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NEUTRON THERMALIZATION IN A HEAVY MODERATOR WITH AN ABSORPTION RESONANCE

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ABSTRACT

The neutron velocity spectrum resulting from interaction of a high-energy neutron source with a spatially infinite, heavy gaseous moderator is obtained by solution of the Wilkins equation for the case of $1/v$ absorption cross section plus a single sharp resonance. The resonance is assumed to be narrow enough so that variations in the flux through the resonance are small with respect to the average flux in the resonance, yet broad with respect to the average energy loss per collision.

The resonance escape probability and the effective resonance integral are defined and calculated. It is shown that the effect of the thermal motion of the moderator on the effective resonance integral can be expressed, in first order, as a correction to the mean logarithmic energy loss per collision. This correction, which can be described as the contribution of energy transfer from moderator to neutron, is the same as the one proposed by Cohen, and increases the resonance integral by ten percent even for resonance energies as high as 20kT.

I. NEUTRON SPECTRUM FOR A MIXED MODERATOR

The neutron spectrum in an infinite heavy moderator in the presence of an absorption cross section with a pure inverse velocity dependence has been the subject of much discussion.[1,2,3,4] Both Wilkins[1] and Hurwitz[2] have shown that the problem can be reduced to the solution of the following differential equation:

$$xN''(x) + (2x^2 - 1)N'(x) + (4x - \Delta)N(x) = 0 \qquad \ldots(1)$$

In this expression, x is proportional to the velocity of the neutron, i.e., $x = \beta v$; β is given by $\beta^2 = 1/2kT$, where T is the moderator temperature and the mass of the neutron is unity. N(x) is the number of neutrons per unit volume having a velocity between x and x + dx, and Δ is the absorption parameter, i.e., $\Delta = 2mx\,\sigma_a(x)/\sigma_s$, where m is the moderator atomic mass in units of neutron mass. Since it is assumed that $\sigma_a(x) = \sigma_o/x$ and since σ_s is constant, $\Delta = 2m\,\sigma_o/\sigma_s$.

Wilkins arrived at (1) by a consideration of the process of diffusion of a neutron gas into a heavy Maxwellian moderator gas under the assumptions that neutron-neutron collisions are vanishingly infrequent, neutron-moderator collisions alter the neutron spectrum only, and a steady state distribution of neutrons exists. Under these assumptions, the space-and-time-independent source-free form of the Boltzman transport equation becomes[2]

$$\int_o^\infty G_s(v' \rightarrow v)N(v')dv' = \left[\gamma(v) + V(v)\right] N(v), \qquad \ldots(2)$$

where $G(v' \rightarrow v)$ is the scattering rate per neutron from velocity v' to velocity v, $\gamma(v)$ is the absorption rate per neutron at velocity v, and

$$V(v) = \int_o^\infty G_s(v \rightarrow v')dv' .$$

For a mixture of heavy gases, (2) may be rewritten as

$$\int_0^\infty \sum_i G_{si}(v' \rightarrow v) N(v') dv' = N(v) \sum_i \left[V_i(v) + \gamma_i(v) \right], \qquad \ldots (3)$$

in which the various symbols are defined as before but apply to the i^{th} component in the mixture.

Analogously to the way in which (1) is derived from (2), the following differential equation is obtained from (3):

$$xN''(x) + (2x^2 - 1)N'(x) + (4x - \bar{\Delta})N(x) = 0, \qquad \ldots (4)$$

where

$$\bar{\Delta} = \frac{4x \sum_i n_i \sigma_{ai}(x)}{\sum_i 2\, n_i \sigma_{si} / m_i} = \frac{4x \sum_i n_i \sigma_{ai}(x)}{\sum_i \xi_i n_i \sigma_{si}} = \frac{4x \Sigma_a}{\overline{\xi \Sigma_s}}, \qquad \ldots (5)$$

n_i is the density of atoms of the i^{th} kind, and ξ_i is their mean logarithmic energy loss per collision. From (5) it is evident that if the $\sigma_{ai}(x)$ are each of the form σ_{oi}/x, $\bar{\Delta}$ is a constant and thus (4) is exactly of the form (1).* Hence the problem of determining the neutron spectrum in a mixture of 1/v-absorbing Maxwellian gases is reduced to that of a single gas having a $\Delta = \bar{\Delta}$.

*If those components of the mixture having absorption cross sections proportional to 1/v are vastly predominant in relative number, $\bar{\Delta}$ is essentially constant, even if there are components which are non–1/v.

II. NEUTRON DENSITY SPECTRUM IN A 1/V ABSORBER WITH A SINGLE SHARP ABSORPTION RESONANCE

This problem is conveniently treated by considering the absorption maximum to be a negative source. The problem is thereby altered to the determination of the neutron spectrum in a two-source system.

Consider a source, S_∞, which introduces neutrons of infinite velocity into a Maxwellian moderator with 1/v absorption. There results a neutron spectrum $N_\infty(x)$ which satisfies Equation (1). Furthermore, consider another source of strength S_∞ but of such a kind that it introduces neutrons of velocity x_1 into the same moderator. In general there results a neutron spectrum which for $x \leq x_1$ is designated by $N_1(x)$, and for $x \geq x_1$ is designated by $N_2(x)$. If now, into the same moderator is introduced at the same time a source, S_∞, of neutrons of infinite velocity and a source, S_1, of neutrons of velocity x_1, then the total neutron spectrum N(x) is given by the sum of the two preceding distributions:

$$\begin{aligned} N(x) &= N_\infty(x) + \left(S_1/S_\infty\right)N_1(x) \qquad x \leq x_1 \\ N(x) &= N_\infty(x) + \left(S_1/S_\infty\right)N_2(x) \qquad x \geq x_1 \end{aligned} \qquad \ldots(6)$$

The functions $N_\infty(x)$, $N_1(x)$, and $N_2(x)$ are to be obtained by solution of (1), which holds for any source-free region, with appropriate boundary conditions.

It has been demonstrated[2] that a first integral of (1) may be written as

$$\frac{\Delta \sigma_s \xi}{4} \int N(x')dx' = \frac{\sigma_s \xi}{2}\left[(x^2-1)N(x) + \frac{1}{2}xN'(x) + C'\right] . \qquad \ldots(7)$$

The quantity on the left is just the neutron absorption rate between whatever limits one cares to place on the integral. Furthermore, $N_\infty(x)$ is known to behave asymptotically as follows:[1]

$$\begin{aligned} N_\infty(x) &\sim x^2 \qquad x \to 0 \\ N_\infty(x) &\sim C/x^2 \qquad x \to \infty \end{aligned} \qquad \ldots(8)$$

At steady state, one has

$$\frac{\Delta \sigma_s \xi}{4} \int_0^{\infty} N_{\infty}(x) dx = S_{\infty} \quad ,$$

and from (7) and (8),

$$C = \frac{2S_{\infty}}{\sigma_s \xi} \quad . \qquad \ldots (9)$$

Also, if one writes

$$\frac{\Delta}{2} \int_0^x N_{\infty}(x) dx = (x^2 - 1) N_{\infty}(x) + \frac{1}{2} x N'_{\infty}(x) \quad ,$$

for which $x^{-3} e^{x^2}$ is an integrating factor, there follows[3]

$$N_{\infty}(x) = x^2 e^{-x^2} \left[\frac{4}{\sqrt{\pi}} + \Delta \int_0^x \frac{e^{u^2}}{u^3} \int_0^u N_{\infty}(t) dt \, du \right] \quad . \qquad \ldots (10)$$

This latter may be used as the basis of an iterative method[3] to determine $N_{\infty}(x)$ as a series in ascending powers of Δ which, because (10), after reversing order of integration, is a Volterra-type integral equation, is convergent for all values of x and Δ. It is to be observed that S_{∞} (and therefore C) has been chosen so that the Maxwellian portion of the solution is normalized.

If neutrons are introduced at some velocity x_1 instead of at infinite velocity, and furthermore are introduced at the rate S_{∞} neutrons per second, then (1) must be solved in two ranges of x values, since it is valid only in a source-free region. Included in the first region, are all values of x between zero and x_1, and in the second region, those values greater than or equal to x_1. The first solution has been called $N_1(x)$ and the second $N_2(x)$; these solutions are still to be determined.

It is convenient to find first another solution of (1), $N_o(x)$, arising from a source of strength S_o neutrons per second introducing neutrons of velocity $x = 0$. Since $N_o(x)$ is a solution of (1), (7) is satisfied by $N_o(x)$. Its asymptotic behavior is given by Wilkins as

$$N_o(x) \sim x^2 e^{-x^2} \qquad \text{as } x \to \infty .$$

Hence

$$\frac{\Delta}{2}\int_x^\infty N_o(x)dx = -\left[(x^2-1)N_o(x) + \tfrac{1}{2}xN_o'(x)\right] . \qquad \ldots (11)$$

From (11), one obtains

$$\frac{d}{dx}\left[\frac{e^{x^2}}{x^2}N_o(x)\right] = -\frac{e^{x^2}}{x^3}\Delta\int_x^\infty N_o(x)dx$$

and

$$N_o(x) = x^2 e^{-x^2}\left[a_o + \Delta\int_x^\infty \frac{e^{u^2}}{u^3}\int_u^\infty N_o(t)dt\,du\right] . \qquad \ldots (12)$$

It is shown (Appendix A) that if one chooses $a_o = 4/\sqrt{\pi}$, then S_o is so normalized that $S_o = S_\infty = \sigma_s C \xi/2$. Hence a source equal in strength to S_∞, but from which neutrons are introduced at velocity $x = 0$, yields a distribution $N_o(x)$ given by

$$N_o(x) = x^2 e^{-x^2}\left[\frac{4}{\sqrt{\pi}} + \Delta\int_x^\infty \frac{e^{u^2}}{u^3}\int_u^\infty N_o(t)dt\,du\right] . \qquad \ldots (13)$$

$N_1(x)$ and $N_2(x)$ can be related to $N_o(x)$ and $N_\infty(x)$, by exploiting the following properties of $N_1(x)$ and $N_2(x)$:

1) Both are solutions to Wilkins' equation in a given region.

2) Because of the thermal motion of the moderator, collisions resulting in increased neutron energy as well as decreased neutron energy occur; hence $N_1(x)$ and $N_2(x)$ are continuous across $x = x_1$ and $N_1(x_1) = N_2(x_1)$.

3) $$\frac{\Delta \xi \sigma_s}{4} \left\{ \int_o^{x_1} N_1(x)dx + \int_{x_1}^{\infty} N_2(x)dx \right\} = S_\infty \quad .$$

It is easily verified (Appendix B) that the three foregoing conditions are satisfied by

$$N_1(x) = \frac{N_o(x_1)}{\frac{4}{\sqrt{\pi}} x_1^2 e^{-x_1^2}} N_\infty(x)$$

and ...(14)

$$N_2(x) = \frac{N_\infty(x_1)}{\frac{4}{\sqrt{\pi}} x_1^2 e^{-x_1^2}} N_o(x) \quad .$$

An absorption resonance at x_1 introduces into (6) a negative source, whose strength S_1 is given by

$$S_1 = -\int_{x_1 - \epsilon}^{x_1 + \epsilon} xN(x)\sigma_a(x)dx \quad . \qquad ...(15)$$

Thus if 2ϵ is small enough so that there is not much variation in $xN(x)$, yet large enough so that the absorption resonance is wide with respect to the scattering kernel $G_s(v' \rightarrow v)$ in (2), the limit of applicability of the Wilkins' equation, there results

$$S_1 \cong - x_1 N(x_1) \int_{x_1 - \epsilon}^{x_1 + \epsilon} \sigma_a(x) dx = -x_1 N(x_1) \hat{\sigma}_a \quad , \qquad \ldots (16)$$

and from (6),

$$N(x_1) = N_{\infty}(x_1) - \frac{x_1 N(x_1) \hat{\sigma}_a}{S_{\infty}} N_1(x_1) \quad .$$

Thus, from (9), (14), and (16), Equation (6) becomes for the case of a resonance

$$N(x) = \frac{1}{1 + D} N_{\infty}(x) \qquad x \leq x_1$$

$$N(x) = N_{\infty}(x) - \frac{N_{\infty}(x_1)/N_o(x_1)}{1 + 1/D} N_o(x) \qquad x \geq x_1 \quad , \qquad \ldots (17)$$

where

$$D = \frac{\sqrt{\pi}\, \hat{\sigma}_a e^{x_1^2}}{2x_1 \sigma_s \xi C} N_o(x_1) N_{\infty}(x_1) \quad ,$$

$$\hat{\sigma}_a = \int_{x_1 - \epsilon}^{x_1 + \epsilon} \sigma_a(x) dx \quad .$$

Figure 1 presents curves for a typical mixture, in which N(x) has been computed at two temperatures. Superimposed upon the plots of N(x) is a curve of $N_{\infty}(x)$ for the same Δ but without a resonance.*

*Although $N_o(x)$ and $N_{\infty}(x)$ were developed for heavy gases, Nelkin[5] has shown that even for a Debye solid, the neutron spectrum is only slightly different from $N_{\infty}(x)$.

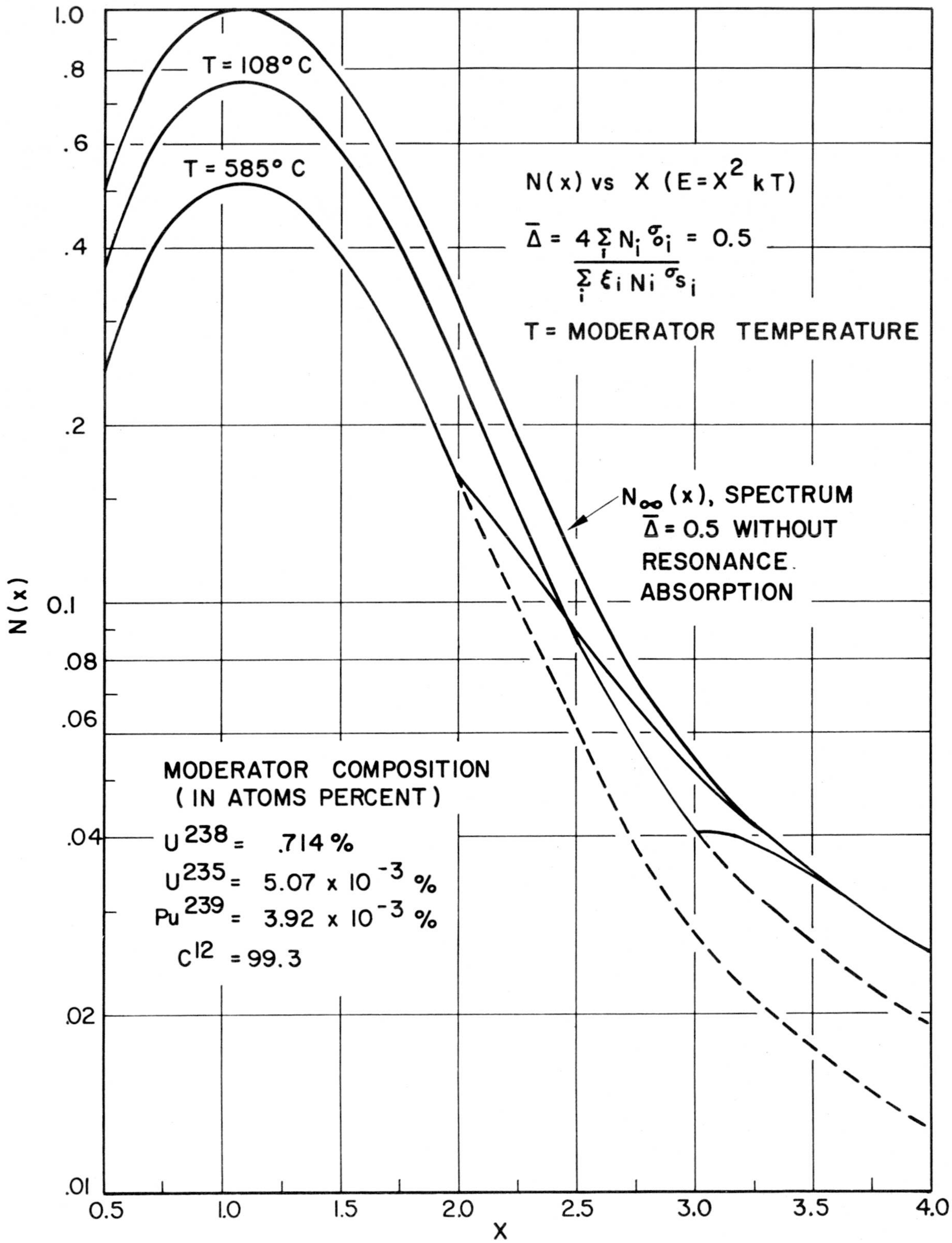

Figure 1. Neutron Velocity Spectrum in a Heavy Moderator With an Absorption Resonance

III. RESONANCE ESCAPE PROBABILITY AND EFFECTIVE RESONANCE INTEGRAL

Figure 1 indicates that the presence of an absorption resonance not only reduces the neutron spectrum generally for energies below the resonance energy, but also introduces a distortion in the neighborhood of the resonance. The extension of the distortion above the resonance is attributed to the loss in the resonance region of neutrons which normally would have been scattered up into the region of the distortion from the low side of the resonance, since it is seen from (17) that the correction to $N_\infty(x)$ above the resonance approaches zero in the same manner as $x^2 e^{-x^2}$, i.e., the moderator distribution.

The definition of the resonance escape probability is complicated by the presence of the distortion above the resonance. The probability that a neutron escapes the resonance is the ratio of the number of neutrons which escape to the number which would have "escaped" had there been no resonance present. Thus,

$$p(x_1, \Delta) = \frac{\dfrac{\Delta \sigma_s \xi}{4} \displaystyle\int_o^{x_1} N(x)dx}{\dfrac{\Delta \sigma_s \xi}{4} \displaystyle\int_o^{x_1} N_\infty(x)dx} \qquad \ldots(18)$$

$$= \frac{1}{1 + D} \quad .$$

The effective resonance integral $I_{eff}(x_1, \Delta)$ is defined[6] as

$$I_{eff}(x_1, \Delta) = \sigma_s \xi \, \frac{1 - P(x_1, \Delta)}{P(x_1, \Delta)}$$

$$I_{eff}(x_1, \Delta) = \frac{\hat{\sigma}_a \sqrt{\pi} e^{x_1^2}}{2Cx_1} N_o(x_1) N_\infty(x_1) \quad . \qquad \ldots(19)$$

Therefore $I_{eff}(x_1, \Delta)$ may be written as

$$I_{eff}(x_1, \Delta) = E(x_1, \Delta) I_{res}(x_1),$$

where $E(x_1, \Delta)$, the enhancement factor, is given by

$$E(x_1, \Delta) = \frac{\sqrt{\pi}\, e^{x_1^2}}{4C} N_o(x_1) N_\infty(x_1) \quad , \qquad \ldots (20)$$

and

$$I_{res}(x_1) = 2 \int_{x_1 - \epsilon}^{x_1 + \epsilon} \sigma_a(x) \frac{dx}{x} \quad . \qquad \ldots (21)$$

$E(x_1, \Delta)$ has been evaluated for various x_1 and Δ and curves are given in Figure 2. The enhancement factor may be studied for large x_1 by use of the asymptotic series for $N_o(x)$ and $N_\infty(x)$ given by Wilkins:[1]

$$N_o(x) = \frac{4}{\sqrt{\pi}} x^2 e^{-x^2} \left[1 + \frac{\Delta}{2x} + \frac{\Delta^2}{8x^2} + \frac{\Delta^3 + 4\Delta}{48x^3} + \frac{\Delta^4 + 16\Delta^2}{384x^4} + \ldots \right],$$

$$N_\infty(x) = \frac{C}{x^2} \left[1 - \frac{\Delta}{2x} + \frac{\Delta^2 + 16}{8x^2} - \frac{\Delta^3 + 76\Delta}{48x^3} + \ldots \right],$$

whence

$$E(x_1, \Delta) \cong \left[1 + \frac{2}{x^2} - \frac{\Delta}{2x^3} + 0\left(\frac{1}{x^4}\right) \right] \qquad \ldots (22)$$

For small Δ, $E(x_1, \Delta)$ is different from unity by 10% for $x^2 = 20$. Since $E(x_1, \Delta)$ is a measure of the effect that the slowing-down tail of the Wilkins distribution has on the resonance escape probability, it is

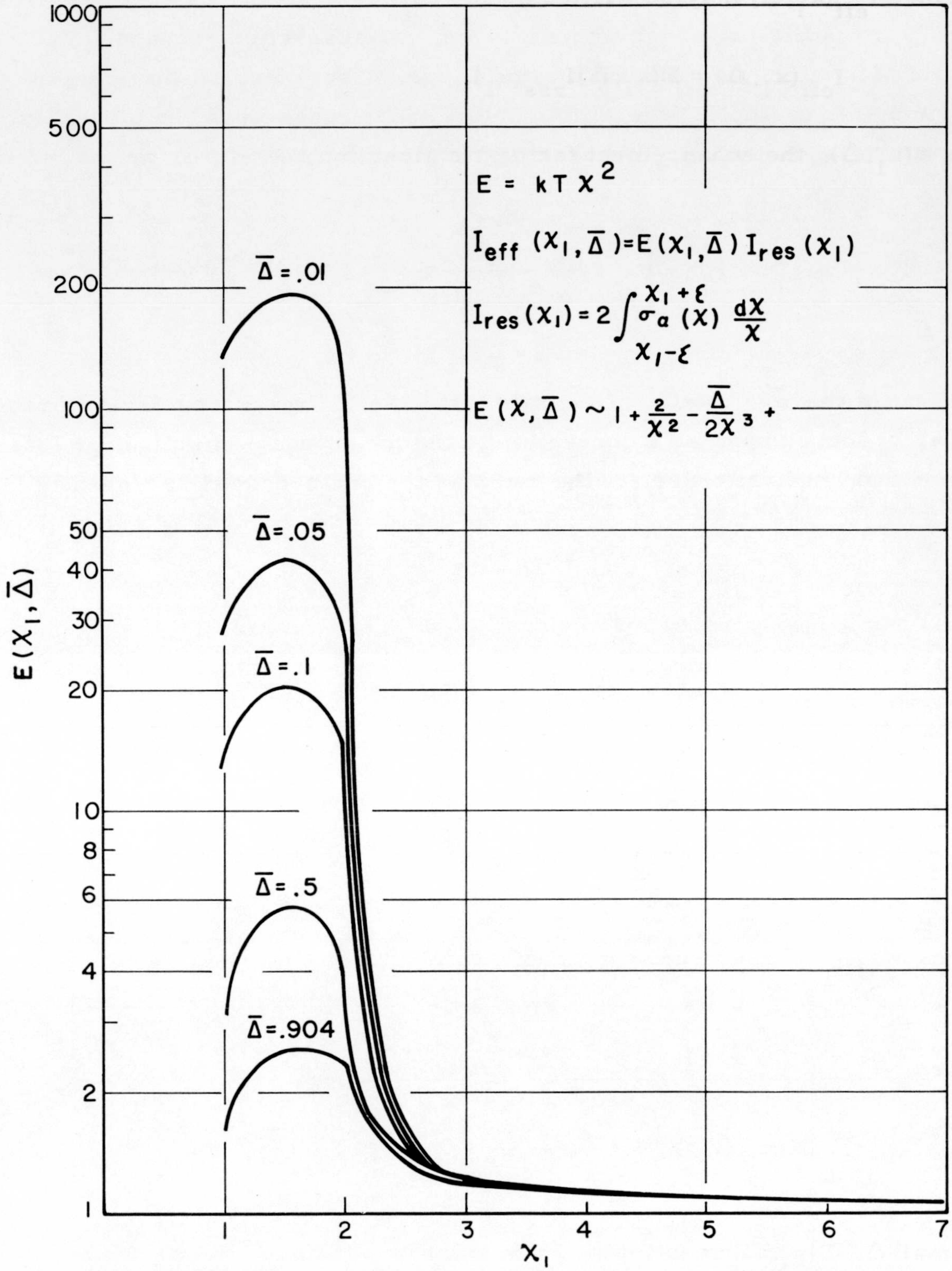

Figure 2. The Resonance Integral Enhancement Factor $E(x_1, \bar{\Delta})$

seen that the effect is noticeable when the resonance occurs at energies as high as 20kT. At sufficiently high temperatures, the absorption resonance of reactor materials might well fall within this range. The 0.8 ev resonance of samarium, for example, is within this 10% error range when the moderator temperature is $\approx 300°C$. To a first approximation, therefore, we may write

$$P(x_1, \Delta) = \exp\left[-\int_{x_1 - \epsilon}^{x_1 + \epsilon} \frac{\sigma_a(x)}{\sigma_s \xi (1 - 2/x^2)} \frac{dx}{x}\right] \quad . \qquad \ldots (23)$$

The effect of thermal motion of the moderator on the resonance escape probability may be looked upon as a correction to the mean logarithmic energy loss per collision and, in first order, is the same as the one proposed by Cohen.[2]

APPENDIX A

THE NORMALIZATION OF $N_O(X)$

If Wilkins' Equation (1) is solved for a source at infinity, S_∞, and for a source at zero, S_o, there result two solutions $N_o(x)$ and $N_\infty(x)$ which are linearly independent of each other. From (10) and (12), there results

$$N_\infty(x) = x^2 e^{-x^2}\left[a_\infty + \Delta\int_o^x \frac{e^{u^2}}{u^3}\int_o^u N_\infty(t)\,dt\,du\right]$$

and ... (A1)

$$N_o(x) = x^2 e^{-x^2}\left[a_o + \Delta\int_x^\infty \frac{e^{u^2}}{u^3}\int_u^\infty N_o(t)\,dt\,du\right] \quad ,$$

where $N_\infty(x)$ and $N_o(x)$ are subject to the normalization conditions

$$\frac{\Delta\sigma_s\xi}{4}\int_o^\infty N_\infty(x)\,dx = S_\infty$$

and ... (A2)

$$\frac{\Delta\sigma_s\xi}{4}\int_o^\infty N_o(x)\,dx = S_o \quad .$$

S_∞ has been chosen such that $a_\infty = \frac{4}{\sqrt{\pi}}$, whence (9) becomes

$$S_\infty = \frac{\sigma_s\xi}{2}C(\Delta), \qquad \text{... (A3)}$$

where $C(\Delta)$ is a known function of Δ.[4]

Since $N_o(x)$ and $N_\infty(x)$ are linearly independent solutions of (1), the Wronskian of (1), $W(x) = W_o x e^{-x^2}$, is given by

$$W(x) = W_o x e^{-x^2} = N_o(x) N'_\infty(x) - N'_o(x) N_\infty(x) \quad . \qquad \ldots (A4)$$

From (A1) it is apparent that

$$N_o(x) \sim a_o x^2 e^{-x^2} \qquad x >> 1 \quad . \qquad \ldots (A5)$$

Hence for large x and from (8), one can write

$$W(x) = W_o x e^{-x^2} \approx 2a_o C(\Delta) x e^{-x^2} \quad ,$$

and consequently

$$W_o = 2a_o C(\Delta) \quad . \qquad \ldots (A6)$$

On the other hand, from (A1),

$$N_\infty(x) \sim a_\infty x^2 e^{-x^2} \qquad x << 1 \quad .$$

Hence for small x,

$$W(x) = W_o x e^{-x^2} \cong N_o(x) \left[a_\infty x^2 e^{-x^2} \right]' - N'_o(x) \left[a_\infty x^2 e^{-x^2} \right] \quad ,$$

whence an integration, using the integrating factor $(x^2 e^{-x^2})^{-2}$, leads to

$$N_o(x) \approx -\frac{W_o}{a_\infty} x^2 e^{-x^2} \left[\int \frac{e^{x'^2}}{x'^3} dx' + C' \right]$$

and

$$\lim_{x \to o} N_o(x) = N_o(0) = \frac{W_o}{2a_\infty} \quad .$$

Hence from (A6), we have

$$N_o(0) = \frac{a_o}{a_\infty} C(\Delta) \quad .$$

Thus if S_o is so chosen that $a_o = a_\infty = \frac{4}{\sqrt{\pi}}$, then

$$N_o(0) = C(\Delta) \quad . \qquad \ldots (A7)$$

It remains to investigate the relationship between S_o and S_∞. From (A2) and (7), one obtains

$$S_o = \frac{\Delta \sigma_s \xi}{4} \int_o^\infty N_o(x)\, dx = \frac{\sigma_s \xi}{2} \left[\lim_{x \to \infty} x^2 N_o(x) + \frac{1}{2} \lim_{x \to \infty} x N_o'(x) + N_o(0) \right],$$

and from (A5) and (A7) ,

$$S_o = \frac{\sigma_s \xi}{2} C(\Delta) \quad . \qquad \ldots (A8)$$

If (A8) is compared with (A3), it is seen that a source S_o equal in magnitude to S_∞ results in a normalization of $N_o(x)$ such that $a_o = a_\infty$. Furthermore, if $S_o = S_\infty = \frac{\xi}{2} \sigma_s C(\Delta)$, then $a_o = a_\infty = 4/\sqrt{\pi}$.

APPENDIX B

THE RELATIONSHIP OF $N_1(x)$ AND $N_2(x)$ TO $N_0(x)$ AND $N_\infty(x)$

It has been shown that the relationship (14) is valid if it satisfies the three conditions on page 6. That condition 1) is satisfied is apparent since $N_o(x)$ and $N_\infty(x)$ are both solutions to Wilkins' equation. Condition 2) is also obviously satisfied. Substitution of (14) into condition 3) yields, with the aid of (7), (8), and (12):

$$S_\infty = \frac{\sigma_s \xi}{4(4/\sqrt{\pi})x_1 e^{-x_1^2}} \left[N_o(x_1)N_\infty'(x_1) - N_o'(x_1)N_\infty(x_1) \right]. \qquad \ldots (B1)$$

Since $N_o(x)$ and $N_\infty(x)$ are linearly independent solutions of (7), the bracketed quantity is the Wronskian of (1), whence from Appendix A, one has

$$S_\infty = \frac{\sigma_s \xi W_o}{4(4/\sqrt{\pi})}$$

and from (A6) and the normalized value of a_o,

$$S_\infty = \frac{\sigma_s \xi}{2} C(\Delta), \qquad \ldots (B2)$$

which is just the expression for S_∞ obtained from (9). Hence (A2) is valid and condition 3), page 6, is satisfied by (14).

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