends on the moderator density and dimensions of the system only in the form of moderator density times the linear dimensions. The cylinder dimensions in

* Private communication from H. Goldstein

** When oxygen moderation is taken into account according to the method given in Appendix I, this value becomes 0.630.

Table I are those of three assemblies used in critical mass experiments (3) at K-25 after a correction for water density was applied. The values of $q(0)$ in Table I do not include the beneficial effect of slowing down due to oxygen. In the one case in which the computation was made, according to Appendix A, the value of $q(0)$ was increased by two percent. Another way of reporting this same result is to say that, in this one case, full density water without oxygen slowing down gave the same q as water with oxygen moderation of 0.97 normal density.

4. Comparison with Critical Experiments. Critical experiments have been carried out at K-25 (3). Using the experimental dimension and composition we have computed, according to the method in section 3, the number of neutrons escaping fast leakage, and from that the theoretical reactivity according to the formula*

$$R = \frac{q(0)\bar{v}}{1 + \frac{\sum_{aH_2O} + DK^2}{\sum_{au}}} = \frac{\bar{v}q(0)}{1 + \frac{\sum_{aH_2O}}{\sum_{au}} \left\{ 1 + L_{H_2O}^2 K^2 \right\}}$$

* This equation assumes the pile is thermal. If this is not the case, then one includes the macroscopic absorption cross section of water and U(25) in \sum_a , computes $q(u)$, and uses the relation

$$R = \int_0^{\infty} (q+g)\bar{v} \frac{\sum_{au}}{\sum_a + DK^2 + \sum_{SH}} du + \frac{\bar{v}q(0)}{1 + \frac{\sum_{aH_2O}}{\sum_{au}} \left\{ 1 + K^2 L_{H_2O}^2 \right\}}$$

R is the reactivity. $\bar{\nu} = 2.10$ neutrons produced per neutron absorbed in U(25). For the absorption cross section of U(25) at .025 ev. we used 645 barns. The parameters for thermal neutrons in water were obtained from reference 6. These are

$$\Sigma_{aH_2O} = 0.68 \text{ barns/molecule}$$

$$L_{H_2O}^2 = 7.13 \text{ cm}^2$$

Table II shows the comparison with three of the experimental critical assemblies.

Table II

Cylinder Dimension (cm)		H/U/25 Atomic Ratio	Water Density (gm/cc)	Theoretical Reactivity
Radius	Height			
19.05	41.7	755	0.992	0.90
25.4	20.5	499	0.997	0.86
12.7	32.3	43.9	0.900	0.82

There are several factors which will tend to improve the agreement shown. The effect of oxygen slowing down increased the reactivity by two percent in the first line of the table and can be expected to make at least that much difference in the other entries. Although epi-thermal fission* did not change the reactivity appreciably in the largest pile, it is anticipated

* See footnote p. 10.

that the increase will be noticeable in the smaller ones. The theoretical results here were compared with the more reactive of the experiments in reference (3). These were the assemblies with iron* containers which in some cases required 5 percent less fuel than their counterparts in aluminum containers.

The poor agreement of the theoretical and experimental results shows that diffusion theory is not adequate to describe the slowing down of fission neutrons in bare, hydrogen moderated reactors whose dimensions are comparable to the diffusion length of high energy neutrons. The critical masses so calculated can be too large by a factor of the order of two in piles of interesting sizes.

However, the method which proceeds from microscopic data only can be used as a starting point for the analysis of metal-water mixtures. This analysis is carried out in the next section.

5. Water-Metal Mixtures. The estimation of the reactivity of water moderated piles containing significant amounts of structural metal is at present difficult because of the scarcity of experimental information. The modification of the method outlined in TAB-53 which was presented earlier was shown to be in only fair agreement with experiments. However, it might be hoped that consistent calculations with this method for all-water-metal reactors would determine more accurately the ratio

* In reflectors around water moderated cores, iron seems to be about as effective a reflector as water (private communication from E. Greuling, based on K-25 experimental data)

of the neutron-stopping power of the metal to that of pure water than either of these quantities themselves. We give below the results of such a calculation for aluminum.

Some slowing down distribution measurements have been made on aluminum-water mixtures (8) and on a zirconium-water mixture (9). The results presented here are found to agree reasonably well with the experimental aluminum-water measurements. Calculations on aluminum are emphasized because the theoretical and experimental values for its transport cross are in good agreement (10). No calculations were made for zirconium. The theoretical transport cross section for iron (the experimental measurements are crude) is nearly the same as that of aluminum (10). Consequently, if the iron slowing down (due to inelastic scattering) is neglected, the calculations for aluminum can be scaled by the ratio of atomic densities into calculations for iron-water mixtures.*

Before turning to the details of the calculations for water-metal mixtures, let us consider the role of the metal component in such mixtures. The scattering cross section of hydrogen falls quite low at high neutron energies, and so in hydrogen moderated reactors much of the neutron leakage occurs

*There is a Canadian experimental result on an iron-water mixture (Can. Jour. Research A, 25, 162, 1947) but it does not seem to be very useful for reactor calculations; the iron was present in large chunks and the measurements were not made with fission neutrons.

at high energies. The cross sections of elements other than hydrogen generally hold up rather better at high energies, and thus while the scattering power of a piece of metal does not compare with that of an equal volume of water at lower energies, it can compare quite favorably at high energies where much of the neutron leakage occurs. This suggests that, for the purpose of preventing fast neutron leakage, a metal can be equivalent to water of some appreciable density x .

If a metal were in fact equivalent to water of density x (for all ratios of metal volume to water volume, and for all size systems) then the equivalent density of a system containing y volumes of metal to 1 volume of full density water would be

$$\bar{\rho} = \frac{1+yx}{1+y} \text{ gm/cc.}$$

If the dimensions of a system are large compared to the total mean free path and scattering mean free path for neutrons in the moderator, then these are the only two lengths which appear in the Boltzmann transport equation. These lengths are both inversely proportional to the moderator density, so that the age (actually one-sixth the mean squared slowing down distance) will be inversely proportional to the density squared. Thus the ratio of the age in a water-metal mixture to that in pure water would be

$$\frac{\tau(y)}{\tau(0)} = \left(\frac{1+y}{1+yx} \right)^2 .$$

For example, the age to indium resonance in a water-zirconium mixture having $y = 0.25$ was measured ⁽⁹⁾ to be 35.7cm^2 , while the age in plain water ($y = 0$) was 30.3cm^2 . With these values the above formula gives $x = 0.59$; thus zirconium appears to be, neutron-stopping-wise, about 0.6 as good as water. Table III shows the age for aluminum-water mixtures as measured by Roberts and Fitch ⁽⁸⁾ and as calculated by the method described below. The calculated values of x are also included.

Table III*

Age for Aluminum-Water Mixtures

y = aluminum to water volume ratio	measured $\gamma(y)/\gamma(0)$	measured x	calculations	
			$\gamma(y)/\gamma(0)$	x
0.4			1.51	.348
0.5	1.62	.355	1.65	.332
0.6			1.80	.318
0.7			1.96	.307
0.8			2.11	.299
0.9			2.26	.294
1.0	2.51	.262	2.40	.291

*The values of x in Tables III and IV are calculated on the basis of q values for plain water without oxygen slowing down. If the only result obtained thus far (that this water is equivalent to actual water of density 0.97 gm/cc) is generally valid, then the values of x in Tables III and IV should be multiplied by 0.97 .

It is seen that the fractional error in $\frac{\tau(y)}{\tau(0)}$ is less than that in x . Hence the quantity x is a "sensitive" parameter and its use tends to magnify discrepancies. Conversely, when the value of x is used to calculate q , the probability of a fission neutron's escaping fast leakage, the result is not very sensitive to small uncertainties in x .

To determine x we first calculated q for bare all-water spherical systems by the method discussed in section 3. For a sphere of radius R , say, containing some aluminum, we calculated $q(0)$. We then determined what density of water, $\bar{\rho}$, in a sphere of radius R would yield the same $q(0)$. x was then determined from the equation on page 14.

The calculation just described makes use of the transport cross section of aluminum and ignores any energy loss due to inelastic collisions with aluminum. The theoretical and experimental values of the aluminum transport cross section are in good agreement ⁽¹⁰⁾, and in between experimental points the theoretical values were used. It is of interest to note that the theoretical $\sigma_{tr}(E)$ values for iron and aluminum are nearly the same ⁽¹⁰⁾. If one assumes that the theoretical values for iron are correct (the measured ones are considered rough) then the above calculations for Al-water mixtures can be considered as calculations for Fe-water mixtures in which the iron slowing down* has been neglected. Since the atomic density of iron is

*The effect of moderation by inelastic scattering can be obtained by a perturbation method. One such calculation was carried out for an iron-water pile ($y = 0.70$) and the effect was to increase x by about 0.1.

1.4 times that of aluminum, the x value for iron is 1.4 times that of aluminum. After correcting the values of y by this same factor, we show the results in Table IV.

Table IV
x for Iron without Slowing Down

y = iron to water volume ratio	Iron Volume (liters)	Total Volume (liters)	calculated x
0.30	88	380	.48
0.30	44	190	.45
0.40	88	308	.45
0.50	88	264	.43
0.50	176	528	.47
0.60	88	235	.42
0.70	88	214	.41

Tables III and IV show that the values of x, as computed here, vary with pile size and composition. However, over the range of compositions and volumes considered here x is a constant to within $\pm 10\%$. As pointed out earlier, $q(o)$ does not depend strongly upon x.

The estimation of the reactivity of bare, water-metal piles by this method would no doubt be subject to as large errors as those for all water piles that were presented in section 4 of this report. However, one might hope that the x values obtained above might be more accurate and could be used along with a method which gives good results for all-water, reflected piles

to obtain good estimates for the critical mass of reflected, water-metal systems.

For example, let us consider a reactor with an infinite water reflector whose core is a sphere of volume 100 liters and which contains 25 liters of iron. Thus $y = \frac{25}{75} = \frac{1}{3}$. From Table IV x is approximately $1/2$, so that the average density is

$$\frac{1 + \frac{1}{3}(1/2)}{1 + \frac{1}{3}} = 0.875.$$

From Greuling's results (11) we find that the critical mass of a sphere of core volume $100(.875)^3$ filled with full density water is 1.56 kg of U(25). Thus a 100 liter core with water of density (.875) requires $1.56/ (.875)^2$ or about 2 kg. The thermal absorption cross section of iron is about 10 times that of water on a volume basis. Thus the core material would be

$$\frac{1 + 10(1/3)}{.875(1 + 1/3)} = 3.71$$

times as absorbing as water of density .875 and the critical mass estimate becomes* 7.5 kg.

*Actually Greuling's results apply only to systems whose core and reflector properties are the same, so the figure of 7.5 kg applies to a reactor whose reflector is also composed of water of density 0.875 gm/cc.

Appendix I

We consider here how the probability of fission neutron becoming thermal changes when a heavy element is also present in the moderator. We define $\Sigma' = \Sigma_a + DK^2$ and rewrite equation (1) in the text in the form

$$A1 \quad \left(\Sigma' + \Sigma_{SH} \right) \phi - \frac{d}{du} \left(\xi \Sigma_S \phi \right) = q(u) + g(u),$$

where, as before [cf. equation (3)] ,

$$\frac{dq}{du} = n - g - Bn = q - \Sigma_{SH} \phi.$$

However, $q(u)$ is no longer the slowing down density. The number of neutrons lost due to leakage and absorption in the interval between u and $u+du$ is $\Sigma' \phi$. Thus the number of neutrons at u which have survived is

$$\begin{aligned} \eta(u) &= \int_u^\infty g(u) du - \int_u^\infty \Sigma' \phi du = - \int_u^\infty \frac{d}{du} \left(\xi \Sigma_S \phi + q \right) \\ &= \xi \Sigma_S \phi + q(u) = q \left(1 + \frac{\xi \Sigma_S}{\Sigma_{SH}} \right) - \frac{\xi \Sigma_S}{\Sigma_{SH}} \frac{dq}{du} \end{aligned}$$

This is the slowing down density in the presence of hydrogen and a heavy moderator element.

We now eliminate ϕ from equation A1 to obtain:

$$A2 \quad \left\{ \frac{\xi \Sigma_S}{\Sigma_{SH}} \frac{d^2 q}{du^2} + \frac{dq}{du} \left[\frac{d}{du} \left(\frac{\xi \Sigma_S}{\Sigma_{SH}} \right) - \frac{\xi \Sigma_S}{\Sigma_{SH}} - \frac{\Sigma' + \Sigma_{SH}}{\Sigma_{SH}} \right] \right\}$$

$$+ q \left\{ \frac{\sum' }{\sum_{SH}} - \frac{d}{du} \left(\frac{\xi \sum S}{\sum_{SH}} \right) \right\} = g(u)$$

Equation A2 is normalized to a fission source of one neutron per second. It is convenient to replace this source by the actual neutron source. If we define f to be the number of fission neutrons produced per neutron becoming thermal, then under this renormalization the number of fission neutrons produced per second is $f \bar{\eta}(0)$, for $\bar{\eta}(0)$ is now the number of neutrons becoming thermal per second. With this renormalization A2 becomes

$$A3 \quad a \frac{d^2 q}{du^2} + b \frac{dq}{du} + cq = f \left[(a+1)q - a \frac{dq}{du} \right]_{u=0} g(u)$$

$$a = \frac{\xi \sum S}{\sum_{SH}}$$

$$b = -\frac{1}{B} - a + \frac{da}{du}$$

$$c = \frac{1}{B} - 1 - \frac{da}{du}$$

The probability of a fission neutron becoming thermal is

$$\frac{\text{rate of neutrons becoming thermal}}{\text{rate of production of fission neutrons}} = \frac{\bar{\eta}(0)}{f \bar{\eta}(0)} = \frac{1}{f}.$$

Equation A3 is an eigenvalue problem for f . We wish to find an expression for f which is invariant to changes in q from its correct value. To do this we multiply A3 by $Q(u)$ and integrate.

$$\text{A4} \quad \int_0^{\infty} Q \left\{ a \frac{d^2 q}{du^2} + b \frac{dq}{du} + cq \right\} du = f \left[(a+1)q - a \frac{dq}{du} \right]_{u=0} \int_0^{\infty} Qg \, du$$

We find this equation for f is invariant to changes in Q and q provided q satisfies A3 with boundary conditions

$$q(\infty) = 0; \quad \frac{dq}{du}(\infty) = 0$$

and Q satisfies

$$\text{A5} \quad \frac{d^2}{du^2}(aQ) - \frac{d}{du}(bQ) + cQ = 0; \quad \text{with the boundary conditions:}$$

$$a(0)Q(0) = a(0)f \int_0^{\infty} Qg \, du$$

and

$$\left[-bQ + \frac{d}{du} aQ \right]_{u=0} = (a+1)_{u=0} f \int_0^{\infty} Qg \, du$$

our invariant expression for f is:

$$\text{A6} \quad f = \frac{\int_0^{\infty} Q \left\{ a \frac{d^2 q}{du^2} + b \frac{dq}{du} + cq \right\}}{\left[(a+1)q - a \frac{dq}{du} \right]_{u=0} \int_0^{\infty} Qg \, du}$$

Our equations for q and Q are homogeneous, so we are free to choose their normalization. For convenience we place:

$$f \int_0^{\infty} Qg \, du = 1$$

$$\text{and } f \left[(a+1)q - a \frac{dq}{du} \right]_{u=0} = 1$$

We take as our zero order or trial functions the solutions of A3 and A5 when $\xi \sum_S = 0$. (This solution for q is the one found in the body of the report). The equations determining these zero order functions are:

$$A3' \quad - \frac{dq_0}{du} + (1-B)q_0 = Bg(u); \quad q(\infty) = 0.$$

and

$$A5' \quad \frac{d(Q_0/B)}{du} + \frac{(1-B)}{B} Q_0 = 0 \quad Q_0(0) = B(0) \cong 1$$

As before, $B = \frac{\sum_{SH}}{\sum_{SH} + \sum_I}$. We have placed $f_0 q_0(0) = 1 = f_0 \int_0^{\infty} Q_0 g \, du$.

Upon substituting A3' into A6 and recalling that $f_0 q_0(0) = 1$, we obtain

$$f/f_0 = \frac{1 + f_0 \int_0^{\infty} Q_0 \frac{d}{du} a \left(\frac{dq_0}{du} - q_0 \right)}{1 + \frac{\xi \sum_S}{\sum_I + \sum_{SH}}} = \frac{1 - f_0 \int_0^{\infty} Q_0 \frac{d}{du} \left(\xi \sum_S \phi_0 \right) du}{1 + \frac{\xi \sum_S}{\sum_I + \sum_{SH}}}$$

Finally, the change in the probability that a neutron will become thermal is

$$\frac{1}{\bar{F}} - \frac{1}{\bar{F}_0} = \frac{\left(\frac{\xi \sum_S}{\sum + \sum_{SH}} q_0 \right)_0 + \int_0^\infty Q_0 \frac{d}{du} \left(\xi \sum_S \phi_0 \right) du}{1 - \frac{1}{q_0(0)} \int_0^\infty Q_0 \frac{d}{du} \left(\xi \sum_S \phi_0 \right) du}$$

The denominator can be put equal to unity with very little error. Now

$$\xi \sum_S \phi_0 = \frac{\xi \sum_S n_0}{\sum + \sum_{SH}} = \frac{\xi \sum_S}{\sum + \sum_{SH}} (q_0 + g) = aB(q_0 + g).$$

and $Q_0 = B(u) e^{-\int_0^u (1-B) du}$ so that

$$\begin{aligned} \text{A7} \quad \frac{1}{\bar{F}} - \frac{1}{\bar{F}_0} &= \frac{1}{\bar{F}} - q_0(0) = \left(\frac{\xi \sum_S}{\sum + \sum_{SH}} q_0 \right)_{u=0} \\ &+ \int_0^\infty B(u) e^{-\int_0^u (1-B) du'} \frac{d}{du} [aB(q_0 + g)] du \end{aligned}$$

This same result can be obtained by direct perturbation of equation (1) in the body of the report. However, the variational procedure gives a stronger proof of the validity of the result.

If we first solve for $q_0(u)$, as in section 3, then equation A7 gives the correction to $q_0(0)$ which has to be applied to take account of the moderation by a heavy element.


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