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INFLUENCE OF ABSORPTION ON THE EFFECTIVE VALUE OF η

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In NAA-SR-Memo-349^{1,2}, a calculation was performed to determine the effect of epithermal capture on the value of η to be used in lattice calculations. The basic physical concepts of the calculation will not be repeated here; however, because of some uncertainty about the magnitude of the effect an independent calculation has now been carried out with essentially the same results.

The present formulation is an approximate one, the purpose of the simplifying assumption being to reduce the analytical difficulties to a point where a solution could be obtained in closed form without the need for numerical integration. The neutron flux density as a function of energy is written in the form

$$\phi(E) = \frac{C}{(kT)^2} e^{-E/kT} \quad \text{for } E/kT \leq x^2 \quad \text{.....(1a)}$$

$$= \frac{g(E)}{\sum_0 \sum_s E} \quad \text{for } E/kT \geq x^2 \quad \text{.....(1b)}$$

Eq. (1b) differs from Eq. (I-8b) in two particulars; the simple slowing down relationship is used in place of Placzek's first order correction, and the mean logarithmic energy loss is assumed constant rather than a function of the neutron energy for energies which are not small compared to the moderator energy. These simplifications will make it possible to carry

* References to this memo will be prefixed with the symbol I.

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out certain integrals which will arise later.

Corresponding to Eq. (I-12) we have the condition

$$\alpha x^2 e^{-x^2} = \frac{q(x)}{\xi_0 \sum_s \Sigma_s} \quad \text{.....(2)}$$

which expresses the continuity of the flux at the point $E = kTx^2$. We must also require that the slowing down density at this point, $q(x)$ shall be sufficient to supply the losses at lower energies

$$q(x) = \int_0^x 0 \sum_s 2v^3 e^{-v^2} dv \quad \text{.....(3)}$$

where $\sum_s = \frac{\sum_a}{v} + \frac{\lambda}{3} H^2$ is the loss coefficient ($v = \sqrt{E/kT}$, and $\sum_a$ is the absorption cross section of the lattice at thermal energies. The energy dependence of the absorption is assumed to be inversely proportional to the neutron velocity.)

$$(I-14) \quad q_1 = q(x) = 0 \sum_a \left\{ \int_0^x e^{-v^2} dv + u - (u + x + ux^2) e^{-x^2} \right\} \dots (4)$$

$$\text{where } u = \frac{\lambda H^2}{3 \sum_a}$$

$$\text{In terms of the function } H(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-v^2} dv, \quad H'(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}$$

which is tabulated in WPA tables we find the following implicit relationship for x , which determines the division point between the Maxwell distribution and the slowing down distribution

$$H = \frac{\sum_a}{\xi \sum_s} = \frac{x H'(x)}{\frac{2u}{\sqrt{\pi}} + H(x) - (u + x + ux^2) H'(x)} \quad \text{.....(5)}$$

The condition that the slowing down density must also in the slowing down region, supply the losses of the flux gives us a relationship which is essentially the differential form of Eq. (3) applied to the slowing

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down region.

$$dq(E) = \sum_{\ell} \beta(E) dE = \sum_{\ell} \frac{q(E)}{E \sum_{\ell} E} \frac{dE}{E} \quad \dots(6)$$

which can be integrated to give

$$\begin{aligned} \ln \frac{q(E)}{q_1} &= \frac{\sum_{\ell} \beta(E)}{\sum_{\ell} E} \int_{\frac{E}{kT}}^E (\sqrt{\frac{E}{kT}} + u) \frac{dE}{E} \\ &= \frac{2M}{x} \int_0^t (e^{-t'} + ux) dt' \\ &= \frac{2M}{x} \left[1 - e^{-t} + uxt \right] \quad \dots(7) \end{aligned}$$

$$\text{where } E = kT x^2 e^{2t}, \quad t = \frac{1}{2} \ln \frac{E}{kT} - \ln ux$$

The flux density in the slowing down region is therefore given by

$$\beta(E) = \frac{q(E)}{E \sum_{\ell} E} = \frac{q_1}{E \sum_{\ell} E} \exp \left\{ \frac{2M}{x} \left[1 - x \sqrt{\frac{kT}{E}} + \frac{ux}{2} \ln \frac{E}{kT} - uxt \right] \right\} \quad \dots(8)$$

The effective value of η is then determined from the condition (Eq. I-19)

$$\eta_{\text{eff}} \frac{q_0}{1 + \mathcal{K}^2 L^2} = \eta \sum_{\ell} \int_0^{E_0} \sqrt{\frac{kT}{E}} \beta(E) dE \quad \dots(9)$$

where $\beta(E)$ is given either by Eq. (1a) or Eq. (8), and $E_0 = kT x^2$ is some unspecified (high) energy. We then can write

$$\begin{aligned} \frac{\eta_{\text{eff}}}{\eta} &= \frac{(1 + \mathcal{K}^2 L^2) q_0}{q_0} \left[\sum_{\ell} \int_0^x 2v^2 e^{-v^2} dv \right. \\ &\quad \left. + \frac{q_1}{E \sum_{\ell} E} \sum_{\ell} \int_x^{\infty} \frac{1}{v} \exp \left\{ -\frac{2M}{v} + 2M \ln \frac{v}{x} \right\} \frac{2M dv}{v^2} \right] \dots(10) \end{aligned}$$

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$$q_2 = q_1 \exp \left\{ \frac{2M}{x} - \frac{2M}{s} + 2M \ln \frac{s}{x} \right\}$$

$$x^2 \tau_s = 2M \ln s \quad x^2 \tau_x^2 = \frac{2M}{x}$$

The first integral of Eq. (10) becomes

$$C \sum_n \int_0^x 2v^2 e^{-v^2} dv = \frac{\sqrt{\pi}}{2} C \sum_n \left[H(x) - x H'(x) \right]$$

and the second reduces to

$$\frac{q_1}{x} \sum_n \exp \left\{ \frac{2M}{x} - 2M \ln \frac{s}{x} \right\} \int_x^s \sqrt{2M} e^{-2M/v} \frac{dv}{v^2}$$

When all the appropriate substitutions are made we find that the variable s occurs only in the upper limit of the second integral (having canceled out everywhere else). Since this integral is absolutely convergent for $2M < 1$ we now let s approach infinity and ultimately reduce the expression to

$$\frac{\eta_{eff}}{\eta} = \left(1 + \frac{2M}{x} \right) \left\{ \frac{1}{x} \left[\frac{H(x)}{x H'(x)} - 1 \right] \exp \left[2M \ln \frac{s}{x} - \frac{1}{x} \right] \right.$$

$$\left. + (2M)^{2M} \int_0^{2M/x} t^{-2M} e^{-t} dt \right\} \quad \dots (11)$$

Since $2M/x < 1$ we may expand e^{-t} inside the integral and integrate termwise. This gives us

$$\exp(2M \ln \frac{s}{x}) \left[\frac{1}{1 - 2M} \left(\frac{2M}{x} \right) - \frac{1}{1! (2 - 2M)} \left(\frac{2M}{x} \right)^2 + \frac{1}{2! (3 - 2M)} \left(\frac{2M}{x} \right)^3 \right.$$

$$\left. - \frac{1}{3! (4 - 2M)} \left(\frac{2M}{x} \right)^4 + \dots \right]$$

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If we now multiply this series by the series for $e^{2u/x}$ this expression becomes

$$\exp 2u \left(\ln x - \frac{1}{x} \right) \left[\frac{1}{1-b} + \frac{b^2}{(1-b)(2-b)} + \frac{b^3}{(1-b)(2-b)(3-b)} + \dots \right] \quad \dots(12)$$

$a = 2u/x, \quad b = 2u.$

The final expression for the epithermal effect therefore becomes

$$\frac{\eta_{eff}}{\eta} = \left(1 + \frac{2u}{\sqrt{\pi}} \right) \exp \left\{ -a + b \ln x \right\} \left[\frac{H(x) - xH'(x)}{H(x) + \frac{2u}{\sqrt{\pi}} - (x + u + ux^2)H'(x)} + \frac{1}{1-b} + \frac{b^2}{(1-b)(2-b)} + \frac{b^3}{(1-b)(2-b)(3-b)} + \dots \right] \quad \dots(13)$$

For values of $a \ll 1$ the series converges rapidly and only two or three terms need to be retained. Numerical calculations yield the results listed in Table I.

TABLE I
VALUES OF η_{eff}/η and M_1 AS FUNCTIONS OF x AND u

		$u = 0.05$	$u = 0.10$	$u = 0.15$
$x = 2.25$	$M_1 \times 10^3$	8.8283		
	η_{eff}/η	1.02663		
$x = 2.50$	$M_1 \times 10^3$	4.0527	7.6976	10.9923
	η_{eff}/η	1.01199	1.02291	1.03288
$x = 2.75$	$M_1 \times 10^3$	1.5899	3.0190	4.3106
	η_{eff}/η	1.00474	1.00902	1.01289

As in the previous results there is almost a one parameter dependence on M_1 in the range of interest and the expression can be written as

$$\frac{\eta_{eff}}{\eta} = 1 + 2.99 M_1 \approx 1 + \frac{2.99^2}{\xi \Sigma_0} \quad \dots(14)$$

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It was pointed out in I that the Maxwell distribution of neutron velocities used in this calculation does not in general correspond to the distribution determined by the temperature of the moderator but by an effective temperature which is somewhat higher. Wilkins² has treated the problem for neutrons in a heavy moderator. He finds that the neutron velocity distribution in an infinite homogeneous medium with constant scattering cross section and $1/v$ absorption is given by

$$N(v)dv = \mu(v)N(v)dv \quad \dots(15)$$

where $N(v)$ is the Maxwell distribution corresponding to the temperature of the medium, $N(v) = v^2 e^{-v^2}$ and $\mu(v)$ is the power series

$$\begin{aligned} \mu(v) &= \sum_{n=0}^{\infty} a_n v^n \\ a_0 &= 1 \quad a_1 = \frac{\Delta}{3} = \frac{\sum \frac{1}{v}}{3 \sum \frac{1}{v}}, \quad a_2 = \frac{\Delta^2}{24} \\ a_n &= \frac{2(n-2)a_{n-2} + \Delta a_{n-1}}{n(n+2)} \quad \dots(16) \end{aligned}$$

The series for $\mu(v)$ is slowly convergent for large values of v , the coefficients a_n approach the limiting recursion formula

$$a_n = \frac{2}{n+2} a_{n-2} \quad n \gg 1$$

which implies that the series is dominated by the expression $v^{-4} e^{-v^2}$ so that for large values of v (i.e. in the slowing down region) we indeed find $N(v) \sim v^{-2}$.

In order to calculate an effective temperature for this distribution we must be careful about what it is we are trying to do. If we define temperature in terms of the mean energy of the neutron we are immediately stymied. The tail of the distribution falls off only as v^{-2}

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so that the mean value of v^2 is infinite. The mean velocity is also infinite. However both of these results are produced by the high energy neutrons and these we can adequately represent in a "slowing down" distribution; the portion of the distribution which interests us most is the region near $v = 1$, near the peak of the distribution. We must therefore choose a criterion which is not strongly affected by the higher energy components.

If we consider the integral

$$F(k) = \int_0^{\infty} v^k H(v) dv = \int_0^{\infty} \sum_{n=0}^{\infty} a_n v^{n+k+2} e^{-v^2} dv \quad \dots(17)$$

as a function of k , we see that it is defined only in the open interval $-3 < k < 1$. We can however use the function $F(k)$ in this region to define an effective temperature; let $G(k)$ be the corresponding function for a Maxwell distribution

$$G(k) = \int_0^{\infty} v^{k+2} e^{-v^2} dv = \frac{1}{2} \Gamma\left(\frac{3+k}{2}\right) \quad \dots(18)$$

and for any value of k we can define T_{eff}/T_0 from the condition

$$\frac{F(k)}{F(0)} = \left(\frac{T_{\text{eff}}}{T_0}\right)^{k/2} \frac{G(k)}{G(0)} = \frac{2}{\sqrt{\pi}} \Gamma\left(\frac{3+k}{2}\right) \left(\frac{T_{\text{eff}}}{T_0}\right)^{k/2} \quad \dots(19)$$

for $k = -1$ we have

$$\frac{T_{\text{eff}}}{T_0} = \frac{4}{\pi} \left[\frac{F(0)}{F(-1)} \right]^2 \quad \dots(19.1)$$

and for $k = -2$

$$\frac{T_{\text{eff}}}{T_0} = 2 \frac{F(0)}{F(-2)} \quad \dots(19.2)$$

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The series for $F(k)$ is readily obtained by direct integration of Eq. (17)

$$F(k) = \frac{1}{2} \sum_{n=0}^{\infty} \sqrt{\left(\frac{3+k+n}{2}\right)} a_n$$

the results of this procedure are collected in Table II and simple fitting to these numbers can be achieved with the expression

$$T_{\text{eff}} = T_0 \left(1 + 0.185 \frac{\sum a_n}{\xi \sum s_n} \right)^2 \quad \text{....(20)}$$

Table II shows the variation in effective Maxwellian temperature as calculated from Eq. (19.1) and from Eq. (19.2) as well as the simple analytic fitting given by Eq. (20). The fact that the temperatures calculated with $k = -1$ are in good agreement with those calculated with $k = -2$ indicates that the neutron distribution does indeed approximate a Maxwellian distribution with a changed "temperature".

The temperature effect calculated here is much smaller than that obtained for example by Karl Cohen³. The reason for this lies in the definition of our terms; in the present analysis we have attempted to fit the shape of the low energy portion of the distribution and essentially to reproduce the shift in the peak. The equivalence set up by K. Cohen involves matching the mean energy of the neutrons below the cadmium cut-off. As we have pointed out the mean energy of the distribution is actually a divergent expression and is made finite only by introducing a cut-off at some epithermal energy. It is reasonable to take this energy as the cadmium cut-off but such a choice is purely arbitrary. The present definition has its disadvantages too; we must consider not only the Maxwell part of the flux but also the epithermal tail, whereas K. Cohen considers everything below cadmium as "thermal".

From the values given by the AEC Neutron Cross Sections Advisory Group⁴ we can now compute the change in η resulting from this change in effective neutron temperature. This calculation is presented in Table III.

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The numbers are based on a moderator temperature corresponding to 0.025 ev. and assume that the absorption cross section of U^{238} is strictly proportional to the reciprocal of the neutron velocity. The values of $\sigma_a^{25}(E)/\sqrt{T/T_0}$ were taken from the smoothed curve of the experimental data normalized arbitrarily to 650 barns at $E = 0.025$ ev. The factor f which represents the effect of the non- $1/v$ character averaged over a Maxwell distribution was also read from an expanded curve and the precision indicated for this quantity in Table III is maintained only to achieve consistency in the numerical calculation; the accuracy of the factor is of course much less. The last column in Table III represents then the variation of η with temperature. The calculated temperature coefficient is not in disagreement with direct experimental data although the accuracy of such a measurement is not high.

Combining the results of Table III with the increase in η due to epithermal captures we have, for a lattice

$$\eta_{\text{eff}} = \eta_0 (1 - 0.0131 \Delta + \frac{\lambda}{\xi \Sigma_s} \Delta^2)$$

where

$$\Delta = \frac{\Sigma_a}{\frac{2}{M} \Sigma_s}$$

and the cross sections should be properly flux-averaged over the lattice cell. In the definition of Δ we have used $2/M$ instead of ξ to indicate specifically that the collision is with the moderator molecule, and not with the individual atoms, since we are dealing mainly with neutrons whose energy is below the chemical binding energy of the molecule. Thus, for D_2O , $M = 20$ and $2/M = 0.10$ in distinction to ξ (evaluated in the epithermal region) = 0.51.

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TABLE II

MAXWELLIAN TEMPERATURE VS ABSORPTION

Δ	$\frac{4}{\sqrt{\pi}} F(0)$	$2F(-1)$	T_{eff}/T_0 $k = -1$	$\frac{2}{\sqrt{\pi}} F(-2)$	T_{eff}/T_0 $k = -2$	$(1 + 0.185\Delta)^2$
0.0	1.000000	1.000000	1.0000	1.000000	1.0000	1.0000
0.1	1.061602	1.041708	1.0386	1.023297	1.0374	1.0373
0.2	1.126201	1.085067	1.0773	1.047279	1.0754	1.0754
0.3	1.193927	1.130137	1.1161	1.071966	1.1138	1.1141
0.4	1.264935	1.176985	1.1550	1.097380	1.1527	1.1535
0.5	1.339329	1.225695	1.1940	1.123547	1.1921	1.1936
1.0	1.767549	1.499172	1.3901	1.266464	1.3957	1.4042
2.0	2.97294	2.27541	1.7071	1.623320	1.8314	1.8769

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TABLE III

VARIATION OF ETA WITH TEMPERATURE OF MAXWELL DISTRIBUTION

ev	$\sqrt{T/T_0}$	$\sigma_a^{25}(E) \sqrt{\frac{T}{T_0}}$	r	$\sigma_a^{25}(kT) \sqrt{\frac{T}{T_0}}$	$\frac{(1-R) \sigma_a^{25}}{R \sigma_a^{25}(kT)}$	η/η_0
0.0250	1.00000	650	0.98500	640.25	0.60303	1.00000
0.0275	1.04881	644.1	0.98518	634.55	0.60844	0.99663
0.0300	1.09545	637.0	0.98558	627.81	0.61497	0.99260
0.0325	1.14018	632.5	0.98618	623.75	0.61898	0.99014
0.0350	1.18322	626.9	0.98702	618.76	0.62397	0.98710
0.0375	1.22474	621.3	0.98816	613.94	0.62887	0.98413
0.0400	1.26491	616.0	0.98960	609.59	0.63336	0.98143

$$R = 0.0772 \quad \sigma_a^{28} \sqrt{\frac{T}{T_0}} = 2.80 \text{ barns}$$

$$\text{whence } \eta/\eta_0 = 1 - 0.0706 (\sqrt{T/T_0} - 1)$$

$$= 1 - (0.0706)(0.185)\Delta$$

$$= 1 - 0.0131 \Delta$$

$$\frac{1}{\eta} \frac{d\eta}{dT} = \frac{-0.0706}{2T_0} = -1.2 \times 10^{-4}/^{\circ}\text{C}$$

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3. K. C. Cooper, "Low Cost Production Reactor", HKF-117, pt. 11.
4. Neutron Cross Sections Advisory Group, BNL-170.

END