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SOME REMARKS ON THE SLOWING DOWN OF NEUTRONS IN HYDROGEN

L. C. Biedenharn
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SOME REMARKS ON THE SLOWING DOWN OF NEUTRONS IN HYDROGEN*

L. C. Biedenharn**
T. A. Welton***

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*This report is a slightly expanded version of a talk presented at an ORNL Reactor Physics Seminar, Spring, 1952.
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SOME REMARKS ON THE SLOWING DOWN OF NEUTRONS IN HYDROGEN

The use of hydrogen as a moderator in certain types of nuclear reactors has stimulated great interest in developing methods to calculate neutron slowing down in mixtures of water and heavier elements.[1,2,3] A unique feature of such moderators is the fact that a neutron can lose all of its energy in a single collision with a hydrogen atom, and this rules out at once any straightforward use of the Fermi Age theory. A very convenient, and ingenious, amalgam of the Fermi Age theory for the heavy elements and an approximate nonage theory for hydrogen has been suggested by Goertzel[1] and Selengut[4] and applied by Shapiro and Preiser among others. This technique, the Goertzel-Selengut approximation as we shall call it, is summarized in Section I.

As shown in Section II, a basic criticism of the Goertzel-Selengut approximation is that it neglects in the hydrogen moderation the strong correlation of the neutron's energy loss with scattering angle. Now the usual P_1 approximation in the Boltzmann equation is already sufficient to handle this complication. Since the P_1 approximation is explicitly made in the age theory, which is used for the heavy element moderation, it remains to be proven that the lesser approximation is justifiable for the hydrogen slowing down in the composition of the two methods as given by Goertzel and Selengut.

1. G. Goertzel, "Criticality of Hydrogen Moderated Reactors," TAB-53 (July 25, 1950).
2. M. Shapiro and S. Preiser, "Criticality Calculations for Hydrogen Moderated Reactors from Microscopic Data," ORNL-1176 (Nov. 29, 1951).
3. H. Hurwitz, Jr. and P. F. Zweifel, "Slowing Down of Neutrons by Hydrogenous Moderators," KAPL-1269 (Feb. 10, 1955).
4. D. Selengut, private communication to G. Goertzel.

It is the purpose of this report to investigate the effect of neglecting this energy loss--angle correlation. To do so, we shall consider the effects of the hydrogen alone in the slowing down. Clearly this is somewhat unfair to the Goertzel-Selengut method, for an essential part of their work was the ease of application to mixed systems. The gain in simplicity, however, offsets this loss in generality.

I. The Goertzel-Selengut Approximation

For convenience we summarize here the contents of TAB-53,[1] since this report is not too generally available.

In the Fermi age theory, with no hydrogen present, the flux $\phi(E)$ obeys the equation:

$$(\Sigma_a + D\Delta)\,\phi(E) = (\partial/\partial E)(E\xi\Sigma_s\phi) + S(E) \qquad (1)$$

where the symbols have their usual significance. In particular, $D = (3\Sigma_{transport})^{-1}$, Δ is the buckling of the reactor, and S is the neutron source function.

For a substance where only hydrogen is effective in slowing down neutrons, Selengut[4] gave the expression:

$$(\Sigma_a + \Sigma_s^{(H)} + D\Delta)\,\phi = \int_E^{\infty} (\Sigma_s^{(H)}\,\phi/E')\,dE' \qquad (2)$$

This has the form of a neutron conservation equation in which the left side represents neutron loss and the right side states that neutrons are gained in a given interval with equal probability of having been scattered out of any higher energy.

From the point of view of neutron conservation, it is reasonable, following Goertzel, to give for the case of mixtures the combined equation:

$$(\Sigma_s^{(H)} + \Sigma_a + D\Delta)\phi = \int_E^\infty \left(\frac{\Sigma_s^{(H)}\phi}{E'}\right) dE' + (\partial/\partial E)(E\xi\Sigma_s^{(Non-H)}\phi) + S \qquad (3)$$

The slowing down density can be seen to be:

$$q(E) = \int_E^\infty \left(\frac{\Sigma_s^{(H)}\phi}{E'}\right) dE' + \xi\Sigma_s^{(Non-H)}\phi \qquad (4)$$

II. The P_1 Approximation for Pure Hydrogen

Let us consider now the case of neutrons slowing down in a medium composed only of hydrogen. Furthermore, let us assume that the hydrogen has no absorption cross section, but only the observed n-p scattering section, Σ.

The Boltzmann equation for this case is then:[5]

$$\vec{\Omega}\cdot\vec{\nabla}F + \Sigma F = \frac{1}{2\pi} \int_E^\infty \int_{\vec{\Omega}'} \Sigma F(dE'/E')\ \delta\left[\mu_o - \mu_o(EE')\right]\ d\Omega' + S \qquad (5)$$

with Fourier transform:

$$ik\mu\phi + \Sigma\phi = \frac{1}{2\pi} \int_E^\infty \int_{\vec{\Omega}'} (\Sigma\phi/E')\ \delta\left[\mu_o - \mu_o(EE')\right]\ d\Omega'\ dE' + \bar{S} \qquad (6)$$

The δ function is expanded in the form:

5. A. M. Weinberg and L. Noderer, "Theory of Neutron Chain Reactions: Extracts from Volume I, Diffusion and Slowing Down of Neutrons," ORNL-CF-51-5-98 (AECD-3471)(May 15, 1951; decl. June 19, 1952).

$$\delta\left[\mu_o - \mu_o(EE')\right] = \sum_{\ell}\left(\frac{2\ell+1}{2}\right) P_{\ell}\left[\mu_o(EE')\right] P_{\ell}(\mu_o) \tag{7}$$

where

$\mu_o(EE') = (E/E')^{1/2}$.

Upon introducing explicitly the P_1 approximation, i.e., that

$$\phi = \sum_{\ell}\left(\frac{2\ell+1}{2}\right) \phi_{\ell} P_{\ell}$$

and terminating the series at $\ell = 1$, one finds the coupled equations:

$$ik\phi_1 + \Sigma\phi_o = \int_E^{\infty} \Sigma \frac{dE'}{E'} \phi_o + S_o \tag{8a}$$

$$\frac{ik}{3} \phi_o + \Sigma\phi_1 = \int_E^{\infty} \frac{dE'}{E'}\sqrt{\frac{E}{E'}} \phi_1 \tag{8b}$$

(In deriving these equations the source has been assumed to be spherically symmetric.)

The last equation is easily solved for ϕ_1 as a function of ϕ_o. This is

$$\phi_1 = -\frac{ik}{3\Sigma}\phi_o + \frac{1}{\Sigma\sqrt{E}} \int_E^{\infty}\left(\frac{-ik}{3}\right)\frac{\phi_o}{\sqrt{E'}}\, dE' \tag{9}$$

Finally one obtains the equation for the flux in the P_1 approximation to be:

$$\phi_o \left[\Sigma + \frac{k^2}{3\Sigma}\right] = \int_E^\infty \frac{dE'}{E'} (\Sigma\phi_o) \left[1 - \sqrt{\frac{E'}{E}} \frac{k^2}{3\Sigma(E)\Sigma(E')}\right] + S_o \tag{10}$$

If we compare this equation with the Goertzel-Selengut approximation, one sees that there are two differences:

1. The term $- \int_E^\infty \frac{dE'}{E'} \left[\phi_o \sqrt{\frac{E'}{E}} \frac{k^2}{3\Sigma(E)}\right]$ on the right of Eq. 10 is missing in the Goertzel-Selengut approximation.
2. The diffusion constant D in the Goertzel-Selengut case involves Σ_{tr}, whereas the above equation involves $\Sigma = 3\Sigma_{tr}$.

In order to compare the predictions of the Goertzel-Selengut approximation with the P_1 approximation, it is convenient to consider the moments of the flux distribution. As is well known, the second moment is yielded exactly by the P_1 approximation. Furthermore, the even moments bear a simple relation to the derivatives of ϕ_o with respect to k^2 at $k^2 = 0$. For example, the second moment is given by:

$$\overline{r^2} = \frac{3! \left.\frac{d\phi_o}{dk^2}\right|_0}{\phi_o(0)} \tag{11}$$

As a result we can compare the exact second moment with the Goertzel-Selengut second moment straight away without having to invert the Fourier transformation. However, the second moment is of direct significance in reactor calculations, and thus we have a convenient "figure of merit" on which to base a comparison of the approximation.

In carrying out this program it is equivalent to expand ϕ_o as a power series in the variable k^2. This effectively "decouples" Eq. 10 and makes it now exactly solvable, even for an arbitrary cross section. Let us carry this out briefly.*

Let

$$\phi_o = \phi^{(o)} + k^2 \phi^{(2)} + \ldots \tag{12}$$

Then Eq. 10 becomes

$$\Sigma\phi^{(o)} = S_o + \int_E^\infty \Sigma \frac{dE'}{E'} \phi^{(o)} \tag{13a}$$

$$\Sigma\phi^{(2)} - \int_E^\infty \Sigma \frac{dE'}{E'} \phi^{(2)} = - \frac{1}{3\Sigma} \phi^{(o)} - \int_E^\infty \frac{dE'}{3E'} \phi^{(o)} \sqrt{\frac{E'}{E}} \frac{1}{\Sigma(E)} \tag{13b}$$

with the solutions:

$$\Sigma\phi^{(o)} = S_o + \frac{\mathbb{1}}{E} \tag{14a}$$

$$\begin{aligned}\Sigma\phi^{(2)} = & - \frac{1}{3\Sigma^2} \left(S_o + \frac{\mathbb{1}}{E}\right) - \frac{\mathbb{1}}{3\Sigma\Sigma_o\sqrt{EE_o'}} \\ & - \frac{\mathbb{1}}{3\Sigma} \int_E^{E_o} \frac{dE'}{(E')^2} \sqrt{\frac{E'}{E}} \frac{1}{\Sigma} \\ & + \frac{1}{E}\left[- \frac{\mathbb{1}}{3\Sigma_o^2} - \frac{\mathbb{1}}{3} \int_E^{E_o} \frac{dE'}{E'\Sigma^2} - \frac{\mathbb{1}}{3\sqrt{E_o'}\,\Sigma} \int_E^{E_o} \frac{dE'}{\sqrt{E'}\,\Sigma} \right. \\ & \left. - \frac{\mathbb{1}}{3} \int_E^{E_o} \frac{dE'}{(E')^{1/2}\Sigma} \int_E^{E_o} \frac{dE''}{(E'')^{3/2}} \cdot \frac{1}{\Sigma} \right]\end{aligned} \tag{14b}$$

*The source S is taken to be a spherically symmetric point source emitting neutrons of energy E_o. The symbol $\mathbb{1}$ is the Heaviside unit function: $\mathbb{1} = 0$ for $E > E_o$ and 1 for $E < E_o$. The notation Σ_o means $\Sigma(E_o)$.

The exact second moment is now readily obtained. This is:

$$\left(\frac{1}{6}\overline{r^2}\right)_{exact} = \frac{1}{3}\left\{\frac{1}{\Sigma^2} + \frac{1}{\Sigma_o^2} + \frac{1}{\Sigma\Sigma_o}\sqrt{\frac{E}{E_o}} + \frac{\sqrt{E}}{\Sigma}\int_E^{E_o}\frac{dE}{E^{3/2}\Sigma}\right.$$

$$+ \int_E^{E_o}\frac{dE}{E\Sigma^2} + \frac{1}{\Sigma_o\sqrt{E_o}}\int_E^{E_o}\frac{dE}{\Sigma\sqrt{E}}$$

$$\left. + \int_E^{E_o}\frac{dE'}{\sqrt{E'}\Sigma}\int_{E'}^{E_o}\frac{dE''}{(E'')^{3/2}\Sigma}\right\} \tag{15}$$

This formula is very well known.[6,7,8]

The equivalent formula for the Goertzel-Selengut approximation is as easily obtained. It turns out that a useful mnemonic is to go through the previous results eliminating square roots and replacing Σ by $\sqrt{\Sigma\Sigma_{tr}}$ (or equivalently multiplying by 3). Thus

$$\left(\frac{1}{6}\overline{r^2}\right)_{G-S} = \left[\frac{1}{\Sigma^2} + \frac{1}{\Sigma_o^2} + \int_E^{E_o}\frac{dE}{E\Sigma^2}\right] \tag{16}$$

As a first example, consider the case of constant cross sections. The result is given in Fig. 1. It is clear that the Goertzel-Selengut approximation overestimates the second moment. The Goertzel-Selengut result, however, becomes asymptotically correct for large lethargy. (It should be pointed out that the second moment is discontinuous at the threshold energy.)

6. E. Fermi, "Sul moto dei neutroni nelle sostange idrogenate," Ricerca Sci. 7(2), 13 (1936).
7. L. S. Ornstein and G. E. Uhlenbeck, "Some Kinetic Problems Regarding the Motion of Neutrons Through Paraffine," Physica 4, 478 (1937).
8. R. E. Marshak, "Theory of the Slowing Down of Neutrons by Elastic Collision with Atomic Nuclei," Revs. Mod. Phys. 19, 185 (1947).

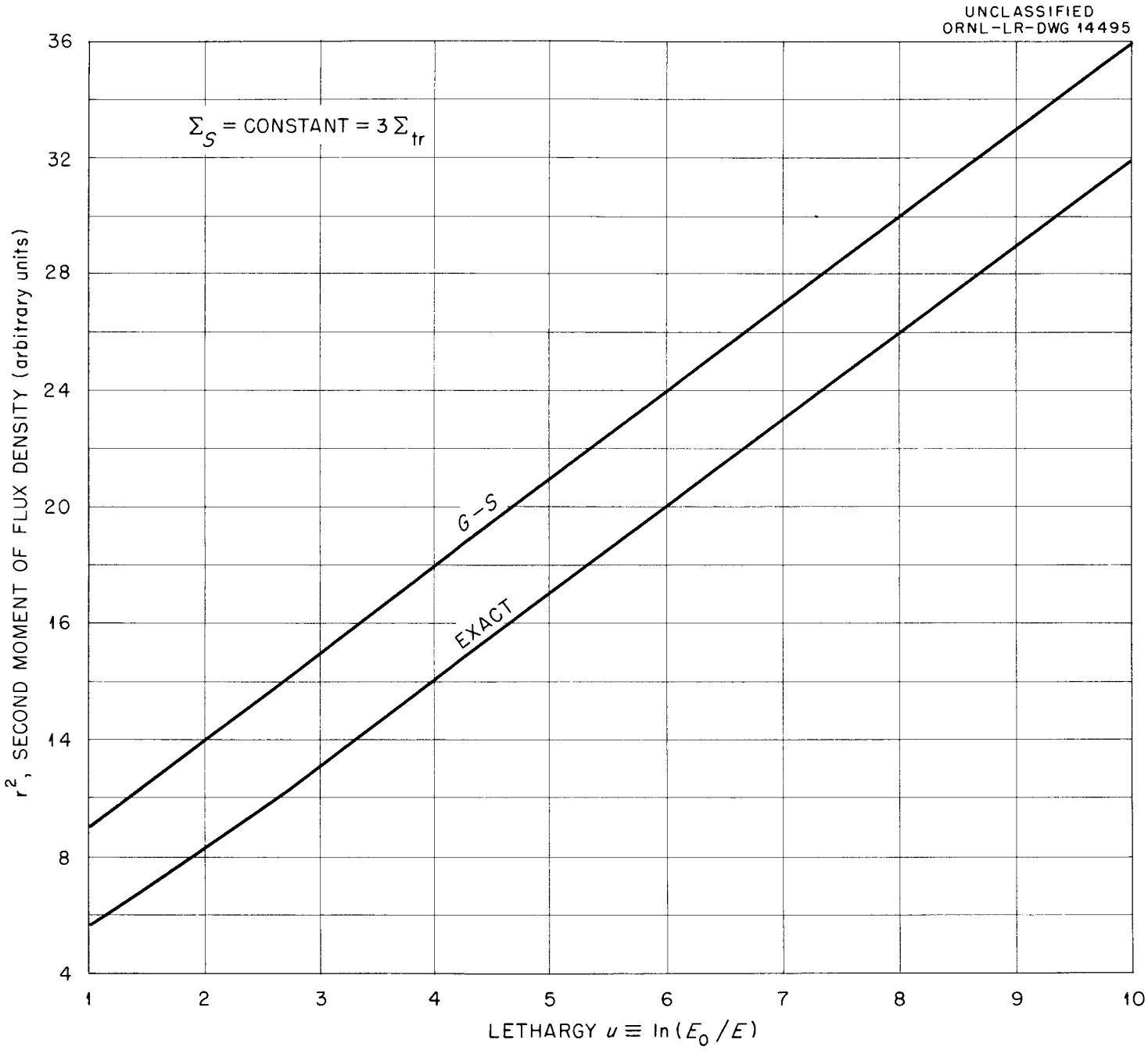

Fig. 1. Constant Cross Section Example.

Before proceeding on to more realistic examples there is something odd about the results so far. Suppose for the sake of discussion we assume that $\bar{\Sigma} = 1/E$. Then one finds that

$$\left(\frac{1}{6}\ \overline{r^2}\right)_{exact} = \frac{1}{6}\left[5E_o^{\,2} - E^2 + 2E^{3/2}\,E_o^{\,1/2}\right] \tag{17}$$

from which we find that

$$\frac{d}{dE}\left(\frac{1}{6}\ \overline{r^2}\right) = -\frac{E}{3} + \frac{1}{2}\sqrt{EE_o} > 0 \tag{18}$$

for $E < E_o$

Hence the "slowing down length" <u>decreases</u> as the energy <u>decreases</u>. This is certainly odd, when one remembers--correctly--that the slowing down length is an <u>increasing</u> function of the lethargy.

The trouble, of course, lies in terminology. The term "slowing down length" has been used in two distinct ways in the literature. The more customary procedure is to use the slowing down length to mean the second moment of the slowing down density. The second way is to mean the second moment of the flux--which was used earlier. The two meanings are equivalent in the age approximation; for hydrogen they are quite distinct.

It is simple enough to correct the preceding results and obtain the true slowing down length. The slowing down density is related to the flux by the equation:

$$q = \int_E^{\infty} \phi_o \frac{dE'}{E'} \tag{19}$$

Since the operations of integrating over E' and expanding in powers of k^2 commute, we can simply alter our previous work accordingly. The results are

$$q^{(o)} = \frac{\mathbb{1}}{E} \tag{20a}$$

$$q^{(2)} = -\frac{\mathbb{1}}{3}\left[\frac{1}{\Sigma_o^2} + \int_E^{E_o} \frac{dE'}{E'\Sigma} + \frac{1}{\Sigma_o\sqrt{E_o}}\int_E^{E_o}\frac{dE'}{(E')^{1/2}\Sigma}\right.$$

$$\left. + \int_E^{E_o}\frac{dE'}{\sqrt{E'}\Sigma}\int_{E'}^{E_o}\frac{dE''}{(E'')^{3/2}\Sigma}\right] \tag{20b}$$

The second moment of the slowing down density is defined customarily as six times the slowing down length (τ). Hence we find

$$\tau_{exact} = \frac{1}{3}\left[\frac{1}{\Sigma_o^2} + \int_E^{E_o}\frac{dE'}{E'\Sigma^2} + \frac{1}{\sqrt{E_o}\,\Sigma_o}\int_E^{E_o}\frac{dE'}{(E')^{1/2}\Sigma}\right.$$

$$\left. + \int_E^{E_o}\frac{dE'}{\sqrt{E'}\Sigma}\int_{E'}^{E_o}\frac{dE''}{(E'')^{3/2}\Sigma}\right] \tag{21}$$

The difference between two second moments is illustrated in Fig. 2. It can be easily verified that τ is indeed an increasing function of the lethargy. Near the threshold energy τ approaches $\frac{1}{3}\,\frac{1}{\Sigma_o^2}$, which is to be expected from the distribution of first collisions.

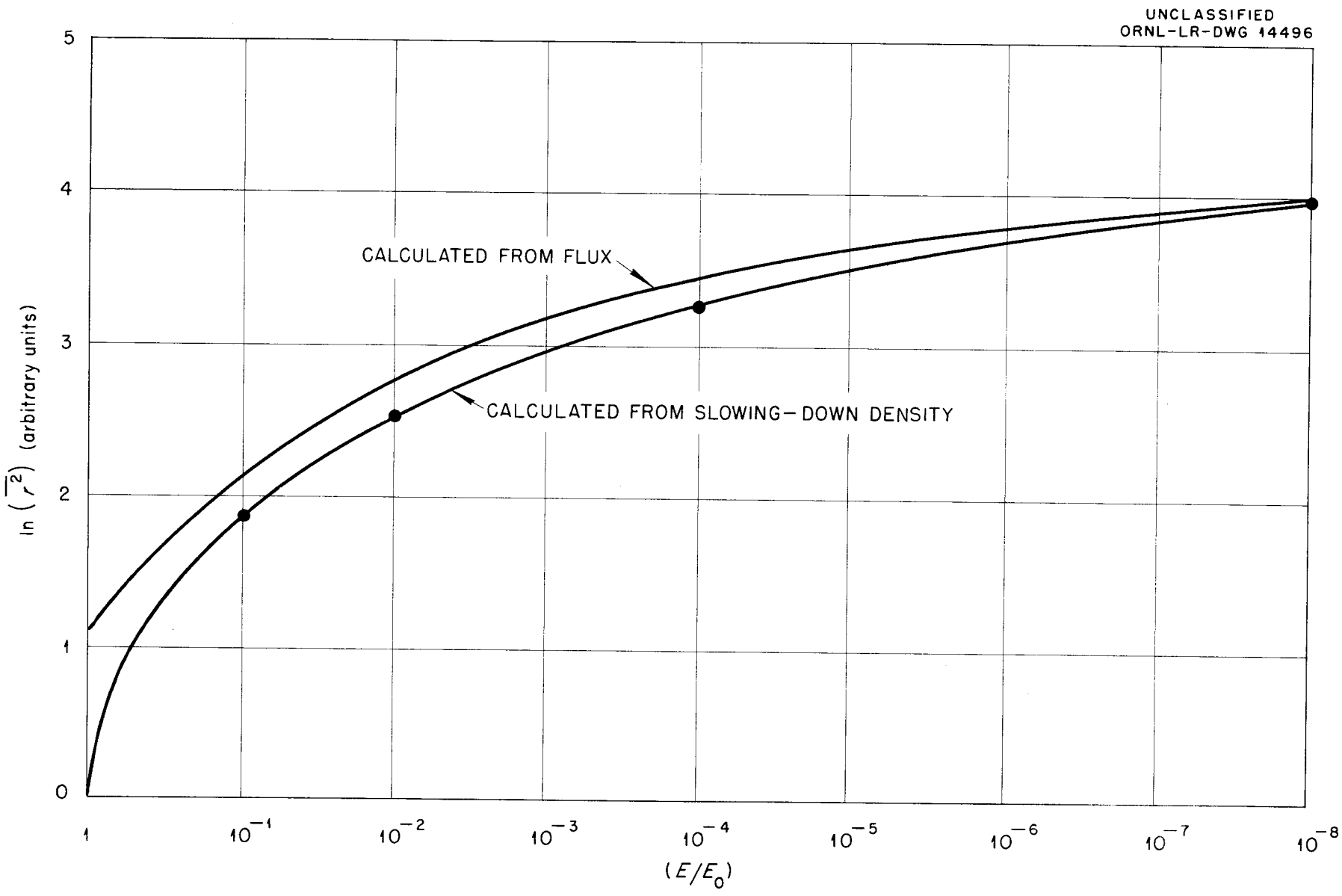

Fig. 2. Second Moment Calculations for Constant Cross Sections.

To calculate τ in the Goertzel-Selengut approximation one can use the mnemonic mentioned earlier and obtain:

$$\tau_{G-S} = \frac{1}{\Sigma_o^2} + \int_E^{E_o} \frac{dE'}{E'\Sigma^2} \tag{22}$$

The terms here have a very simple interpretation. The first term is <u>three</u> times the result to be expected from the distribution of first collisions; this arises from the Goertzel-Selengut use of $\Sigma_{tr} = \frac{1}{3}\Sigma$ in the diffusion constant. The second term can be written as

$$\int_E^{E_o} \frac{dE'}{3\xi\Sigma_{tr}\Sigma_{E'}} \; - -$$

which is just the Fermi age. A large part of the Goertzel-Selengut overestimate of the age comes from the $\frac{1}{\Sigma_o^2}$ term. In a crude way one sees that the neglect of the energy loss-angle correlation does lead to such a result, for the use of the transport cross section neglects the fact that the collisions cause an effective absorption of the neutrons. On the other hand, the Goertzel-Selengut use of Σ_{tr} is necessary in the Fermi age term in order to obtain asymptotic agreement for large lethargy. (The constant cross-section examples show that if $\Sigma \longrightarrow$ constant as $E \longrightarrow 0$, then the Goertzel-Selengut result must approach the exact result for $E \longrightarrow 0$.)

In order to give a realistic comparison of the slowing down length in the two cases, we have calculated using the observed n-p scattering cross section. The constants of the effective range theory give an

excellent fit from 0 up to, say 10 Mev.[9] If we neglect the E^2 term in the triplet case, and put the singlet range to zero, i.e., use:

$$\sigma_H(\text{barns}) = \frac{2.605}{E + 0.1476} + \frac{11.424}{E + 4.171} \quad (E \text{ in Mev}) \tag{23}$$

then this fits the observed cross section from 1 Mev to 0 with an error of better than 1%. (The error increases rapidly with E, but is only 10% at 10 Mev.) The advantages of such a form is that it can be integrated in closed form.

Figures 3 and 4 illustrate the results obtained.

III. Conclusions

It is clear from the foregoing that the Goertzel-Selengut approximation--that is, the neglect of the neutron's energy loss with scattering angle--causes appreciable error in the slowing down length in hydrogen. Nevertheless, the approximation has had very good success in predicting the observed slowing down lengths in water, and it is, of course, undeniably convenient. While no conclusion can be drawn without much further study, such as begun by Hurwitz and Zweifel, there is some indication that the fission source distribution might possibly be the source of the discrepancy. Since the hydrogen cross section varies so rapidly near 1 Mev, the age should be quite sensitive to the exact form of the fission spectrum in this region.

The authors would like to thank Dr. Mathew Shapiro for his helpful discussions and his aid, particularly in pointing out the significance of the use of Σ_{tr} in the Goertzel-Selengut approximation.

9. J. M. Blatt and V. F. Weisskopf, Theoretical Nuclear Physics, John Wiley and Sons, New York, 1952.

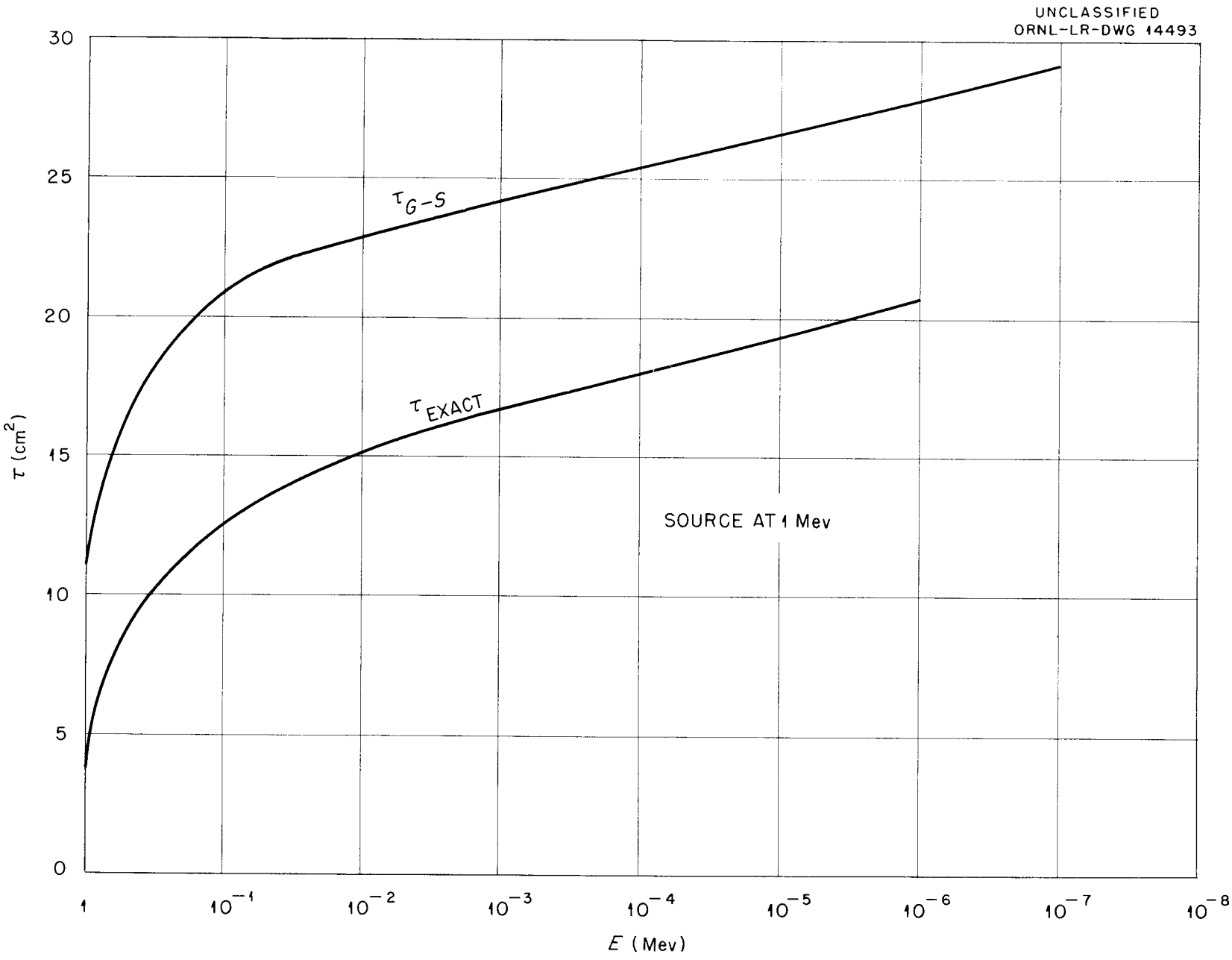

Fig. 3. Values of τ_{EXACT} and τ_{G-S} for Water, Considering Only the Hydrogen Effective and Using the Experimental Σ_H.

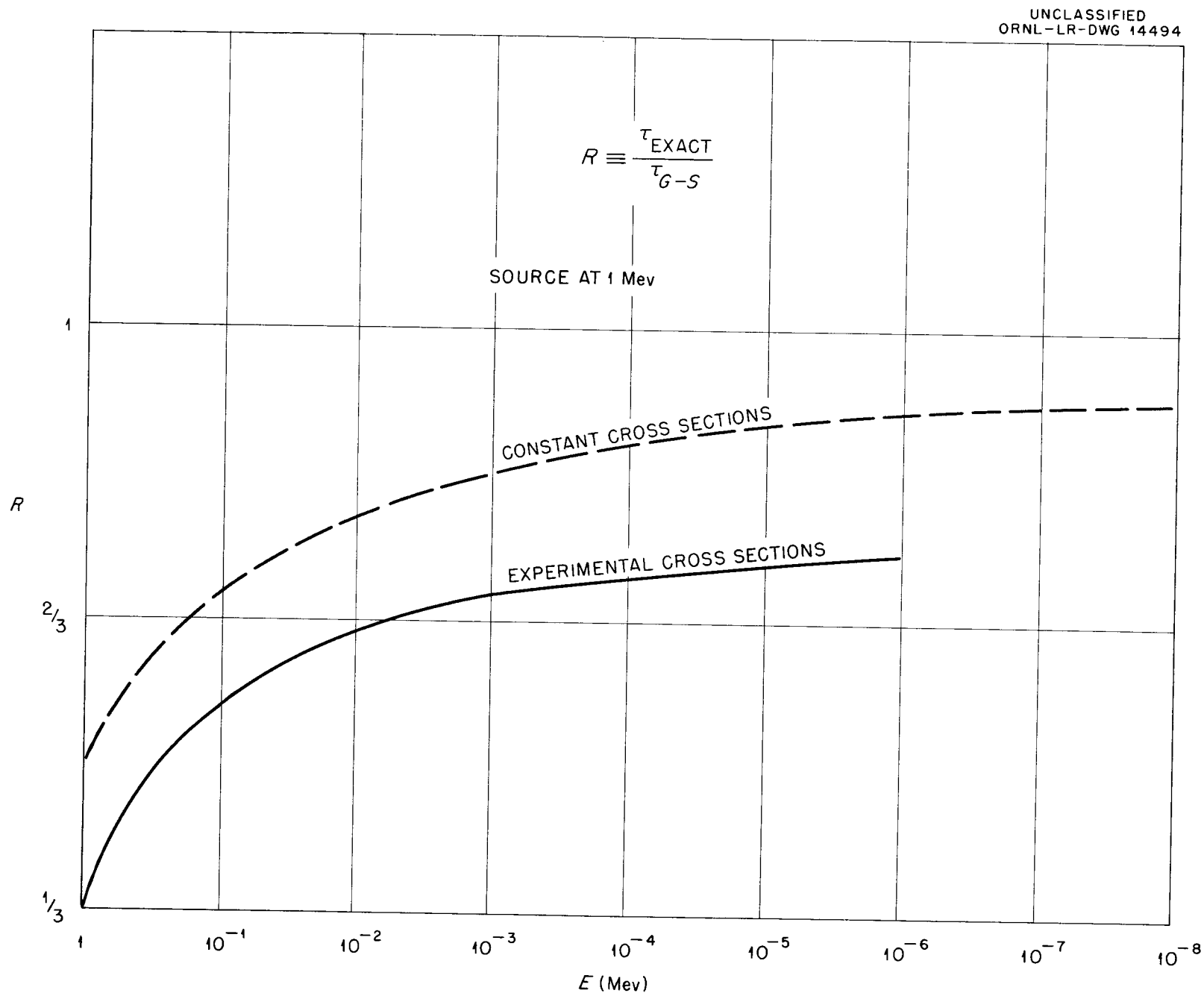

Fig. 4. Ratio of Slowing-Down Lengths in Hydrogen with Various Cross Sections.