

Disordering of Solids by Neutron Radiation

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A general method is outlined for determining the number of vacant lattice sites or interstitial atoms in a monatomic solid exposed to neutron radiation. The colliding atoms are assumed to be within the energy range for which the orbital picture can be applied. Following the treatment of Bohr, the scattering regions of excessive and moderate screening, Rutherford distribution, and electronic collisions are considered separately. The number of vacancies or interstitial atoms as a function of the energy of the primary knocked-out atom is given by the solution of certain integral equations that are different for various energy regions considered. It is found that if the velocity of a recoil atom resulting from neutron collision is less than e^2/\hbar (region of elastic collisions) approximately half of its energy is used up to produce vacancies

or interstitials. If the velocity of the recoil atom is above e^2/\hbar (region of inelastic collisions) then the energy used up to produce vacancies and interstitials is approximately constant for medium and heavy elements. A simple formula has been derived expressing the average number of vacant lattice sites or interstitials produced in a collision of a neutron having energy E in a monatomic solid composed of medium or heavy elements having atomic mass M . The formula is as follows:

$$G(E) \sim (nE - \alpha)^2 / 4cnE \quad \text{for } E \leq \gamma/n,$$

$$G(E) \sim [(nE - \alpha)^2 - (1 - \bar{R})(nE - \alpha - \gamma)^2] / 4cnE \quad \text{for } E \geq \gamma/n,$$

where $\gamma = Me^4/2\hbar^2$; $n = 4M/(M+1)^2$, α is the binding energy of an atom in the lattice, and \bar{R} is a slowly varying function of Z .

I. INTRODUCTION

HEAVY corpuscular radiations such as neutrons or ionizing particles which enter a solid dissipate a portion of their energy in close encounters with the constituent atoms of the solid and eject some of them irreversibly from their normal positions thus producing vacant lattice sites and interstitial atoms which we shall designate as "displacements" and "displaced atoms." The properties of the solid change with the number of the displaced atoms and it is the purpose of the present investigation to determine the number of such displacements.

Wigner was the first to call attention to these phenomena and the earlier treatments of this subject are based largely on the pioneer work of Seitz¹ and utilize the Born approximation for determining the elastic collisions of atoms. The Born approximation is, however, applicable in a range of velocities considerably higher than those encountered in this problem. We are, therefore, applying classical considerations based on an extended study of the subject made by Bohr.² Also, we give a more detailed analysis of the cumulative processes leading to the atomic displacements.

If the atom knocked out from its normal lattice position has acquired a relatively high velocity, it will lose much of its energy by colliding with the individual electrons and thereby excite and ionize other atoms in the solid. These processes are designated as "inelastic collisions." As the atom slows down, the relative amount of energy lost by inelastic collisions decreases and most of the energy loss is due to direct hits on other atoms in the solid. The latter process is designated as an

"elastic collision" and is effective in producing atomic displacements.

We consider a monatomic solid composed of atoms having atomic number Z . Following Bohr, we shall use a simplified picture assuming that the stopping of a knocked-out atom having energy x is due almost entirely to inelastic collision if

$$\omega > 1 \quad \text{or} \quad x > \gamma = Me^4/2\hbar^2. \quad (1)$$

ω designates the velocity of the atom and is measured in "atomic units," i.e.,

$$\omega = v/v_0, \quad (2)$$

where v_0 is the "velocity" of the electron in the hydrogen orbit:

$$v_0 = e^2/\hbar = 2.18 \times 10^8 \text{ cm/sec.} \quad (3)$$

We shall also assume that the stopping is entirely due to elastic collisions if

$$\omega < 1 \quad \text{or} \quad x < \gamma. \quad (4)$$

II. ELASTIC COLLISIONS

A. Formulation of the Problem

The mechanism of collisions is assumed to be the same as in the previous treatments and is based on the existence of a binding energy α of the lattice atoms. In determining the energy distribution of the struck atoms, we use the cross section for collisions with free atoms. If the energy acquired by this atom as a result of a collision exceeds α , we assume that it leaves its cell in the crystal and produces a permanent displacement. If, however, this energy is below α , then we assume that the lattice acquires vibrational energy which becomes eventually dissipated without producing any permanent changes. The value of α is not accurately determined and has been taken in the past to be of the order of 25 ev.

¹ F. Seitz, *Discussions Faraday Soc.* 5, 271 (1949).

² N. Bohr, *Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd.* 18, No. 8 (1948).

Each atom knocked out of the lattice as a result of a collision gradually loses its energy in secondary collisions, thus generating secondary particles. Each secondary particle thus released moves through the lattice and releases by the same mechanism tertiary particles. This process may continue for several generations until the energy of the particles released after several stages is insufficient to knock out any additional particles of the lattice and is dissipated in the form of heat.

Assume that as a result of the mechanism described above, a primary knocked-out atom having energy x produces $g(x) - 1$ displacements in all successive stages, i.e., the total number of displacements is $g(x)$ including the primary atom. If the atoms in the solid were free (i.e., if we neglect their binding energy) then the energy y acquired by each atom would be used entirely to produce further collisions. Since the atoms are not free, a portion of the acquired energy is used to free the atom from its bond and the remainder $(y - \alpha)$ is the kinetic energy that is effective in producing further collisions. Thus

$$g(x) = 1 \quad \text{for } x < \alpha. \quad (5)$$

Let $K(x, y)$ be the probability that the primary atom loses energy in dy about y in an elastic collision. We have

$$K(x, y) = \sigma(x, y) / \sigma(x), \quad (6)$$

where $\sigma(x, y)dy$ is the differential cross section for an atom of energy x to lose an amount of energy in dy about y in an elastic collision and $\sigma(x)$ is the corresponding total cross section for an elastic collision.

Assume that the struck atom gets energy in dy at y and then the primary atom has energy $x - y$. If $y \geq \alpha$, then the number of displacements is $g(x - y) + g(y - \alpha)$, but if $y < \alpha$ then the struck atom is not displaced and the number is $g(x - y)$.

Thus for $x > \alpha$, $g(x)$ is a solution of the integral equation

$$g(x) = \int_0^x g(x - y)K(x, y)dy + \int_\alpha^x g(y - \alpha)K(x, y)dy. \quad (7)$$

If we define $g(x) = 0$ for $x \leq 0$, then (7) is satisfied also for $0 \leq x \leq \alpha$.

B. Determination of the Kernel

1. General

We are dealing with a collision of two identical atoms which, in the center-of-mass coordinates, is represented as an interaction of a heavy particle having mass

$$M_0 = M/2, \quad (8)$$

with a screened field characterized by

$$V = (Z^2 e^2 / r) \exp(-r/a), \quad (9)$$

with the screening parameter

$$a = \hbar^2 / (\sqrt{2} m e^2 Z^3). \quad (10)$$

We shall apply the orbital picture to the study of the collisions of particles in the field (9). Since previous investigations utilized the Born approximation it appears to be desirable to consider the range of validity of the two methods and their possible applicability to this problem.

2. Region of Validity of the Born Approximation and of the Orbital Picture

A convenient criterion for the validity of the Born approximation is that the scattered field is small when compared to the incident field at the source. When applied to the screened Coulomb field, this criterion can be expressed as follows³:

$$\frac{Z^2 e^2}{\hbar v} \ln \left(\frac{M_0 v a}{\hbar} \right) \ll 1. \quad (11)$$

The inequality (11) should be satisfied for velocities $\omega \gg 2\sqrt{2}Z^3 m / M$, which are those encountered in the present problem.

Substituting (2) and (3) in (11) and taking into account the fact that the term under the logarithm in (11) is considerably larger than one, we obtain

$$\omega \gg Z^2. \quad (12)$$

Thus, the Born approximation is not applicable to medium and heavy elements and for the light elements its applicability is limited to a relatively high-energy region.

The criterion for the validity of the classical picture has been established by Williams⁴ and can be expressed as follows: (a) the wavelength of the moving particle is very small when compared to the screening parameter and (b) the uncertainty in the momentum of the particle is much less than the disturbance caused by the deflection in the field V .

The assumption (a) leads to the following inequality:

$$(\hbar/a) \ll M_0 v. \quad (13)$$

Taking into account (2), (3), (8), and (10), we can express (13) as follows:

$$\omega \gg 2\sqrt{2}Z^3 m / M. \quad (14)$$

This inequality is satisfied in all practical cases.

The assumption (b) leads to the following inequality:

$$Vr / \hbar v \gg 1. \quad (15)$$

Substituting (2), (3), and (9), in (15), we obtain

$$(Z^2 / \omega) \exp(-r/a) \gg 1. \quad (16)$$

³ L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), p. 169.

⁴ E. J. Williams, *Revs. Modern Phys.* **17**, 217 (1945).

It is noted that for a given value of Z and ω the condition (16) can never be satisfied for the *whole* region of space and, consequently, the orbital picture cannot be generally applied. We may associate with each value of ω a radius

$$R = a \ln(Z^2/\omega), \quad (17)$$

such that only for $r \ll R$ is the orbital picture valid. If, however, the region defined by the radius R is sufficiently large so as to include most of the space occupied by the scattering potential, i.e., if

$$R \gg a \quad \text{or} \quad \ln(Z^2/\omega) \gg 1, \quad (18)$$

we may assume that the orbital picture applies to the whole space.

Since in the present problem $\omega \ll Z^2$, we are dealing with a problem in which the orbital picture is valid.

3. Scattering of Particles in the Screened Coulomb Field

A complete study of the scattering of particles in a screened Coulomb field has been given by Bohr. Bohr divides the space in which the scattering occurs into regions defined by a screening parameter⁵

$$\zeta = b/a, \quad (19)$$

where b designates the collision diameter, i.e.,

$$b = 2Z^2e^2/M_0v^2. \quad (20)$$

Taking into account (8), (19), (20) and putting $x = Mv^2/2$, we obtain

$$x = 2Z^2e^2/\zeta a. \quad (21)$$

The character of the problem depends essentially upon the value of the screening parameter ζ . Following Bohr, we shall simplify the picture by assuming that, for relatively slow particles such that

$$\zeta > 1 \quad \text{or} \quad x < \beta = 2Z^2e^2/a, \quad (22)$$

the nuclei of the two colliding atoms will not penetrate substantially within each others electronic shells and the scattering has a spherically symmetrical angular distribution in the center-of-mass coordinates. We shall designate this region as the "region of isotropic scattering."

If, however, the particle has a relatively high energy, such that

$$\zeta < 1 \quad \text{or} \quad x > \beta, \quad (23)$$

we assume that the nuclei of the colliding atoms will penetrate substantially within each others electronic shells and the scattering in the center-of-mass coordinates will conform over a considerable angular interval with the Rutherford law. This region shall be designated as the "region of Rutherford scattering."

(a) *Region of isotropic scattering* ($x < \beta$).—We have⁶

$$\sigma(x, y) = \sigma(x)/x. \quad (24)$$

The total cross section $\sigma(x)$ depends upon the effectiveness of screening. For very low velocity in the region of excessive screening ($\zeta \gg 1$) it is of the order of magnitude of the gas kinetic cross section and for higher velocities in the region of moderate screening ($\zeta \sim 1$) it has the form $\sigma(x) \sim \pi \zeta a^2/\epsilon$, where $\epsilon = 2.74$. Taking into account (6) and (22), we have

$$K(x, y) = 1/x \quad \text{for} \quad 0 < y < x < \beta. \quad (25)$$

(b) *Region of Rutherford scattering*.—Bohr has replaced the screened field by a Coulomb field confined within a sphere of radius a . Consequently,

$$\sigma(x) = \pi a^2. \quad (26)$$

The cutoff introduced by the maximum impact parameter equal to a is equivalent to an angular cutoff θ_{\min} defined by⁷

$$\tan(\theta_{\min}/2) = b/2a. \quad (27)$$

Substituting (20) and (22) in (27) we obtain

$$\sin^2 \theta_{\min} = \beta^2/(4x^2 + \beta^2). \quad (28)$$

Consequently, the amount of energy y lost by the particle during the collision is comprised within the energy range

$$y_{\min} < y < x, \quad (29)$$

where

$$y_{\min} = x \sin^2 \theta_{\min} = x\beta^2/(4x^2 + \beta^2). \quad (30)$$

The cutoff value associated with an energy x will be denoted by x_1 in all that follows. Thus

$$x_1 = x\beta^2/(\beta^2 + 4x^2). \quad (31)$$

The solution of our problem is found to depend, in part, on the ratio of x_1 to α .

From (22) and (10), we have (assuming that $\alpha = 25$ ev),

$$\frac{\beta}{\alpha} = \frac{2\sqrt{2}me^4}{\hbar^2\alpha} Z^{2+\frac{1}{2}} \sim 3.078 Z^{2+\frac{1}{2}} \geq 39.95 \quad \text{for} \quad Z \geq 3; \quad (32)$$

and from (1) we have that

$$\gamma/\alpha = Me^4/2\hbar^2\alpha \sim 2 \times 10^3 Z \geq 6 \times 10^3 \quad \text{for} \quad Z \geq 3. \quad (33)$$

It is clear that x_1 is a decreasing function of x and we have

$$x_1 = \alpha \quad \text{for} \quad x = \frac{\beta^2}{8\alpha} \left[1 + \left(1 - \frac{16\alpha^2}{\beta^2} \right)^{\frac{1}{2}} \right]. \quad (34)$$

We shall denote this value by β' . Similarly, for

$$x = \beta'' = \frac{\beta^2}{16\alpha} \left[1 + \left(1 - \frac{64\alpha^2}{\beta^2} \right)^{\frac{1}{2}} \right], \quad (35)$$

the cutoff value is $(\beta'')_1 = 2\alpha$.

⁵ Reference 2, p. 20.

⁶ Reference 2, p. 49, Eq. (2.2.8).

⁷ Reference 2, p. 6, Eq. (1.1.3).

TABLE I. Numerical values of the parameters, for $\alpha = 25$ ev.

Z	β/α	γ/α	β'/α	γ/α	β''/α
7	286.8	1.381×10^4	20560	1.489	10280
6	200.12	1.183×10^4	10020	0.8463	5006
5	130.08	1.067×10^4	4276	0.4008	2137
4	78.71	8.893×10^3	1509	0.1697	752.9
3	39.72	6.844×10^3	393.3	0.05762	195.1

For the convenience of the reader, the following table of numerical values is given (Table I). In calculating these values, it has been assumed that $\alpha = 25$ ev. It is easily seen that these quantities are increasing functions of Z . Since⁸

$$\sigma(x, y) = \pi Z^4 e^4 / xy^2, \quad (36)$$

we obtain, taking into account (6), (26), and (36),

$$K(x, y) = \beta^2 / 4xy \quad \text{for } x\beta^2 / (4x^2 + \beta^2) < y < x, \quad (37)$$

$$K(x, y) = 0 \quad \text{for } y < x\beta^2 / (4x^2 + \beta^2).$$

C. Determination of the Number of Displacements

We shall proceed now to determine $g(x)$ from (7) in the region of isotropic scattering and Rutherford scattering.

Substituting $K(x, y)$ as defined by (25) and (37) in (7), we obtain

$$g(x) = 1 + \frac{1}{x} \int_{\alpha}^x dug(u) \quad \text{for } \alpha < x < 2\alpha, \quad (38)$$

$$g(x) = \frac{2\alpha}{x} + \frac{1}{x} \int_{\alpha}^x dug(u) + \frac{1}{x} \int_{\alpha}^{x-\alpha} dug(u) \quad (39)$$

for $2\alpha < x < \beta$,

$$g(x) = \int_{x_1}^x \frac{dt\beta^2}{4xt^2} g(x-t) + \int_{[\alpha, x_1]_>} \frac{dt\beta^2}{4xt^2} g(t-\alpha) \quad (40)$$

for $\beta < x < \gamma$,

where x_1 is defined by (31) and $[\alpha, x_1]_>$ designates the larger of values α and x_1 .

As shown in the Appendix, the solution of (38), (39) and (40) is as follows:

For $\alpha \leq x \leq \beta$, we have

$$A(x+\alpha)/2\alpha \leq g(x) \leq B(x+\alpha)/2\alpha, \quad (41)$$

with $A = 1$ and $B = 8/7$.

For $\beta \leq x \leq [\beta', \gamma]_<$, where $[\beta', \gamma]_<$ indicates the smaller of β' and γ , $A = 1$ is also valid and $\beta' > \gamma$ if $Z > 6$. For $Z \leq 6$ and $\beta' \leq x \leq \gamma$, A may be taken from the table:

Z	6	5	4	3
A	1	0.9627	0.8770	0.7542

⁸ Reference 2, p. 42, Eq. (2.2.2).

For $\beta \leq x \leq [\beta'', \gamma]_<$, we may take $B = 1.15$ and for $Z \leq 7$, $\beta'' > \gamma$. If $Z \leq 7$ and $\beta'' \leq x \leq \gamma$, then we take $B = (8/7) + 0.07$. (See Appendix 109a.)

On the basis of the above results, we may assume that in the region of elastic collisions, i.e., for $0 < x < \gamma$, the following relation is approximately correct

$$g(x) = x/2\alpha; \quad (42)$$

i.e., approximately half of the energy of a recoil atom is used to produce displacements.

III. INELASTIC COLLISIONS

A. General

We are dealing here with a region in which the velocity of the moving particle is less than the orbital electron velocities in the solid and at the present time there is no exact theory to evaluate the excitation and ionization losses in this region. Our computation of energy losses will be based on certain assumptions made by Bohr that are applicable to intermediate and heavy elements.

In the case of lighter elements it is necessary to compute separately the effectiveness of each electronic orbit as done by Livingston and Bethe,⁹ Hirschfelder and Magee,¹⁰ and Neufeld.¹¹

B. Calculation of the Energy Loss

According to Bohr the rate of energy loss of a particle in the above range moving through a medium composed of intermediate or heavy elements is as follows¹²:

$$dx/dz = NB_e n_e (3[\kappa]^{-1/3} + [\kappa]^{-1}), \quad (43)$$

where z is the length of the particle track, N is the number of atoms per cm³ of the solid,

$$B_e = \frac{2\pi(Z^*)e^4}{mv^2}; \quad n_e = Z^3 \frac{2v}{v_0}; \quad \kappa = \frac{2Ze^2}{\hbar v},$$

$$[\kappa] = \kappa \quad \text{for } \kappa > 1 \quad \text{and} \quad [\kappa] = 1 \quad \text{for } \kappa < 1. \quad (44)$$

Here Z^* represents the charge of the moving particle and can be assumed to vary with the velocity as follows:

$$Z^* = Z^{3/2} v / v_0. \quad (45)$$

We take $\kappa > 1$. From this it follows that $\omega < 2Z$ and, consequently, the formula (43) is valid for $\gamma < x < 4Z^2\gamma$. Substituting (44) and (45) in (43), we obtain

$$dx/dz = C\sqrt{x}, \quad (46)$$

where

$$C = \frac{4\pi\sqrt{2}NZ\hbar^3}{M^{3/2}me^2} [3(2Z^{3/2})^{-1} + 2(Z^{3/2})^{-1}]. \quad (47)$$

⁹ M. S. Livingston and H. A. Bethe, Revs. Modern Phys. **9**, 263 (1937).

¹⁰ J. O. Hirschfelder and J. L. Magee, Phys. Rev. **73**, 207 (1948).

¹¹ J. Neufeld, Proc. Phys. Soc. **A66**, 590 (1953).

¹² Reference 2, p. 102, Eq. (3.5.7).

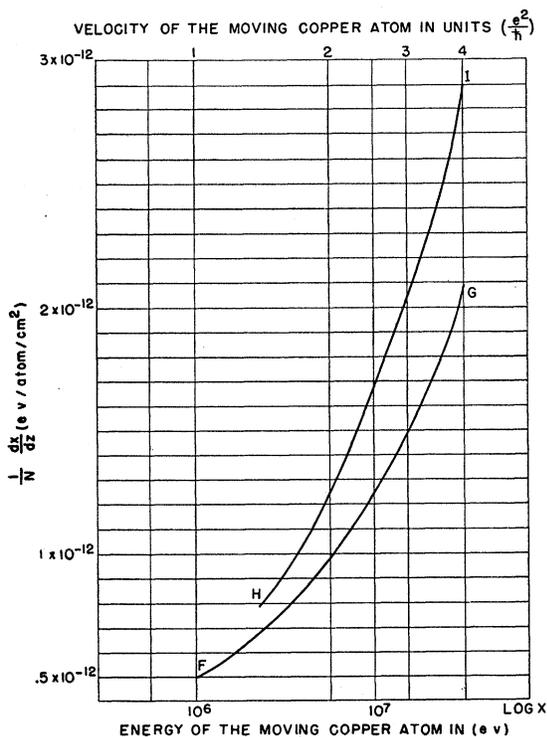


FIG. 1. Stopping power of copper ions in copper.

In view of the complete lack of experimental evidence, we are not able to verify the results expressed by (46). Some approximate estimates show, however, that this expression gives at least the right order of magnitude for the energy loss. In Fig. 1, the line *FG* is based on (46) and represents the stopping power of recoil atoms in copper. The line *HI* shows a rough estimate of the stopping power which has been obtained by assuming

$$\frac{1}{N} \frac{dx}{dz} = (Z^2)_{Av} \sigma, \quad (48)$$

where σ designates the "specific electronic cross section" and $(Z^2)_{Av}$ is the average of the square of the moving charge.¹³ Using the experimental data of Warshaw¹⁴ giving $(1/N)(dx/dz)$ for protons in copper, and the experimental data of Hall¹⁵ for (Z_{Av}) for protons, we derived from (48) the specific electronic cross section σ for copper corresponding to various velocities of the moving ion. The stopping power due to inelastic collisions has been calculated by using

$$\frac{1}{N} \frac{dx}{dz} = (Z^*)^2 \sigma, \quad (49)$$

where Z^* for copper has been determined from (45). It

is noted that the curve *HI* gives values of the same order of magnitude than those shown on the curve *FG*. The assumptions leading to the curve *HI* have been very rough and, therefore, the above calculations are not considered as a verification of the formula (43). They do indicate, however, that this formula is of the right order of magnitude.

C. Determination of the Number of Displacements

We consider here a particle having energy $x > \gamma$. While slowing down the particle loses its energy by inelastic collisions in accordance with (43) and also participates in elastic collisions in accordance with (37). Only the latter process is effective in producing lattice holes and interstitial atoms.

The probability that the particle has traversed a distance z without suffering an elastic collision is $\exp(-N\pi a^2 z)$, where πa^2 is the scattering cross section.

Thus, the probability that the striking atom has its first elastic collision while traversing an element of path length dz after going a distance z along its path without an elastic collision is

$$\exp(-N\pi a^2 z) N\pi a^2 dz. \quad (50)$$

Using (46), we have that

$$z = (2/C)(x^{\frac{1}{2}} - t^{\frac{1}{2}}), \quad (51)$$

and

$$dz = -dt/Ct^{\frac{1}{2}}. \quad (52)$$

Substituting (51) and (52) in (50), the probability that the striking atom has its first elastic collision in an energy interval dt about t is given by

$$\exp\left[\frac{-2N\pi a^2}{C}(x^{\frac{1}{2}} - t^{\frac{1}{2}})\right] \times \frac{dt \times N\pi a^2}{Ct^{\frac{1}{2}}}. \quad (53)$$

Once an elastic collision has occurred, the probability distribution for the energy lost by the striking atom is given by (37), and thus the probability that the striking atom having energy x will have an elastic collision in an energy interval dt about t where $t > \gamma$, and that it loses energy dy about $y < t$ is given by

$$\exp\left[\frac{-2N\pi a^2}{C}(x^{\frac{1}{2}} - t^{\frac{1}{2}})\right] \frac{N\pi a^2 dt}{t^{\frac{1}{2}}} \times \frac{dy\beta^2}{4ty^2} \quad (54)$$

for $t\beta^2/(\beta^2 + 4t^2) < y < t$, and is 0 for $0 \leq y \leq t\beta^2/(\beta^2 + 4t^2)$.

Then the average number of displacements produced by the particle which had its first collision within an interval dt about t is

$$\int_{t\beta^2/(\beta^2 + 4t^2)}^t \frac{dy\beta^2}{4ty^2} g(t-y) + \int_{[\alpha, t\beta^2/(4t^2 + \beta^2)]}^t \frac{dy\beta^2}{4ty^2} g(y-\alpha). \quad (55)$$

If the striking atom reaches energy γ without an elastic collision, then its first elastic collision is at

¹³ J. Knipp and E. Teller, Phys. Rev. **59**, 659 (1941).

¹⁴ S. D. Warshaw, Phys. Rev. **76**, 1759 (1949).

¹⁵ T. Hall, Phys. Rev. **79**, 504 (1950).

energy γ since it can, in our model, lose no more energy by inelastic collisions. The probability that the first collision is at energy γ is given by

$$\exp\left[-\frac{2N\pi a^2}{C}(x^{\frac{1}{2}}-\gamma^{\frac{1}{2}})\right]. \quad (56)$$

Consequently $g(x)$ can be expressed as follows:

$$\begin{aligned} g(x) = & g(\gamma) \exp[-2N\pi a^2(x^{\frac{1}{2}}-\gamma^{\frac{1}{2}})/C] \\ & + \int_{\gamma}^x dx \frac{N\pi a^2}{Cl} \exp[-2N\pi a^2(x^{\frac{1}{2}}-t^{\frac{1}{2}})/C] \\ & \times \int_{t\beta^2/(4t^2+\beta^2)}^{t'} dy \frac{\beta^2}{4ty^2} g(t-y) \\ & + \int_{[\alpha, t\beta^2/(4t^2+\beta^2)]}^{t'} dy \frac{\beta^2}{4ty^2} g(y-\alpha). \end{aligned} \quad (57)$$

In the right-hand side of the above expression, the first term represents the number of displacements produced by the particle after it had slowed down from the initial energy x to γ , and the second term represents the number of displacements produced while the particle is slowing down from x to γ .

The solution of (57) is found to satisfy the inequality:

$$\begin{aligned} \frac{R_1}{2\alpha}(x-\gamma+\gamma_1) + \frac{\gamma-\gamma_1+\alpha}{2\alpha} & \leq g(x) \\ & \leq \frac{R_2}{2\alpha}(x-\gamma) + \frac{1.15\gamma+2\alpha}{2\alpha}, \end{aligned} \quad (58)$$

for $\gamma \leq x \leq 20$ Mev and $Z \geq 16$. R_1 and R_2 are defined by (120) and (123) respectively and are shown graphically on Fig. 2.

The average of these bounds will be taken as the approximate solution for $g(x)$ for $x > \gamma$. Neglecting terms of minor importance, we have

$$g(x) \approx \frac{\bar{R}}{2\alpha}(x-\gamma) + \frac{\gamma}{2\alpha}, \quad (59)$$

with $\bar{R} = (R_1 + R_2)/2$.

It is clear that for $x > \gamma$ the slope of the function $g(x)$ is substantially less than for $x < \gamma$, and the curve seems to be nearly constant for low values of Z .

The values of R_1 and R_2 are graphed for $Z \geq 16$ which we take as the lower limit of the range in Z for energies above γ . (See Fig. 2.)

Refinements of the arguments given in the Appendix show that instead of being constant, R_1 and R_2 are decreasing functions of x . While $g(x)$ increases the rate of increase is generally much less than for $x < \gamma$.

We can thus assume that $g(x)$ is constant, i.e.,

$$g(x) = g(\gamma) \sim \gamma/2\alpha. \quad (60)$$

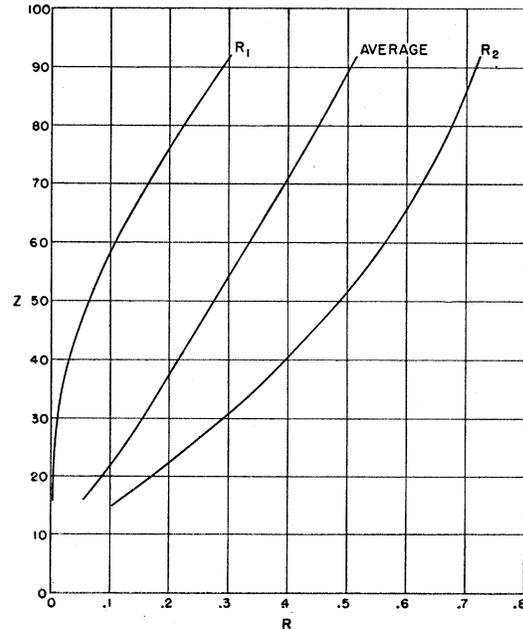


FIG. 2. Variation of R_1 and R_2 with Z .

IV. IRRADIATION BY NEUTRONS

We assume that the solid is irradiated by a flux of neutrons of known spectrum and that the scattering is isotropic in center-of-mass coordinates. Let $H(E,x)dx$ represent the number of primary knock-outs assumed initially as free, with energy in dx about x that result from a collision with a neutron having energy E . We have

$$\begin{aligned} H(E,x) &= dx/nE \quad \text{for } x < nE, \\ H(E,x) &= 0 \quad \text{for } x > nE, \end{aligned} \quad (61)$$

where $n = 4M/(M+1)^2$.

Consequently, the average number of displacements produced in the solid by a single collision of neutrons is

$$G(E) = \int_{\alpha}^{nE} H(E,x)g(x-\alpha)dx = \frac{1}{nE} \int_0^{nE-\alpha} g(x)dx. \quad (62)$$

Substituting in (62) the simplified expressions for $g(x)$ given by (42) and (60), we obtain

$$G(E) \sim nE/4\alpha \quad \text{for } E \leq \gamma/n, \quad (63)$$

$$G(E) \sim [(nE-\alpha)^2 - (1-\bar{R})(nE-\alpha-\gamma)^2]/4n\alpha E \quad \text{for } E > \gamma/n. \quad (64)$$

We assume that the solid is irradiated by a flux comprising $N(E)dE$ neutrons having energy in dE about E and velocity $v_n = (2E/1.662 \times 10^{-24})^{1/2}$. Then the number of displacements produced by this flux in one cm³ per second is

$$J = \int v_n N(E) \sigma(E) G(E) dE, \quad (65)$$

where $\sigma(E)$ is the cross section for the collision of a neutron with the atom of the solid and the integral extends over the whole range of the neutron spectrum.

For a neutron spectrum comprising only energies $E \leq (A+1)^2 6.25 \times 10^8$ ev, the total amount of energy used up to produce displacements is equal to the half of the energy absorbed by the solid (for any solid having $Z > 3$).

APPENDIX

For the range $\alpha \leq x \leq \gamma$, we have from (7) the equation

$$g(x) = \int_0^x dy K(x,y)g(x-y) + \int_\alpha^x dy K(x,y)g(y-\alpha). \quad (66)$$

Equation (66) is easily seen to be of Volterra type:

$$g(x) = s(x) + \int_\alpha^x dy \mathcal{K}(x,y)g(y), \quad (67)$$

where $\mathcal{K}(x,y)$ is non-negative and bounded on the range $\alpha \leq x \leq \gamma, \alpha \leq y \leq \gamma$.

It follows from the standard theory of such equations that there is a unique solution of (66) given by the formula:

$$g(x) = F_0(x) + \sum_{n=1}^{\infty} [F_n(x) - F_{n-1}(x)], \quad (68)$$

where F_0 is an arbitrary bounded integrable function on the range $\alpha \leq x \leq \gamma$ and

$$F_{n+1}(x) = s(x) + \int_\alpha^x dy \mathcal{K}(x,y)F_n(y), \quad n=0, 1, 2, \dots \quad (69)$$

Our method of obtaining an approximate solution of (166) depends upon the following theorem, which does not seem to be standard in the literature:

Theorem I. If the kernel \mathcal{K} of (67) is non-negative and bounded and if $F_0(x) \geq F_1(x)$ on the interval $[\alpha, \gamma]$, then for every $n \geq 0$,

$$F_n(x) \geq g(x), \quad \alpha \leq x \leq \gamma.$$

If the inequalities are reversed, the statement remains true.

Proof. Clearly $F_n(x) \geq F_{n-1}(x), \alpha \leq x \leq \gamma$ implies $F_{n+1}(x) \geq F_n(x), \alpha \leq x \leq \gamma$ and the theorem follows from (68).

Corollary I. If $F_0(x) \geq g(x)$ on the interval $[\alpha, c]$ and if $F_0(x) \geq F_1(x)$ on the interval $[c, \gamma]$ then $F_0(x) \geq g(x)$ on the interval $[c, \gamma]$ also. If the inequalities are reversed, the statement is also true.

Proof. For x in the interval $[c, \gamma]$, we may rewrite (67) as

$$g(x) = \left\{ s(x) + \int_\alpha^c dy \mathcal{K}(x,y)g(y) \right\} + \int_c^x dy \mathcal{K}(x,y)g(y), \quad (70)$$

which is again of the same form as (67) but with the bracketed quantity as source term. Then, for x in the interval $[c, \gamma]$,

$$\left\{ s(x) + \int_\alpha^c dy \mathcal{K}(x,y)g(y) \right\} + \int_c^x dy \mathcal{K}(x,y)F_0(y) \leq F_1(x) \leq F_0(x), \quad (71)$$

and hence the result follows from the preceding theorem.

For x in the interval $[\alpha, 2\alpha]$, Eq. (66) becomes [see (38)]:

$$g(x) = 1 + \frac{1}{x} \int_\alpha^x dy g(y), \quad (72)$$

and it is easy to verify that the exact solution is given by

$$g(x) = 1 + \ln(x/\alpha). \quad (73)$$

For x in the interval $[2\alpha, \beta]$, Eq. (66) becomes [see (39)]:

$$g(x) = \frac{2\alpha}{x} + \frac{1}{x} \int_\alpha^x dy g(y) + \frac{1}{x} \int_\alpha^{x-\alpha} dy g(y). \quad (74)$$

If we take $F_0(x) = B(x+\alpha)/2\alpha$, then

$$F_1(x) - F_0(x) = \alpha(8-7B)/4x, \quad (75)$$

and this is positive or negative according as $B < 8/7$ or as $B > 8/7$.

To apply the corollary, we also need that for x in the interval $[\alpha, 2\alpha]$,

$$\frac{x+\alpha}{2\alpha} \leq 1 + \ln \frac{x}{\alpha} \quad \text{for a lower bound,} \quad (76)$$

or that

$$\frac{x+\alpha}{2\alpha} \geq 1 + \ln \frac{x}{\alpha} \quad \text{for an upper bound.} \quad (77)$$

It is easy to verify that $B=1$ is the largest value of B for which (76) holds, and that (77) holds if $B=8/7$. Thus, we have, for x in the interval $[\alpha, \beta]$,

$$(x+\alpha)/2\alpha \leq g(x) \leq 4(x+\alpha)/7\alpha. \quad (78)$$

For x in the interval $[\beta, \gamma]$, Eq. (66) becomes [see (40)]:

$$g(x) = \int_{x_1}^x \frac{dy \beta^2}{4xy^2} g(x-y) + \int_{[\alpha, x_1]}^x \frac{dy \beta^2}{4xy^2} g(y-\alpha), \quad (79)$$

where x_1 is equal to y_{\min} as defined by (31).

For all elements $Z > 6$ we have $\beta' > \gamma$ see (34) and thus (79) becomes

$$g(x) = \int_{x_1}^x \frac{dy \beta^2}{4xy^2} [g(x-y) + g(y-\alpha)]. \quad (80)$$

An exact solution of (80) is given by

$$g(x) = B \left(\frac{x+\alpha}{2\alpha} \right), \quad B = \text{any constant.} \quad (81)$$

Taking $B=1$ and applying Corollary I, we have

$$(x+\alpha)/2\alpha \leq g(x), \quad \begin{cases} Z > 6, & \beta \leq x \leq \gamma \\ Z \leq 6, & \beta \leq x \leq \beta'. \end{cases} \quad (82)$$

For $Z \leq 6$, $\beta' \leq x \leq \gamma$, the equation determining $g(x)$ becomes

$$g(x) = \int_{x_1}^x \frac{dy\beta^2}{4xy^2} g(x-y) + \int_{\alpha}^x \frac{dy\beta^2}{4xy^2} g(y-\alpha), \quad (83)$$

but we may continue to write (83) as

$$g(x) = \int_{x_1}^x \frac{dy\beta^2}{4xy^2} [g(x-y) + g(y-\alpha)], \quad (84)$$

if we agree to define $g(x) = 0$ for $x < 0$.

To obtain a lower bound for $g(x)$, define

$$\begin{aligned} f(x) &= 0, & x < 0; \\ f(x) &= 1, & 0 \leq x \leq \alpha; \\ f(x) &= (x+\alpha)/2\alpha, & \alpha \leq x \leq \beta' - \alpha; \\ f(x) &= \frac{x+\alpha}{2\alpha} - \frac{k}{2\alpha}(x-\beta'+\alpha), & \beta' - \alpha \leq x \leq \gamma; \end{aligned} \quad (85)$$

where $k = \text{constant}$.

To determine $k \geq 0$ so that $f(x)$ will be a lower bound, we note that $f(x) \leq g(x)$ for $x \leq \beta'$, and so $f(x)$ will be a lower bound also for $\beta' \leq x \leq \gamma$ provided

$$\int_{x_1}^x \frac{dy\beta^2}{4xy^2} [f(x-y) + f(y-\alpha)] - f(x) \leq 0. \quad (86)$$

Substituting for $f(x)$ and integrating, (86) becomes

$$\begin{aligned} & \int_{x-\alpha}^x \frac{dy\beta^2}{4xy^2} \left[1 - \frac{x-y+\alpha}{2\alpha} \right] + \int_{\alpha}^{2\alpha} \frac{dy\beta^2}{4xy^2} \left[1 - \frac{y}{2\alpha} \right] \\ & - \int_{x_1}^{\alpha} \frac{dy\beta^2}{4xy^2} \frac{y}{2\alpha} - \frac{k}{2\alpha} \int_{x_1}^x \frac{dy\beta^2}{4xy^2} (x-y-\beta'+\alpha) \\ & - \frac{k}{2\alpha} \int_{\beta'}^x \frac{dy\beta^2}{4xy^2} (y-\beta') + \frac{k}{2\alpha} (x-\beta'+\alpha) \geq 0. \end{aligned} \quad (87)$$

The first integral of (87) is small compared to the second and will be replaced by

$$\frac{\beta^2\alpha}{16\alpha^3} = \int_0^{\alpha} \frac{dy\beta^2(\alpha-y)}{8\alpha x^3} \leq \int_{x-\alpha}^x \frac{dy\beta^2}{4xy^2} \left(1 - \frac{x-y+\alpha}{2\alpha} \right). \quad (88)$$

Substituting from (88) for the first integral and integrating in (87), the condition for a lower bound becomes

$$\begin{aligned} & \frac{\beta^2\alpha}{16x^3} + \frac{\beta^2}{4x} \left\{ \frac{1}{2\alpha} - \frac{1}{2\alpha} \ln \frac{2\alpha}{x_1} \right. \\ & \left. + \frac{k}{2\alpha} \left[1 - \frac{\alpha}{x} + \ln \frac{\beta'(x-\beta'+\alpha)}{xx_1} \right] \right\} \geq 0. \end{aligned} \quad (89)$$

Multiplying by $8\alpha x/\beta^2$, Eq. (89) becomes

$$1 + \frac{\alpha^2}{2x^2} + \ln \frac{x_1}{2\alpha} + k \left[1 - \frac{\alpha}{x} + \ln \frac{\beta'(x-\beta'+\alpha)}{xx_1} \right] \geq 0. \quad (90)$$

An elementary argument shows that

$$1 - \alpha/x + \ln[\beta'(x-\beta'+\alpha)/xx_1]$$

is an increasing function of x and is positive for $x > \beta'$.

Dividing (90) by $1 - \alpha/x + \ln[\beta'(x-\beta'+\alpha)/xx_1]$, the condition becomes

$$k + \frac{1 + (\alpha/x^2) + \ln(x_1/2\alpha)}{1 - (\alpha/x) + \ln[\beta'(x-\beta'+\alpha)/xx_1]} \geq 0. \quad (91)$$

Since (91) is a decreasing function of x , (91) will be true for $\beta' \leq x \leq \gamma$ provided

$$k = \max \left[0, \frac{-1 - (\alpha^2/2\gamma^2) - \ln(\gamma_1/2\alpha)}{1 - (\alpha/\gamma) + \ln[\beta'(\gamma-\beta'+\alpha)/\gamma\gamma_1]} \right]. \quad (92)$$

For $Z \leq 6$, Eq. (92) gives the following values for k :

Z	6	5	4	3
k	0	0.0622	0.1481	0.2607

Thus

$$\frac{x+\alpha}{2\alpha} - \frac{k}{2\alpha}(x-\beta'+\alpha) = f(x) \leq g(x) \quad (93)$$

for $Z \leq 6$, $\beta' \leq x \leq \gamma$.

Since $A(x+\alpha)/2\alpha \leq f(x)$, $\alpha \leq x \leq \gamma$, where $A = 1 - [k(\gamma-\beta'+\alpha)/(\gamma-\alpha)]$, we have

$$A(x+\alpha)/2\alpha \leq g(x), \quad 0 \leq x \leq \gamma, \quad (94)$$

with $A = 1$ for $Z > 6$; and for $Z \leq 6$, A is given by the accompanying table.

Z	6	5	4	3
A	1	0.9627	0.8770	0.7542

Now consider a function $h(x)$ defined by

$$\begin{aligned} h(x) &= 0, & x < 0; \\ h(x) &= 1, & 0 \leq x \leq \alpha; \\ h(x) &= 4(x+\alpha)/7\alpha, & \alpha < x \leq \beta-\alpha; \\ h(x) &= \left(\frac{8}{7}+k\right)\frac{x+\alpha}{2\alpha}, & \beta-\alpha < x \leq \gamma, \end{aligned} \tag{95}$$

where k = constant.

Let β^* be the energy x , where $x_1 = x - \beta + \alpha$. It is easily seen that $\beta < \beta^* < \beta''$ (see 35). Then for $\beta \leq x \leq \beta^*$ we have $x_1 - \alpha > \alpha$, and so

$$h_1(x) = \frac{8}{7} \left(\frac{x+\alpha}{2\alpha} \right) + \frac{\beta^2}{4x} \left[\frac{3\alpha-4x}{7x(x-\alpha)} + \frac{4}{7\alpha} \ln \frac{x}{x-\alpha} + \frac{k}{2\alpha} \ln \frac{x}{\beta} \right]. \tag{96}$$

Hence, the condition $h_1(x) \leq h(x)$ is equivalent to

$$\frac{3\alpha-4x}{7x(x-\alpha)} + \frac{4}{7\alpha} \ln \frac{x}{x-\alpha} + k \left[\frac{1}{2\alpha} \ln \frac{x}{\beta} - \frac{2x(x+\alpha)}{\alpha\beta^2} \right] \leq 0. \tag{97}$$

Since $\ln[x/(x-\alpha)] < [\alpha/(x-\alpha)]$, Eq. (97) will be satisfied if

$$\frac{3\alpha}{7x(x-\alpha)} + k \left[\frac{1}{2\alpha} \ln \frac{x}{\beta} - \frac{2x^2}{\alpha\beta^2} \right] \leq 0, \quad \beta \leq x \leq \beta^*. \tag{98}$$

For $k > 0$, the left member of (98) is a decreasing function of x , and hence (98) is satisfied for $\beta \leq x \leq \beta^*$ if

$$k \geq \frac{3\alpha^2}{14\beta(\beta-\alpha)}. \tag{99}$$

Since $\beta/\alpha \geq 39.71$, we have

$$k = 1.377 \times 10^{-4} \tag{100}$$

as an admissible value of k , and thus

$$\left(\frac{8}{7} + 1.377 \times 10^{-4} \right) \frac{x+\alpha}{2\alpha} \geq g(x), \quad \beta \leq x \leq \beta^*. \tag{101}$$

For $\beta^* \leq x \leq \beta''$, we only need to add the term

$$\frac{k}{2\alpha} \int_{x_1}^{x-\beta+\alpha} \frac{dy\beta^2}{4xy^2} (x-y+\alpha)$$

to (97), so that on this range $h_1(x) \leq h(x)$ is equivalent to

$$\begin{aligned} &\frac{3\alpha-4x}{7x(x-\alpha)} + \frac{4}{7\alpha} \ln \frac{x}{x-\alpha} \\ &+ \frac{k}{2\alpha} \left[\ln \frac{xx_1}{\beta(x-\beta+\alpha)} + \frac{\alpha}{x} - \frac{\beta}{x-\beta+\alpha} \right] \leq 0. \end{aligned} \tag{102}$$

Since $x_1 < \beta^2/4x$, $\ln[x/(x-\alpha)] < [\alpha/(x-\alpha)]$, Eq. (102) will be true if

$$\frac{6\alpha^2}{7x(x-\alpha)} + k \left[\ln \frac{\beta}{4(x-\beta+\alpha)} - \frac{\beta-\alpha}{x-\beta+\alpha} \right] \leq 0. \tag{103}$$

The function in square brackets in (103) has a maximum at $x = 2(\beta-\alpha)$, and this maximum is

$$\ln(\beta/4\beta-\alpha) - 1 < \alpha/(\beta-\alpha) - 2.386.$$

Thus (103) is satisfied if we take

$$k = 2.7 \times 10^{-4} > \frac{3\alpha^2}{7\beta^2} > \frac{6\alpha^2}{7\beta(\beta-\alpha)[2.386-\alpha/(\beta-\alpha)]}. \tag{104}$$

Thus

$$\left(\frac{8}{7} + 2.7 \times 10^{-4} \right) \frac{x+\alpha}{2\alpha} \geq g(x), \quad \alpha \leq x \leq \beta''. \tag{105}$$

For $\beta'' \leq x \leq \gamma$ we have to add the term

$$\int_{[x, x_1] > y^2}^{2\alpha} \frac{dy}{y^2} \left[1 - \frac{4y}{7\alpha} \right] \leq \int_{\alpha}^{2\alpha} \frac{dy}{y^2} \left[1 - \frac{4y}{7\alpha} \right] = \frac{1}{2\alpha} - \frac{4}{7\alpha} \ln 2$$

to (102). Thus, on the range $\beta'' \leq x \leq \gamma$, $h_1(x) \leq h(x)$ is true if

$$\begin{aligned} &\frac{3\alpha-4x}{7x(x-\alpha)} + \frac{1}{2\alpha} - \frac{4}{7\alpha} \ln 2 + \frac{4}{7\alpha} \ln \frac{x}{x-\alpha} \\ &+ \frac{k}{2\alpha} \left[\ln \frac{xx_1}{\beta(x-\beta+\alpha)} + \frac{\alpha}{x} - \frac{\beta}{x-\beta+\alpha} \right] \leq 0. \end{aligned} \tag{106}$$

Making the same substitutions as before, we get

$$\frac{6\alpha^2}{7x(x-\alpha)} + 1 - \frac{8}{7} \ln 2 + k \left[\ln \frac{\beta}{4(x-\beta+\alpha)} - \frac{\beta-\alpha}{x-\beta+\alpha} \right] \leq 0. \tag{107}$$

Since $x \geq \beta'' > 2(\beta-\alpha)$, (107) is a decreasing function of x for $x \geq \beta''$. Putting $x = \beta''$ and using $\beta/\alpha \geq 39.71$, we get as an admissible value for k :

$$k = 0.068 > \frac{1 - \frac{8}{7} \ln 2 + \frac{6\alpha^2}{7\beta''(\beta''-\alpha)}}{\frac{\beta-\alpha}{\beta''-\beta+\alpha} + \ln \frac{4(\beta''-\beta+\alpha)}{\beta}}. \tag{108}$$

Thus

$$\left(\frac{8}{7} + 0.07 \right) \frac{x+\alpha}{2} \geq g(x), \quad \alpha \leq x \leq \gamma, \quad Z \geq 3. \tag{109a}$$

For $Z > 7$, β'' exceeds γ and so

$$\left(\frac{8}{7} + 2.7 \times 10^{-4} \right) \frac{x+\alpha}{2\alpha} \geq g(x), \quad \alpha \leq x \leq \gamma, \quad Z > 7. \tag{109b}$$

In the energy region $x > \gamma$, the equation to be solved is given by [see (57); we have substituted λ for $(N\pi a^2/C)\gamma^{\frac{1}{2}}$]:

$$g(x) = g(\gamma) \exp\left[-2\lambda\left(\frac{x}{\gamma}\right)^{\frac{1}{2}} - 1\right] + \int_{\gamma}^x d\lambda \left(\frac{\gamma}{x}\right)^{\frac{1}{2}} \times \exp\left[-2\lambda\left(\frac{x}{\gamma}\right)^{\frac{1}{2}} - \left(\frac{t}{\gamma}\right)^{\frac{1}{2}}\right] \times \int_{t_1}^t \frac{dy\beta^2}{4ty^2} [g(t-y) + g(y-\alpha)]. \quad (110)$$

The energy

$$\beta' = \frac{\beta^2}{8\alpha} \left[1 + \left(1 - \frac{16\alpha^2}{\beta^2} \right)^{\frac{1}{2}} \right],$$

where $(\beta')_1 = \alpha$, exceeds 20 Mev if $Z \geq 16$ and $[\alpha, t_1]_> = t_1$ if we require $Z \geq 16$ and $x < \beta'$.

It is easy to see that (110) may be written in the form (67) and is also an integral equation of Volterra type. A function f which is an upper (lower) bound for g in the region $x \leq \gamma$ and which satisfies

$$g(\gamma) \exp\{-2\lambda[(x/\gamma)^{\frac{1}{2}} - 1]\} + \int_{\gamma}^x \frac{d\lambda}{\sqrt{t}} \exp\{-2\lambda[(x/\gamma)^{\frac{1}{2}} - (t/\gamma)^{\frac{1}{2}}]\} \times \int_{t_1}^t \frac{dy\beta^2}{4ty^2} [f(t-y) + f(y-\alpha)] - f(x) \leq 0 (\geq 0) \quad (111)$$

will give an upper (lower) bound for g in the region $\gamma \leq x$.

Now (111) is certainly true for $x = \gamma$ if $f(\gamma) \geq g(\gamma)$ [$f(\gamma) \leq g(\gamma)$], and thus f will be an upper (lower) bound for $x \geq \gamma$ if f is an upper (lower) bound for $x \leq \gamma$ and if the derivative of (111) is negative (positive) for all $x > \gamma$.

The same is true if we multiply (111) by

$$\exp\{2\lambda(x/\gamma)^{\frac{1}{2}} - 1\}.$$

Thus we obtain the conditions $f(x) \geq g(x)$, [$f(x) \leq g(x)$] for $x \leq \gamma$ and

$$\int_{x_1}^x \frac{dy\beta^2}{4xy} [f(x-y) + f(y-\alpha)] - f(x) - \frac{f'(x)(x\gamma)^{\frac{1}{2}}}{\lambda} \leq 0 (\geq 0) \quad (112)$$

for an upper (lower) bound.

Let

$$f(x) = A \frac{x+\alpha}{2\alpha} + B, \quad x \leq \gamma - \gamma_1;$$

$$f(x) = \frac{R}{2\alpha}(x-\gamma) + D, \quad x \geq \gamma - \gamma_1;$$

where A, B, R , and D are constants. Substituting in (112), the left side becomes

$$2\alpha B - \frac{R(x\gamma)^{\frac{1}{2}} + \beta^2}{\lambda} \left\{ (A-R) \ln \frac{(x-\gamma+\gamma_1)(\gamma-\gamma_1+\alpha)}{xx_1} - (A-R) \frac{\alpha}{x} + \frac{A(\gamma+\alpha) + (B-D)2\alpha - (A-R)\gamma_1}{x-\gamma+\gamma_1} + \frac{(D-B)2\alpha - R(\gamma+\alpha)}{\gamma-\gamma_1+\alpha} \right\}. \quad (113)$$

Taking

$$B=0, \quad A=1, \quad D = \frac{R\gamma_1}{2\alpha} + \frac{\gamma-\gamma_1+\alpha}{2\alpha}, \quad R < 1,$$

$$f(x) \leq g(x) \quad \text{for } x \leq \gamma,$$

and substituting these values in (113), the condition for a lower bound is that for $x \geq \gamma$,

$$-1 + (1-R) \left[1 + \frac{\lambda\beta^2}{4\gamma^{\frac{1}{2}}x^{\frac{3}{2}}} \times \left\{ 1 - \frac{\alpha}{x} + \ln \frac{(x-\gamma+\gamma_1)(\gamma-\gamma_1+\alpha)}{xx_1} \right\} \right] \geq 0. \quad (114)$$

Taking $A = 1.15, B = 0.425, D = 1 + (1.15\gamma/2\alpha)$, and substituting in (113), the condition for an upper bound is that for $x \geq \gamma$,

$$\frac{0.85\alpha\lambda}{(x\gamma)^{\frac{1}{2}}} - 1.15 + (1.15-R) \left[1 + \frac{\lambda\beta^2}{4\gamma^{\frac{1}{2}}x^{\frac{3}{2}}} \left\{ 1 - \frac{\alpha}{x} + \frac{\gamma_1}{\gamma-\gamma_1+\alpha} - \frac{\gamma_1}{x-\gamma+\gamma_1} + \ln \frac{(x-\gamma+\gamma_1)(\gamma-\gamma_1+\alpha)}{xx_1} \right\} \right] \geq 0. \quad (115)$$

Since

$$\frac{5}{\beta^2} > \frac{1}{xx_1} = \frac{4}{\beta^2} + \frac{1}{x^2} > \frac{4}{\beta^2}, \quad \frac{\alpha}{\gamma} < \frac{\alpha}{\gamma}$$

Eq. (114) will be satisfied for $x \geq \gamma$ if

$$-1 + (1-R) \left[1 + \frac{\lambda\beta^2}{4\gamma^{\frac{1}{2}}x^{\frac{3}{2}}} \times \left\{ 1 - \frac{\alpha}{x} + \ln \frac{4(x-\gamma+\gamma_1)(\gamma-\gamma_1+\alpha)}{\beta^2} \right\} \right] \geq 0; \quad (116)$$

and (115) will be satisfied for $x \geq \gamma$ if

$$\frac{0.85\alpha\lambda}{\gamma} - 1.15 + (1.15-R) \left[1 + \frac{\lambda\beta^2}{4\gamma^{\frac{1}{2}}x^{\frac{3}{2}}} \left\{ 1 + \frac{\gamma_1}{\gamma-\gamma_1+\alpha} - \frac{\gamma_1}{x-\gamma+\gamma_1} + \ln \frac{5(x-\gamma+\gamma_1)(\gamma-\gamma_1+\alpha)}{\beta^2} \right\} \right] \geq 0. \quad (117)$$

Now x occurs in (116) and (117) only in the form

$$H(x) = x^{-3} \left[a - \frac{b}{x - \gamma + \gamma_1} + \ln \frac{\tau(x - \gamma + \gamma_1)(\gamma - \gamma_1 + \alpha)}{\beta^2} \right], \tag{118}$$

with a nearly 1, b either 0 or γ_1 , and $\tau = 4$ or 5.

The derivative of (118) is

$$2x^{-5/2} \left[2 - 3a + \frac{5b + \gamma - \gamma_1}{x - \gamma + \gamma_1} + \frac{2b(\gamma - \gamma_1)}{(x - \gamma + \gamma_1)^2} - 3 \ln \frac{\tau(x - \gamma + \gamma_1)(\gamma - \gamma_1 + \alpha)}{\beta^2} \right]. \tag{119}$$

It is easily seen that the bracketed quantity in (119) is a decreasing function of x which is positive at $x = \gamma$ and negative at $x = \infty$, and thus (119) changes sign exactly once for $x > \gamma$.

It follows that both (116) and (117) are concave downward for $x \geq \gamma$ and hence attain a maximum at some value of $x_{\max} > \gamma$ while the minimum is attained at one end of the range of x .

Thus for a lower bound on the range $\gamma \leq x \leq \delta$ we may take $R = R_1$ where

$$1 - R_1 = \frac{1}{2\alpha [1 + (\lambda\beta^2/4\gamma^3) \min[H(\gamma), H(\delta)]]}, \tag{120}$$

where H is defined by (118).

It is not difficult to show that (119) is negative for $x = 4\gamma/3$, and thus the value x_{\max} where H attains its maximum satisfies $x_{\max} < 4\gamma/3$. Since

$$a - \frac{b}{x - \gamma + \gamma_1} + \ln \frac{\tau(x - \gamma + \gamma_1)(\gamma - \gamma_1 + \alpha)}{\beta^2}$$

is an increasing function of x , we have

$$H(x_{\max}) < T = \gamma^{-3} \left[\frac{\gamma}{\gamma + 3\gamma_1} + \frac{\gamma_1}{\gamma - \gamma_1 + \alpha} + \ln \frac{5(\gamma + 3\gamma_1)(\gamma - \gamma_1 + \alpha)}{3\beta^2} \right]; \tag{121}$$

and hence for an upper bound, we take $R = R_2$ where

$$1.15 - R_2 = \frac{1.15 - (0.85\alpha\lambda/\gamma)}{1 + (\lambda\beta^2/4\gamma^3)T}. \tag{122}$$

Neglecting the term $(0.85\alpha\lambda/\gamma)$, which is very small, we may take

$$R_2 = \frac{1.15}{1 + (4\gamma^3/\lambda\beta^2)T}. \tag{123}$$

Thus

$$\begin{aligned} \frac{R_1}{2\alpha}(x - \gamma + \gamma_1) + \frac{\gamma - \gamma_1 + \alpha}{2\alpha} &\leq g(x) \\ &\leq \frac{R_2}{2\alpha}(x - \gamma) + 1 + \frac{1.15\gamma}{2\alpha}, \end{aligned} \tag{124}$$

where R_1 is the value of R defined by (121) and R_2 the value or R defined by (123).

The values of R_1 and R_2 are plotted in Fig. 2, with the value $\delta = 800\gamma/A$ which corresponds to an energy of 20 Mev.

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