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Inelastic Scattering of Slow Neutrons

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The total polycrystalline elastic and inelastic scattering cross sections are computed by means of the Born approximation with use of the Fermi (δ function) interaction between slow neutrons and bound nuclei. Isotopic disorder and magnetic interaction are neglected. Numerical calculation for iron scattering "300-degree" neutrons yields an inelastic cross section which rises from 0.006 at $T=0°K$ to 0.192 for a scatterer temperature of 1000°K, in units of the "free" nuclear elastic scattering cross section. The total (elastic plus inelastic) cross section remains constant for scatterer temperature up to 250°K, but falls off from 0.97 at $T=0°K$ to 0.90 at $T=1000°K$. High and low temperature approximate results are also computed. Comparison of the results for inelastic scattering with the theory of the diffuse scattering of x-rays as developed by Zachariasen is successful in the limiting cases in which the two theories overlap.

I. INTRODUCTION

IF a neutron scattered by polycrystalline matter possesses the same amount of kinetic energy that it had upon incidence, then it is said to have been scattered elastically. If the scattering results in a decrease or an increase in the neutron's kinetic energy, then the process is said to have been inelastic. In any given experiment, elastic and inelastic processes occur simultaneously, so that by mere measurement upon the intensity of the transmitted beam one is not able to separate the contributions of the two types of scattering. Comparison with theory thus requires theoretical knowledge of both the elastic and inelastic scattering cross sections. The present work includes, in addition to a presentation of the theory of elastic scattering, a theoretical treatment of inelastic processes in which energy is given to or absorbed from the elastic vibrations of the scatterer by the neutron. Loss of energy by the neutron is accompanied by the excitation of one or more elastic vibrations—the emission of one or more sound quanta, or "phonons;" gain of energy by the neutron is accompanied by the quenching of one or more elastic vibrations—the absorption of one or more phonons.

Although Halpern, Hamermesh, and Johnson[1] have treated the elastic scattering of slow neutrons by polycrystals, the subject is retained here since the present derivation is more complete and somewhat more general. Also, elastic scattering is here treated as a special case of inelastic scattering—zero-order process.[2]

In all the expressions derived herein, there is a constant factor left undetermined, which in general can be determined only by experiment;

[1] O. Halpern, M. Hamermesh, and M. H. Johnson, Phys. Rev. 59, 981 (1941), henceforth referred to as HHJ.

[2] HHJ gives no explicit derivation of the crystal temperature dependence of elastic scattering; instead it borrows the exponential factor from the earlier x-ray theory as developed by Debye, Waller, *et al.* This procedure is justified explicitly in the present work.

this is the total nuclear elastic scattering cross section for the free nucleus. That this quantity should differ from the average cross section per nucleus for nuclei bound in a crystal lattice arises from the fact that nuclei so bound do not scatter independently; but interference influences completely analogous to the familiar x-ray interference effects occur in the scattering of neutrons as well. In the present state of the understanding of nuclear forces, theoretical calculation of the free nuclear cross section is in general not at all possible; only the knowledge that nuclear forces are of short range ($\sim 10^{-12}$ cm) is certain in the realm of features relevant to the present problem. This fact is expressed in the particular analytical form of the neutron-nucleus interaction employed. What is here sought is a comparison of the average elastic and inelastic nuclear cross sections, and the variation with scatterer temperature of these quantities as well as of their sum.

For the calculation of all scattering cross sections, the present work employs the Born approximation with use of the Fermi (δ function) interaction between slow neutrons and bound nuclei. Attention is apparently limited to spin-free nuclei, but a slightly more detailed analysis reveals that the results are spin independent; for all scattering cross sections (including the free nucleus cross section) are multiplied by the same spin dependent factor in the case of scattering by nuclei of spin different from zero.

Initially, consideration is restricted to a single crystal as scattering body. Since, however, we are concerned with the scattering from polycrystalline substances, it is necessary to average the single crystal results over all possible crystal orientations. The single crystal is assumed sufficiently large to be approximated, for our purposes, by an infinite crystal. On the other hand, it is assumed that the crystal is sufficiently small to neglect the influence of the so-called "secondary extinction" in the polycrystal. This refers to the fact that the incident beam, in traversing the scattering specimen, is being depleted because of scattering by individual crystals, so that crystals farther back in the polycrystal are shielded from the full intensity of the beam. In HHJ, it is shown that for reasonably small crystals this secondary extinction is negligible.

Throughout, it is assumed that the neutron beam is monochromatic: Every incident neutron possesses a definite energy, the same for all in the beam. By the use of velocity selectors, such beams are approximately attainable.

From the outset, it will be assumed that every nucleus of the crystal scatters neutrons in precisely the same way. Thus we shall be limited to scattering by elements, and only those elements in which the abundance of the possible rarer isotopes is negligible. In addition, the interaction between the magnetic moment of the neutron and the inhomogeneous atomic magnetic fields in the case of magnetic substances is neglected. Actually, its contribution to the scattering is always quite small compared with the purely nuclear part, if not completely negligible.

The most significant result of the present work from the point of view of comparison with experiment is embodied in the variation of the total (elastic plus inelastic) scattering cross section with the temperature of the scattering polycrystal. So far as the author is aware, there have been no experiments performed which could provide the necessary check, so that the test of the theory must await more favorable times.

On the theoretical side, however, there is an interesting check provided by a close similarity between the inelastic scattering of slow neutrons and the diffuse scattering of monochromatic x-rays. Except that the scattering of x-rays from the single atom is by no means isotropic, the only significant point of departure of the two problems is that for x-rays the energy of the scattered photon may always be set equal to the incident energy. That is, the photon energy is always large compared with its energy change in an inelastic process. For slow neutrons, the incident energy and probable energy changes are in general of the same order of magnitude. If, however, the energy change were negligible for neutrons as well, then the results should be precisely the same as one would obtain for x-rays of equal wave-length assumed to undergo isotropic scattering by the individual atom. For constant neutron wave-length—hence constant momentum—the energy is inversely proportional

to the mass, so that in the limit of neutron mass equal to zero the equivalence with the case of the supposedly isotropic x-rays is complete. (Actually the mass needs to be only so small as to render the neutron energy large compared with energy changes probable.) Modification and further development of the work of Zachariasen[3] on diffuse x-ray scattering provide a result suitable for the required comparison, as we shall see in full detail in III.

Owing to the great complexity of the resulting mathematical expression for the inelastic cross section, it is difficult to obtain much useful information from mere inspection of the formula. In the special cases of high and low temperatures —compared with both the Debye temperature of the scatterer and the neutron "temperature" —simplifications occur, however, to render obvious a number of interesting qualitative results. The work is then completed with a numerical computation of the nuclear elastic and inelastic cross sections for polycrystalline iron as a function of the temperature, for 300-degree neutrons. The strict calculations are supplemented by the low and high temperature approximate calculations. The results are discussed in the final section.

II. ANALYTICAL TREATMENT

The fundamental question is, then: Given a crystal in a definite state described by the wave function Φ_n and a neutron incident with a definite momentum $\mathbf{p}$, what is the probability that, as a result of the interaction between crystal and neutron, the neutron will later be found to possess a momentum $\mathbf{p}'$, and the crystal will be found in the state $\Phi_{n'}$? To this end, we employ the Born approximation, justified by Fermi[4] for the case of slow neutrons scattered elastically by bound nuclei. The justification of its use for inelastic scattering lies in the circumstance, as will be shown, that the inelastic amplitude is in general small compared with the elastic.

It is necessary to know the solutions of the Schrödinger equation corresponding to all states of the neutron and crystal in which the interaction between them is neglected—that is, the product of neutron wave functions by crystal wave functions. The neutron functions are merely $\exp(i\mathbf{k}\cdot\mathbf{r})$ for all $\mathbf{k}$, where $\mathbf{k}=(\mathbf{p}/\hbar)$ is the propagation vector of the neutron; $\mathbf{r}$ is the neutron coordinate vector.

The treatment of the crystalline potential energy by the introduction of normal coordinates is carried out in the standard fashion of expanding the individual nuclear displacements from equilibrium in terms of a series of plane polarized standing elastic waves, each of which is characterized by a propagation vector $\mathbf{q}$ and one of three mutually orthogonal polarization directions ($j=1, 2, 3$) corresponding to the given $\mathbf{q}$. Most of the details are omitted, since they are abundantly covered in the literature.[5]

If the position of each nucleus in the crystal at any instant is given by the vectors $\mathbf{R}_\sigma$, we may write:

$$\mathbf{R}_\sigma=\boldsymbol{\sigma}+\mathbf{u}_\sigma, \tag{1}$$

where $\boldsymbol{\sigma}$ is the equilibrium position of the σth nucleus and $\mathbf{u}_\sigma$ the instantaneous deviation from equilibrium. For not too high temperatures, the potential energy of the crystal is expressible as a quadratic form involving the components of all the displacements $\mathbf{u}_\sigma$. To obtain the most simple expression for this energy, we introduce the variables γ_s and μ_s, where

$$\mathbf{u}_\sigma=(2/mN)^{\frac{1}{2}}\sum_s \boldsymbol{\alpha}_s(\gamma_s\cos\boldsymbol{\sigma}\cdot\mathbf{q}_s-\mu_s\sin\boldsymbol{\sigma}\cdot\mathbf{q}_s). \tag{2}$$

The index s stands for the double index $(\mathbf{q}, j)$, and the range of values assumed by s is such that for each $\mathbf{q}$ the three mutually orthogonal directions of $\boldsymbol{\alpha}_s$ (unit polarization vector) are summed over, and then *one-half* (determined by any plane intersecting the origin) of the $\mathbf{q}$ space to be defined presently. N is the number of scattering centers in the crystal, m the mass at each scattering center.

In terms of the γ_s and μ_s, the crystalline potential energy may be written

$$U=\sum_s (1/2)\omega_s^2(\gamma_s^2+\mu_s^2). \tag{3}$$

Because of the fact that U may be so written, the γ_s and μ_s, the "normal coordinates," may be regarded as the coordinates of harmonic oscillators of unit mass and circular frequencies ω_s.

[3] W. H. Zachariasen, Phys. Rev. **57**, 597 (1940).
[4] E. Fermi, Ricerca Scient. **7**, Part 2, 13 (1936).
[5] M. Born and K. Sarginson, Proc. Roy. Soc. **A179**, 69 (1941).

To each s, then, there are both a "γ-oscillator" and a "μ-oscillator"—therefore one of each to every $(\mathbf{q}, j)$ combination.

The definition of the $\mathbf{q}$ space over which summation is taken is fixed by the usual requirement of periodicity of $\mathbf{u}_\sigma$ in a "fundamental parallelopiped" of the crystal. Since all results must be independent of the size of this parallelopiped, we take it to be that containing the N lattice points of our crystal, for sake of definiteness. We write:

$$\boldsymbol{\sigma}=\sigma_1\mathbf{a}_1+\sigma_2\mathbf{a}_2+\sigma_3\mathbf{a}_3, \tag{4}$$

where $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ are the basic vectors of the lattice (of dimensions length), and σ_1, σ_2, σ_3 are integers peculiar to the $\boldsymbol{\sigma}$th lattice point. If $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ are the basic vectors of the reciprocal lattice—$\mathbf{b}_1=(\mathbf{a}_2\times\mathbf{a}_3)/[\mathbf{a}_1\cdot(\mathbf{a}_2\times\mathbf{a}_3)]$, etc.—we have:

$$\mathbf{q}=q_1\mathbf{b}_1+q_2\mathbf{b}_2+q_3\mathbf{b}_3. \tag{5}$$

Then

$$\boldsymbol{\sigma}\cdot\mathbf{q}=\sigma_1q_1+\sigma_2q_2+\sigma_3q_3. \tag{6}$$

Thus q_i must have only such values that if σ_i runs through its "fundamental interval," then σ_iq_i changes by some integral multiple of 2π; for only then will $\mathbf{u}_\sigma$, given by (2), remain unaltered. If the fundamental parallelopiped is such that it is traversed exactly once when all three of the σ_i are augmented by the integers g_i, then we have

$$q_i=2\pi Q_i/g_i, \tag{7}$$

where Q_i is a positive or negative integer.

Also, $\mathbf{q}$ space is limited by the fact that each oscillator actually represents a plane polarized standing wave of half-interval of periodicity in any of the three basic directions $\mathbf{a}_i$ equal to (π/q_i). Since it is physically meaningless for the half wave-length of a sound wave to be less than the distance between successive lattice points in the crystal, we must have $(\pi/|q_i|)\geqslant 1$, or $-\pi\leqslant q_i\leqslant\pi$. By (7), then, the integers Q_i are limited by the inequalities $-(g_i/2)\leqslant Q_i\leqslant(g_i/2)$, whence $\mathbf{q}$ space is limited to $g_1g_2g_3=N$ points. (Unity is neglected compared with g_i.) We employ this fact later to determine the upper limit of the absolute value of $\mathbf{q}$.

Now, the potential energy U, given by (3), is that of a system of $3N$ uncoupled harmonic oscillators of circular frequencies ω_s and each of mass unity. (There are $N/2$ points of *half* $\mathbf{q}$ space, to each $\mathbf{q}$ the three values $j=1, 2, 3$; to each $(\mathbf{q}, j)$ combination are both a γ and a μ—that is, $3N$ terms in (3) altogether.) The wave functions are well known to be[6] Hermite functions of argument $\gamma(\omega/\hbar)^{\frac{1}{2}}$ and $\mu(\omega/\hbar)^{\frac{1}{2}}$ for the respective cases. The normalized solution for a γ-oscillator in the nth energy state is

$$\phi_n(\gamma(\omega/\hbar)^{\frac{1}{2}})=[(\omega/\hbar\pi)^{\frac{1}{4}}/(2^nn!)^{\frac{1}{2}}]\times\exp(-\omega\gamma^2/2\hbar)H_n(\gamma(\omega/\hbar)^{\frac{1}{2}}), \tag{8}$$

where H_n is the nth Hermite polynomial defined by the generating function

$$\exp(-z^2+2zx)=\textstyle\sum_n (z^n/n!)H_n(x).$$

The energy of the oscillator in the nth state is $(n+1/2)\hbar\omega$.

Thus we may write the total wave function describing the thermal agitation of the crystal as the product

$$\Phi_n=\prod_{s_1s_2}\phi_{n_{s_1}}\phi_{n_{s_2}},$$

where $\phi_{n_{s_1}}=\phi_{n_s}(\gamma_s(\omega_s/\hbar)^{\frac{1}{2}})$, $\phi_{n_{s_2}}=\phi_{n_s}(\mu_s(\omega_s/\hbar)^{\frac{1}{2}})$.

Each of the indices s_1, s_2 clearly takes on the $3N/2$ values assumed by s.

Finally, the total wave function of the system neutron plus crystal without interaction is

$$\Psi=\exp(i\mathbf{k}\cdot\mathbf{r})\Phi_n=\exp(i\mathbf{k}\cdot\mathbf{r})\prod_{s_1s_2}\phi_{n_{s_1}}\phi_{n_{s_2}}.$$

Because of the interaction between crystal and neutron, the state of either or both may be changed, so that we denote the wave function after interaction by

$$\Psi'=\exp(i\mathbf{k}'\cdot\mathbf{r})\prod_{s_1s_2}\phi_{n'_{s_1}}\phi_{n'_{s_2}}.$$

In the Born approximation, the probability of transition from a state Ψ to a state Ψ' because of the interaction energy V between neutron and crystal is proportional to $|M|^2$, where

$$M=\int\int\int\Psi'^*V\Psi d\mathbf{r}d\gamma d\mu;$$

the integrations are carried out over the complete ranges of the variables; $d\mathbf{r}$ = volume element in neutron coordinate space,

$$d\gamma=\prod_s d\gamma_s,\quad d\mu=\prod_s d\mu_s.$$

[6] Any elementary text on quantum mechanics—e.g., V. Rojansky, *Introductory Quantum Mechanics* (Prentice-Hall, Inc., New York, 1938), first edition.

Fermi has shown[4] that for bound nuclei scattering neutrons of wave-length long compared with nuclear dimensions, the interaction energy between the neutron and individual nucleus, position $\mathbf{R}_\sigma$, is given by

$$V_\sigma = A_\sigma \delta(\mathbf{r}-\mathbf{R}_\sigma),$$

where, for spin-free nuclei (cf. introductory remarks that the results also apply to a spin dependent interaction) A_σ is a scalar depending upon the type of scattering nucleus. We are restricted to scattering by identical nuclei by setting $A_\sigma = A$, a constant for all σ. $\delta(\mathbf{r}-\mathbf{R}_\sigma)$ is a three-dimensional Dirac δ function. For "room temperature" neutrons, the wave-lengths are of the order of atomic dimensions, so that we may employ the above form of V_σ. The total interaction between neutron and crystal is given by:

$$V = \sum_\sigma A_\sigma \delta(\mathbf{r}-\mathbf{R}_\sigma) = A\sum_\sigma \delta(\mathbf{r}-\mathbf{R}_\sigma),$$

where the summation is taken over all the nuclei of the crystal.

We write, therefore, since $\Phi_{n'}$ is a real function,

$$\begin{aligned} M &= A\int\int\int \exp[i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')] \times \sum_\sigma \delta(\mathbf{r}-\mathbf{R}_\sigma)\Phi_n\Phi_{n'} d\mathbf{r}d\gamma d\mu \\ &= A\sum_\sigma \int\int \exp[i\mathbf{R}_\sigma\cdot(\mathbf{k}-\mathbf{k}')] \times \prod_{s_1}\phi_{n_{s_1}}\phi_{n'_{s_1}}d\gamma_{s_1}\prod_{s_2}\phi_{n_{s_2}}\phi_{n'_{s_2}}d\mu_{s_2} \\ &= A\sum_\sigma \exp[i\sigma\cdot(\mathbf{k}-\mathbf{k}')] \times \int\int \exp[i\mathbf{u}_\sigma\cdot(\mathbf{k}-\mathbf{k}')]\prod_{s_1}\phi_{n_{s_1}}\phi_{n'_{s_1}}d\gamma_{s_1} \times \prod_{s_2}\phi_{n_{s_2}}\phi_{n'_{s_2}}d\mu_{s_2}, \end{aligned}$$

with the use of (1). The expansion of $\mathbf{u}_\sigma$ according to (2) gives, finally,

$$M = A\sum_\sigma \exp[i\sigma\cdot(\mathbf{k}-\mathbf{k}')]\prod_{s_1 s_2} I^\sigma_{n'_{s_1}n_{s_1}} I^\sigma_{n'_{s_2}n_{s_2}}, \tag{9}$$

where

$$I^\sigma_{n'_s n_s} = \int \exp(iF^\sigma_s\gamma_s)\phi_{n'_s}\phi_{n_s}d\gamma_s,$$

$$F^\sigma_{s_1} = (2/mN)^{\frac{1}{2}}(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\alpha}_{s_1}\cos\boldsymbol{\sigma}\cdot\mathbf{q}_{s_1}$$

and

$$F^\sigma_{s_2} = -(2/mN)^{\frac{1}{2}}(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\alpha}_{s_2}\sin\boldsymbol{\sigma}\cdot\mathbf{q}_{s_2}. \tag{10}$$

It is necessary, then, to evaluate integrals of the form

$$I_{n+\lambda,n}(t) = \int_{-\infty}^{\infty}\exp(tx/a)\phi_{n+\lambda}(x/a)\phi_n(x/a)dx \qquad (t = iaF^\sigma_s,\ a = (\hbar/\omega_s)^{\frac{1}{2}}). \tag{11}$$

For n' has been written $n+\lambda$; i.e., the result corresponds to a change from state n to state $n+\lambda$ of the given oscillator. λ may be positive or negative, but necessarily an integer (as is n). The evaluation follows:

According to (8),

$$\begin{aligned} I_{n+\lambda,n}(t) &= [2^{2n+\lambda}n!(n+\lambda)!\pi]^{-\frac{1}{2}}\int_{-\infty}^{\infty}\exp(tx/a)\exp(-x^2/a^2)H_{n+\lambda}(x/a)H_n(x/a)d(x/a) \\ &= [2^{2n+\lambda}n!(n+\lambda)!\pi]^{-\frac{1}{2}}\int_{-\infty}^{\infty}\exp(tx)\exp(-x^2)H_{n+\lambda}(x)H_n(x)dx \\ &= [2^{2n+\lambda}n!(n+\lambda)!\pi]^{-\frac{1}{2}}\int_{-\infty}^{\infty}\exp[-(x-t/2)^2]\exp(t^2/4)H_{n+\lambda}(x)H_n(x)dx \\ &= [2^{2n+\lambda}n!(n+\lambda)!\pi]^{-\frac{1}{2}}\exp(t^2/4)\int_{-\infty}^{\infty}\exp(-z^2)H_{n+\lambda}(z+t/2)H_n(z+t/2)dz \\ &= \frac{\exp(t^2/4)}{[2^{2n+\lambda}n!(n+\lambda)!\pi]^{\frac{1}{2}}}\sum_{\nu=0}^{m}\sum_{\beta=0}^{m+\lambda}\binom{n}{\nu}\binom{n+\lambda}{\beta}t^{\nu+\beta}\int_{-\infty}^{\infty}\exp(-z^2)H_{n+\lambda-\beta}(z)H_{n-\nu}(z)dz \\ &= \frac{\exp(t^2/4)}{[2^{2n+\lambda}n!(n+\lambda)!\pi]^{\frac{1}{2}}}\sum_{\nu\beta}\binom{n}{\nu}\binom{n+\lambda}{\beta}t^{\nu+\beta}\delta^{n-\nu}_{n+\lambda-\beta}2^{n-\nu}(n-\nu)!\pi^{\frac{1}{2}} \\ &= \frac{\exp(t^2/4)}{[n!(n+\lambda)!]^{\frac{1}{2}}}\sum_\nu\binom{n+\lambda}{\nu+\lambda}\frac{n!}{\nu!}\left(\frac{t^2}{2}\right)^{\nu+\lambda/2}. \end{aligned} \tag{12}$$

The second-from-last step is obtained through the use of the expansion

$$H_n(x+y)=\sum_{\nu=0}^{n}\binom{n}{\nu}(2y)^\nu H_{n-\nu}(x),$$

as one may show from the familiar recursion formula $(d/dx)H_n(x)=2nH_{n-1}(x)$ and use of the Taylor expansion of $H_n(x+y)$ about the point x in powers of y. Otherwise, the expansion of $H_n(x+y)$ may be obtained directly through use of the generating function for Hermite polynomials. The next-to-last step in the sequence above is given by the orthogonality relation

$$\int_{-\infty}^{\infty}\exp(-z^2)H_\nu(z)H_\beta(z)dz=\delta_\nu{}^\beta 2^\nu\nu!\pi^{\frac{1}{2}}.$$

The summation limits for ν (and β above) are provided naturally by the presence of denominator factorials; the result is unchanged if one sums from zero to infinity.

The quantity $|M|^2$ (proportional to the scattering cross section), for scattering processes in which the quantum number of the sth oscillator changes by the (positive or negative) integer λ_s, is given according to (9) by

$$|M|^2=|A|^2\sum_{\sigma\sigma'}\exp[i(\boldsymbol{\sigma}-\boldsymbol{\sigma}')\cdot(\mathbf{k}-\mathbf{k}')]\times\prod_{s_1s_2}J^{\sigma\sigma'}_{n_{s_1}+\lambda_{s_1},n_{s_1}}J^{\sigma\sigma'}_{n_{s_2}+\lambda_{s_2},n_{s_2}},\quad(13)$$

where

$$J^{\sigma\sigma'}_{n'_sn_s}=I^{\sigma}_{n'_sn_s}I^{\sigma'*}_{n'_sn_s}.$$

If for all s, $\lambda_s=0$, the scattering is elastic; this is the case which has been considered by HHJ. Positive λ_s means loss of energy, of an amount $\lambda_s\hbar\omega_s$, by the neutron to the sth oscillator; negative λ_s means the absorption of this amount of energy by the neutron from the sth oscillator.

According to (11) and (10), t is proportional to $N^{-\frac{1}{2}}$; since $N\gg1$, then (for $\omega_s\neq0$) $t\ll1$. Thus it is necessary to keep only the lowest powers of t in the expression (12) for $I_{n+\lambda,n}(t)$. For $\lambda=0$, it is necessary to expand to the quadratic term in t; to this approximation,

$$I_{n,n}(t)=1+(1+2n)(t^2/4).\quad(14)$$

The term in t^2, proportional to N^{-1}, must be kept since the quantity M involves the product of approximately $3N$ such factors; higher order terms involve higher powers of N^{-1} and are therefore negligible for $N\gg1$.

For $\lambda=\pm1$, only the linear term must be kept:

$$I_{n+1,n}(t)=[(n+1)/2]^{\frac{1}{2}}t;\quad I_{n-1,n}(t)=(n/2)^{\frac{1}{2}}t.\quad(15)$$

In the transition probability, proportional to $|M|^2$, the lowest appearing power of t due to $\lambda=\pm1$ for just one oscillator (and $\lambda=0$ for all the others) is the second, which is proportional to N^{-1}. Since, however, there are $3N$ oscillators which may so participate, the probability that *any* oscillator so participate is the sum of the single probability over all the oscillators. The probability is thus rendered finite, no matter how large N; the terms in higher powers of t still contribute negligibly for large N. If more than one oscillator, say $\beta(\ll N)$ in all, undergo changes in n by $\lambda=\pm1$, then the factor $N^{-\beta}$ appears in the quantity $|M|^2$. Summation over the $\binom{3N}{\beta}$ combinations of $3N$ oscillators taken β at a time renders the total probability finite, but the contribution of higher powers of t remains negligible.

It is next shown that processes for which $|\lambda|\geqslant2$ are completely negligible so long as $N\gg1$. By (12), to the lowest power of t:

$$I_{n+\lambda,n}(t)=[n!(n+\lambda)!]^{-\frac{1}{2}}[(n+\lambda)!/\lambda!]t^\lambda 2^{-\lambda/2};$$

$$I_{n-\alpha,n}(t)=[n!(n-\alpha)!]^{-\frac{1}{2}}(n!/\alpha!)t^\alpha 2^{-\alpha/2}\quad(\alpha=-\lambda>0).$$

For $|\lambda|\geqslant2$, the squares of these quantities are proportional to N^{-2}, or higher powers of N^{-2}. Thus even summation over the $3N$ oscillators still renders the probability negligible for $N\gg1$.

From the expansions (14), (15), it is seen that for $N\gg1$ the ratio $|I_{n\pm1,n}|^2/|I_{nn}|^2$ is proportional to $|t|^2$, or to $(\hbar/\omega_s)(F_s^\sigma)^2$, by (11). Since $|I_{n\pm1,n}|^2$ must be summed over all $3N$ oscillators, the ratio of the probability of a first-order process to that of a zero-order process is roughly proportional to

$$L=N(\hbar/\omega_s)(F_s^\sigma)^2\leqq(\hbar k^2/2m\omega_s)=\frac{(\hbar^2k^2/2m_0)}{\hbar\omega_s}\left(\frac{m_0}{m}\right)$$

to order of magnitude, according to (10). Here m_0 is the neutron mass, so that $(\hbar^2k^2/2m_0)$ is the incident neutron energy; $\hbar\omega_s$ is of the order of

the energy of the sth oscillator. For room temperature neutrons the ratio of these energies is, on the average, of the order of unity for many substances. Hence for such cases, what counts in the ratio L is the factor (m_0/m), the ratio of the neutron mass to the mass of the scattering nucleus. Thus, in general, for elements of large nuclear mass L is small compared with unity; i.e., inelastic processes are much less probable than elastic ones. Also, since this same ratio L is involved in the comparison of the probability of processes involving two oscillators with the probability of those involving only one, the former are much less likely than the latter for $(m_0/m)\ll 1$. It is for this reason that the present work shall confine itself to single oscillator first-order processes only, in addition to zero-order processes. For Fe as scatterer, $(m_0/m)\leqq 1/56$, so that the limited consideration is well justified in this case. The role of the factor, ratio of incident neutron energy to $\hbar\omega_s$, in L is not so clearly defined as a function of neutron energy. This is because of crystal interference effects, which depend, for processes of all orders, quite strongly upon the incident energy and, therefore, may play a far greater part in determining the relative magnitudes of types of scattering than do these simple ratio considerations.

To find the actual probability (eventually the cross section) of each of the oscillators performing the transition from n_s to $n_s+\lambda_s$ ($\lambda_s=\pm\delta_s{}^f$ or 0 for all s, for our purposes), it is necessary to multiply $|M|^2$, (13), by the probability that the oscillators originally be in the states n_s. Since before interaction with the incoming neutron the crystal is in thermal equilibrium, the Boltzmann probability that the sth oscillator be in the state n_s (energy $=(n_s+\frac{1}{2})\hbar\omega_s$) is given by $(1-x_s)x_s{}^{n_s}$, where

$$x_s=\exp(-\hbar\omega_s/k_0T),\quad x_s{}^{n_s}=\exp(-n_s\hbar\omega_s/k_0T),$$

$k_0=$ Boltzmann's constant, and $T=$ crystal temperature, Kelvin. Hence the probability that all the oscillators initially be in the states n_s is

$$\prod_{s_1s_2}(1-x_{s_1})x_{s_1}{}^{n_{s_1}}(1-x_{s_2})x_{s_2}{}^{n_{s_2}}$$—the indices s_1, s_2 referring, respectively, to the γ and μ oscillators, as previously. We form, then, the product

$$Q=\prod_{s_1s_2}(1-x_{s_1})x_{s_1}{}^{n_{s_1}}(1-x_{s_2})x_{s_2}{}^{n_{s_2}}|M|^2,$$

whence from (13),

$$Q=|A|^2\sum_{\sigma\sigma'}\exp[i(\boldsymbol{\sigma}-\boldsymbol{\sigma}')\cdot(\mathbf{k}-\mathbf{k}')]\prod_{s_1s_2}(1-x_{s_1})$$
$$\times x_{s_1}{}^{n_{s_1}}J^{\sigma\sigma'}_{n_{s_1}+\lambda_{s_1},n_{s_1}}(1-x_{s_2})x_{s_2}{}^{n_{s_2}}J^{\sigma\sigma'}_{n_{s_2}+\lambda_{s_2},n_{s_2}}.$$

Owing to the circumstance that the energy levels of the harmonic oscillator are equidistantly spaced, an important quantity is the quantity Q summed over all n_s (zero to infinity) for all s. This gives (when properly normalized) the probability of oscillator transitions by energies $\lambda_s\hbar\omega_s$, regardless of the initial states n_s. Applied to Q, this operation gives:

$$P=|A|^2\sum_{\sigma\sigma'}\exp[i(\boldsymbol{\sigma}-\boldsymbol{\sigma}')\cdot(\mathbf{k}-\mathbf{k}')]$$
$$\times\prod_{s_1s_2}(1-x_{s_1})(1-x_{s_2})Y^{\sigma\sigma'}_{s_1\lambda_{s_1}}Y^{\sigma\sigma'}_{s_2\lambda_{s_2}},\quad(16)$$

where

$$Y^{\sigma\sigma'}_{s\lambda_s}=\sum_{n_s}x_s{}^{n_s}J^{\sigma\sigma'}_{n_s+\lambda_s,n_s}.$$

Dropping for the moment excess indices, we write

$$Y_\lambda=\textstyle\sum_n x^nJ_{n+\lambda,n},$$

with $J_{n+\lambda,n}=I_{n+\lambda,n}(t)I_{n+\lambda,n}(w)$, and $t=iaF_s{}^\sigma$, $w=-iaF_s{}^{\sigma'}$, $a=(\hbar/\omega_s)^{\frac{1}{2}}$. The calculations of Y_0, $Y_{\pm1}$ follow:

According to (14)

$$J_{n,n}=1+(1+2n)(t^2+w^2)/4,$$

so that

$$Y_0=\textstyle\sum_n x^n+[(t^2+w^2)/4][\sum_n x^n+2\sum_n nx^n]$$
$$=(1-x)^{-1}+[(t^2+w^2)/4]$$
$$\times[(1-x)^{-1}+2x(1-x)^{-2}],$$

since

$$\textstyle\sum_n x^n=(1-x)^{-1},\quad(x<1),$$

and

$$\textstyle\sum_n nx^n=x(d/dx)\sum_n x^n=x(1-x)^{-2}.$$

Finally,

$$Y_0=(1-x)^{-1}\exp[(t^2+w^2)(1+x)/4(1-x)],$$

since $1+z=\exp(z)$ for $z\ll 1$. Or, if we restore the missing indices,

$$Y^{\sigma\sigma'}_{s,0}=(1-x_s)^{-1}\exp[-(\hbar/\omega_s)$$
$$\times\{(F_s{}^\sigma)^2+(F_s{}^{\sigma'})^2\}(1+x_s)/4(1-x_s)],\quad(17)$$

t and w having been replaced by their respective values given directly above.

In what follows, it is convenient to obtain the quantities $Y_{\pm 1}$ as multiples of Y_0. To this end, it is necessary to expand $I_{n\pm 1,\,n}$ to powers higher than the first of t (or w), as in (15). From (12), we get

$$I_{n+1,\,n}(t) = t \exp(t^2/4)[(n+1)/2]^{\frac{1}{2}}[1+n(t^2/4)],$$

whence

$$J_{n+1,\,n} = (tw/2)\exp[(t^2+w^2)/4](n+1) \times[1+n(t^2+w^2)/4],$$

$$Y_1 = \sum_n x^n J_{n+1,\,n} = (tw/2)(1-x)^{-2} \times \exp[(t^2+w^2)(1+x)/4(1-x)] = (tw/2)(1-x)^{-1} Y_0,$$

as one finds by applying $\sum_n n^2 x^n = x(d/dx)\sum_n nx^n = x(1+x)(1-x)^{-3}$ (the sums $\sum_n x^n$ and $\sum_n nx^n$ having been evaluated to obtain Y_0), and $1+z=\exp(z)$ for $z \ll 1$. Finally,

$$Y_{s,\,1}^{\sigma\sigma'} = [\hbar F_s^{\sigma} F_s^{\sigma'}/2\omega_s(1-x_s)]\, Y_{s,\,0}^{\sigma\sigma'}. \tag{18}$$

Similarly, it is found that

$$Y_{s,\,-1}^{\sigma\sigma'} = [\hbar x_s F_s^{\sigma} F_s^{\sigma'}/2\omega_s(1-x_s)]\, Y_{s,\,0}^{\sigma\sigma'} = x_s Y_{s,\,1}^{\sigma\sigma'}.$$

Since $x_s = \exp(-\hbar\omega_s/k_0 T)$ is less than unity for finite T, the relation $Y_{-1} = xY_1$ expresses the physically obvious fact that processes in which the neutron loses energy are more likely to occur than those in which it gains the same amount; at $T=0$, it is impossible for a neutron to absorb energy from a crystal lattice. Only for temperatures such that $k_0 T \gg \hbar\omega_s$ are energy gain and loss equally probable.

For elastic scattering, the quantity P given by (16) is denoted by P_0; for first-order processes in which the fth oscillator undergoes a change n_f by ± 1, P is denoted by $P^f{}_{\pm 1}$. According to (16), (17), and (18),

$$P_0 = |A|^2 \exp(-2W) \times |\textstyle\sum_\sigma \exp[i\boldsymbol{\sigma}\cdot(\mathbf{k}-\mathbf{k}')]|^2, \tag{19}$$

$$P_1{}^f = |A|^2 \exp(-2W)[\hbar/2\omega_f(1-x_f)] \times |\textstyle\sum_\sigma \exp[i\boldsymbol{\sigma}\cdot(\mathbf{k}-\mathbf{k}')] F_f^{\sigma}|^2, \tag{20}$$

and

$$P_{-1}^f = x_f P_1{}^f; \tag{21}$$

$$W = \textstyle\sum_{s_1}[(\hbar/\omega_{s1})(F_{s1}^{\sigma})^2(1+x_{s1})/4(1-x_{s1})] + \sum_{s_2}[(\hbar/\omega_{s2})(F_{s2}^{\sigma})^2(1+x_{s2})/4(1-x_{s2})].$$

The removal of $\exp(-2W)$ to the left of $\sum_\sigma$ is justified directly; W is actually independent of $\boldsymbol{\sigma}$.

Since there is a one-to-one correspondence between the terms of the two sums of W, this quantity may be simplified by dint of the fact that $\omega_{s1} = \omega_{s2} = \omega_s$ (and therefore $x_{s1} = x_{s2} = x_s$) for corresponding terms. From (10), we obtain, for corresponding s_1, s_2,

$$(F_{s1}^{\sigma})^2 + (F_{s2}^{\sigma})^2 = (2/mN)[(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\alpha}_s]^2.$$

Consequently,

$$W = (\hbar/2mN)\textstyle\sum_s [(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\alpha}_s]^2(1+x_s)/\omega_s(1-x_s)$$

has clearly no dependence on $\boldsymbol{\sigma}$.

In the usual fashion, the sum over s is replaced by an integral over the half of $\mathbf{q}$ space. For $N \gg 1$, this is valid. Also, we employ the Debye approximation for the frequency spectrum—namely, $\omega = cq$, where c is the constant average sound velocity. (We adopt the average sound velocity—to be characterized in terms of the average Debye temperature—instead of keeping the individual transverse and longitudinal velocities for the sake of great simplification of the work involved.) The assumption of a sound velocity independent of wave-length actually holds in a continuum, therefore for wave-lengths long compared with the lattice constant. That it breaks down for short wave-lengths (large ω) is not a serious difficulty so long as we use only integral properties of the frequency spectrum.

With an average sound velocity assumed, the values of ω_s (and hence x_s) are the same for the three mutually orthogonal directions of the unit vectors $\boldsymbol{\alpha}_s$ *for a given* $\mathbf{q}$. Thus we may write

$$W = (\hbar/2mN)(\mathbf{k}-\mathbf{k}')^2 \textstyle\sum_s{}' (1+x_s)/\omega_s(1-x_s),$$

where the prime of $\sum_s{}'$ indicates that only the $N/2$ points of half $\mathbf{q}$ space need be summed over —the summation over j (indicating the three directions of polarization) having been carried out for all $\mathbf{q}$. Now $\sum_s{}'$ actually means summation over the three sets of discrete variables q_1, q_2, q_3, given by (7). To convert this sum into an integral, we must first multiply the summand by $[N/(2\pi)^3]dq_1 dq_2 dq_3$ since (7) shows that there are $N/(2\pi)^3$ points per unit "volume" of $q_1 q_2 q_3$ space. It is yet more convenient to convert $\sum_s{}'$ into an integral over the variables q_{x1}, q_{x2}, q_{x3}, where these are the Cartesian components of $\mathbf{q}$

(and of dimensions inverse length). This necessitates further multiplication by B, where

$$dq_1dq_2dq_3 = Bdq_{x1}dq_{x2}dq_{x3}. \tag{22}$$

For regular lattices, the transformation from reciprocal lattice to Cartesian components is linear, the Jacobian B constant. It will be shown in Section VI that B is the volume per nucleus in the crystal. Finally, we employ the usual artifice of replacing the region of $\mathbf{q}$ space by a sphere containing the same number—$N/2$—of points. The volume element is thus a hemispherical shell, or $dq_{x1}dq_{x2}dq_{x3} = 2\pi q^2 dq$; the radius of the sphere, to be determined directly, is q_0. To insure that the number of points in the hemisphere is $N/2$, we must have

$$(N/2) = [N/(2\pi)^3]B\int_0^{q_0} 2\pi q^2 dq;$$
$$q_0{}^3 = (6\pi^2/B). \tag{23}$$

At length, with application of $cq = \omega$, $cq_0 = \omega_0$ (the maximum circular frequency), we find (the now unnecessary index s having been dropped):

$$W = (3\hbar/4m\omega_0{}^3)(\mathbf{k}-\mathbf{k}')^2\int_0^{\omega_0}[\omega(1+x)/(1-x)]d\omega$$
$$= (3\hbar^2/2mk_0\Theta)(\mathbf{k}-\mathbf{k}')^2 \times\{(1/4)+(T/\Theta)^2Q_1(\Theta/T)\}, \tag{24}$$

where use has been made of the fact that $x = \exp(-\hbar\omega/k_0T)$, and $\Theta = (\hbar\omega_0/k_0)$ is the Debye temperature of the scattering substance. Here,

$$Q_1(z) = \int_0^z \{\beta/[\exp(\beta)-1]\}d\beta. \tag{25}$$

A. Elastic Scattering

In order to convert P_0, (19), to an actual cross section (per unit solid angle and per scattering nucleus), we must multiply by $(m_0{}^2/4\pi^2\hbar^4N)$, where m_0 is the neutron mass. Thus

$$G_0(\mathbf{k}-\mathbf{k}') = (X/4\pi N)\exp(-2W) \times|\textstyle\sum_\sigma \exp[i\boldsymbol{\sigma}\cdot(\mathbf{k}-\mathbf{k}')]|^2, \tag{26}$$

is the elastic scattering cross section per nucleus per unit solid angle for the single crystal; here $X = (m_0{}^2/\pi\hbar^4)|A|^2$ is the total elastic cross section of the free scattering nucleus.

Our system of basic lattice vectors is necessarily such that for each integer triple $\sigma_1\sigma_2\sigma_3$ $(0 \leqslant \sigma_i \leqslant g_i)$ there is one and only one crystal lattice point. [The definition of g_i—$\gg 1$—precedes relation (7) directly; we shall often neglect unity in comparison with g_i.] Thus, since

$$\boldsymbol{\sigma} = \sum_{i=1}^3 \sigma_i\mathbf{a}_i, \quad (\mathbf{k}-\mathbf{k}') = \sum_{i=1}^3 (k_i-k_i')\mathbf{b}_i,$$

and

$$\boldsymbol{\sigma}\cdot(\mathbf{k}-\mathbf{k}') = \sum_{i=1}^3 \sigma_i(k_i-k_i'),$$

following (4), (5), (6) (where k_i and k_i' are clearly the reciprocal lattice components of $\mathbf{k}$ and $\mathbf{k}'$, respectively),

$$|\textstyle\sum_1|^2 = |\sum_\sigma \exp[i\boldsymbol{\sigma}\cdot(\mathbf{k}-\mathbf{k}')]|^2$$
$$= \prod_{i=1}^3 \left|\sum_{\sigma_i=0}^{g_i} \exp[i\sigma_i(k_i-k_i')]\right|^2$$
$$= \prod_{i=1}^3 \frac{\sin^2[g_i(k_i-k_i')/2]}{\sin^2[(k_i-k_i')/2]}$$
$$= (2\pi)^3N\prod_{i=1}^3 \delta(k_i-k_i'-2\pi\tau_i). \tag{27}$$

Here $\delta(k_i-k_i'-2\pi\tau_i)$ is a Dirac δ function defined by the integral property $\int f(x)\delta(x-b)dx = f(b)$ for b within the range of integration, $=0$ for b without the range of integration; τ_i is a positive or negative integer. The vector

$$\boldsymbol{\tau} = \sum_{i=1}^3 \tau_i\mathbf{b}_i$$

therefore connects two points of the reciprocal lattice, and is loosely referred to as a "reciprocal lattice vector." The validity of replacing the sine-squared ratios by δ functions rests upon the facts that $g_i \gg 1$ and that functions by which $|\textstyle\sum_1|^2$ is multiplied undergo no violent variation in the region in which $|\textstyle\sum_1|^2$ differs appreciably from zero; also, only the integral properties of $|\textstyle\sum_1|^2$ are required in the present work.

If instead of using δ functions whose arguments are reciprocal lattice components of vectors, we introduce δ functions in which the arguments are the Cartesian components of these same vectors, we find from the definition of $\delta(x-b)$ above that

$$\prod_{i=1}^3 \delta(k_i-k_i'-2\pi\tau_i) = B^{-1}\delta(k_{x1}-k_{x1}'-2\pi\tau_{x1}) \times\delta(k_{x2}-k_{x2}'-2\pi\tau_{x2})\delta(k_{x3}-k_{x3}'-2\pi\tau_{x3})$$
$$= B^{-1}\delta(\mathbf{k}-\mathbf{k}'-2\pi\boldsymbol{\tau}),$$

where B^{-1} is the reciprocal of the Jacobian, defined by (22), for the transformation from reciprocal lattice to Cartesian components. The three-dimensional, or vector, δ function is merely an abbreviated way of writing the triple product for which it stands. It has the additional advantage of independence upon the orientation of the Cartesian coordinate system. Thus (26) finally becomes

$$G_0(\mathbf{k}-\mathbf{k}')_\tau = 2\pi^2 B^{-1} X \exp(-2W)\delta(\mathbf{k}-\mathbf{k}'-2\pi\boldsymbol{\tau}).$$

This result expresses for neutrons the familiar x-ray Laue conditions for elastic scattering by a single crystal—namely, that only for well-defined (the better the larger N) angles of incidence is there elastic scattering at all for an incident monochromatic beam, and then only at certain angles defined with the same degree of sharpness as is required of the angles of incidence.

We now pass to the case of the polycrystal by averaging over all crystal orientations. We do this by averaging over all directions of $\boldsymbol{\tau}$, which for any given value has a fixed orientation relative to the crystal axes. We choose a polar axis along the direction of $(\mathbf{k}-\mathbf{k}')$ and denote the polar coordinates of $\boldsymbol{\tau}$ by τ, θ_τ, φ_τ, so that

$$E_0(\mathbf{k}-\mathbf{k}')_\tau = (1/4\pi)\int_0^{2\pi} d\varphi_\tau \int_0^{\pi} G_0(\mathbf{k}-\mathbf{k}')_\tau \sin\theta_\tau d\theta_\tau$$
$$= (\pi/2)B^{-1}X \exp(-2W)S_1 \qquad (28)$$

is the polycrystalline elastic cross section corresponding to the reciprocal lattice vector $\boldsymbol{\tau}$. Here, clearly,

$$S_1 = \int_0^{2\pi} d\varphi_\tau \int_0^{\pi} \delta(\mathbf{k}-\mathbf{k}'-2\pi\boldsymbol{\tau}) \sin\theta_\tau d\theta_\tau$$
$$= (1/4\pi^2\tau^2)\int\int \delta(\tau x_1)\delta(\tau x_2) \times \delta(|\mathbf{k}-\mathbf{k}'|-2\pi\tau x_3)\,|\cos\theta_\tau|^{-1} d\tau x_1 d\tau x_2,$$

since the x_1 and x_2 components of $(\mathbf{k}-\mathbf{k}')$ vanish owing to the choice of polar axis, and the Jacobian

$$D(-2\pi\tau x_1,\ -2\pi\tau x_2/\theta_\tau,\ \varphi_\tau) = 4\pi^2\tau^2 \sin\theta_\tau \cos\theta_\tau.$$

For a non-vanishing integrand, $\tau x_3 = \tau$, so that $\cos\theta_\tau = 1$. Hence the polycrystal cross section per unit solid angle per scattering nucleus for given $\boldsymbol{\tau}$ is, on substitution of the result for S_1 into (28),

$$E_0(\mathbf{k}-\mathbf{k}')_\tau = (X/8\pi B\tau^2)\exp(-2W) \times \delta(|\mathbf{k}-\mathbf{k}'|-2\pi\tau)$$
$$= (X/8\pi B\tau^2)\exp(-2W_0{}^\tau) \times \delta(2k\sin(\theta/2)-2\pi\tau), \qquad (29)$$

since for $k=k'$ (elastic scattering), $|\mathbf{k}-\mathbf{k}'| = 2k\sin(\theta/2)$; θ is the angle of scattering. This result expresses for neutrons scattered elastically the familiar polycrystalline (or powder) scattering of x-rays along certain right circular cones about the line of incidence—so called "Debye-Scherer rings." The particular cone depends, of course, on the magnitude only of $\boldsymbol{\tau}$, but we must keep in mind that in general there are several examples of $\boldsymbol{\tau}$ in the reciprocal lattice to a single absolute value τ. Since $\sin(\theta/2) \leqslant 1$, only those vectors $\boldsymbol{\tau}$ for which $\tau \leqslant (k/\pi)$ provide Debye-Scherer rings of scattering.

To obtain the total polycrystal cross section per nucleus, we integrate over all θ, φ—the polar angles of neutron scattering. For simplification, in the exponent W of (29) we have replaced $(\mathbf{k}-\mathbf{k}')$ by $2\pi\boldsymbol{\tau}$, its equivalent for permissible angles of scattering, and have so replaced W by $W_0{}^\tau$. Then the only θ, φ dependence is in the δ-function factor. By (24),

$$W_0{}^\tau = (6\pi^2\hbar^2\tau^2/mk_0\Theta) \times \{(1/4)+(T/\Theta)^2 Q_1(\Theta/T)\}. \qquad (30)$$

It is here for the first time that we use the independence of X on θ, φ—i.e., the fact that purely nuclear scattering of slow neutrons is isotropic from the single isolated scatterer.

Since $E_0(\mathbf{k}-\mathbf{k}')_\tau$ is independent of φ, the total cross section for given $\boldsymbol{\tau}$ is

$$E_{el}^\tau = 2\pi\int_0^{\pi} E_0(\mathbf{k}-\mathbf{k}')_\tau \sin\theta d\theta$$
$$= (X/4B\tau^2)\exp(-2W_0{}^\tau)S_2,$$

where

$$S_2 = \int_0^{\pi} \delta(2k\sin(\theta/2)-2\pi\tau)\sin\theta d\theta$$
$$= (1/k^2)\int_0^{\pi} \delta(2k\sin(\theta/2)-2\pi\tau) \times \{2k\sin(\theta/2)\}d\{2k\sin(\theta/2)\}$$
$$= 2\pi\tau/k^2,$$

whence, finally,

$$E_{el}^\tau = (\pi X/2B\tau k^2)\exp(-2W_0{}^\tau). \qquad (31)$$

For simple cubic structure ($B=a^3$, volume of unit cell), this reduces to the result of HHJ for elastic scattering.

The total elastic polycrystal cross section per nucleus is obtained by summing over all reciprocal lattice vectors $\boldsymbol{\tau}$ for which $\tau \leqslant (k/\pi)$ is satisfied, together with other conditions on $\boldsymbol{\tau}$ depending upon the type of lattice:

$$E_{el}=\sum_\tau E_{el}^\tau = (\pi X/2Bk^2)\sum_\tau (1/\tau)\exp(-2W_0{}^\tau). \quad (32)$$

B. Inelastic Scattering

We pass now to inelastic scattering processes of first order; initially, consideration is confined to phonon emission—loss of energy by the neutron in exciting a sound quantum. From the definition (10) of $F_f{}^\sigma$, we write (20):

$$P_1{}^f=|A|^2[\hbar/4m\omega_f(1-x_f)N][(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\alpha}_f]^2 \times\exp(-2W)\,|\sum_\sigma\{\exp[i\boldsymbol{\sigma}\cdot(\mathbf{k}-\mathbf{k}'+\mathbf{q}_f)] \pm\exp[i\boldsymbol{\sigma}\cdot(\mathbf{k}-\mathbf{k}'-\mathbf{q}_f)]\}|^2. \quad (33)$$

The $\pm$ sign arises from the fact that $F_f{}^\sigma$ may contain either a cosine or sine factor (according to whether f refers to a γ- or μ-oscillator). The ambiguity may be removed by recollection of the limitation to consideration of just one-half of $\mathbf{q}$ space (determined by any plane through the origin). For $\mathbf{q}_f\neq 0$ and $N\gg 1$, only one term of the summand in (33) will give a contribution appreciably different from zero for suitable $\mathbf{k}$, $\mathbf{k}'$; each sum is essentially a δ function of argument different from that of the other. Hence, if we now open consideration to all of $\mathbf{q}$ space, thereby departing from the earlier restriction, it is permissible to omit one of the terms of the summand. That is, the one term provides for the "non-zeros" of the other by the mere introduction of the previously eschewed values of $\mathbf{q}_f$ of opposite sign.

To convert $P_1{}^f$ to the cross section per unit solid angle per scattering nucleus, one multiplies by $(m_0{}^2k'/4\pi^2k\hbar^4N)$. Thus

$$G_1{}^f(\mathbf{k}-\mathbf{k}')=[k'\hbar X/16\pi km\omega_f(1-x_f)N^2] \times[(\mathbf{k}-\mathbf{k}')\cdot\boldsymbol{\alpha}_f]^2\exp(-2W) \times|\sum_\sigma\exp[i\boldsymbol{\sigma}\cdot(\mathbf{k}-\mathbf{k}'+\mathbf{q}_f)]|^2 \quad (34)$$

[where again $X=(m_0{}^2/\pi\hbar^4)|A|^2$ is the total elastic cross section for the free nucleus] is the inelastic scattering cross section per unit solid angle per nucleus for single phonon emission, corresponding to the fth oscillator.

From (21), one finds directly that

$$G_{-1}^f(\mathbf{k}-\mathbf{k}')=x_fG_1{}^f(\mathbf{k}-\mathbf{k}'). \quad (35)$$

Comparison with the treatment given the quantity $|\sum_1|^2$, (27), yields the result:

$$G_1{}^f(\mathbf{k}-\mathbf{k}')_\tau=[\pi^2k'\hbar X/2km\omega_f(1-x_f)BN] \times[(2\pi\boldsymbol{\tau}-\mathbf{q}_f)\cdot\boldsymbol{\alpha}_f]^2 \times\exp(-2W_f{}^\tau)\delta(\mathbf{k}-\mathbf{k}'+\mathbf{q}_f-2\pi\boldsymbol{\tau}), \quad (36)$$

where $\boldsymbol{\tau}$ is a reciprocal lattice vector of the type introduced in (27). Since $G_1{}^f(\mathbf{k}-\mathbf{k}')_\tau$ vanishes unless $\mathbf{k}-\mathbf{k}'=2\pi\boldsymbol{\tau}-\mathbf{q}_f$, this substitution has been made in (36); thus W has been replaced by

$$W_f{}^\tau=(3\hbar^2/2mk_0\Theta)(2\pi\boldsymbol{\tau}-\mathbf{q}_f)^2 \times\{(1/4)+(T/\Theta)^2Q_1(\Theta/T)\}.$$

Now the only dependence upon the angle of scattering rests in the δ function.

We next compute the total single crystal scattering cross section for given k', but integrated over all orientations of $\mathbf{k}'$. The quantity required is

$$G_1{}^{f,\tau}=\int_0^{2\pi}d\varphi'\int_0^{\pi}G_1{}^f(\mathbf{k}-\mathbf{k}')_\tau\sin\theta'd\theta' =[\pi^2k'\hbar X/2km\omega_f(1-x_f)BN] \times[(2\pi\boldsymbol{\tau}-\mathbf{q}_f)\cdot\boldsymbol{\alpha}_f]^2\exp(-2W_f{}^\tau)S_3, \quad (37)$$

where k', θ', φ' are the polar coordinates of $\mathbf{k}'$, and

$$S_3=\int_0^{2\pi}d\varphi'\int_0^{\pi}\delta(\mathbf{k}-\mathbf{k}'+\mathbf{q}_f-2\pi\boldsymbol{\tau})\sin\theta'd\theta'. \quad (38)$$

We choose as polar axis the direction of $(2\pi\boldsymbol{\tau}-\mathbf{q}_f)$, so that the x_1 and x_2 components of this vector difference vanish. Also, we use the variables

$$k'_{x1}=k'\sin\theta'\cos\varphi' \quad\text{and}\quad k'_{x2}=k'\sin\theta'\sin\varphi'$$

for the integration, the Jacobian of the transformation being

$$D(k'_{x1},\,k'_{x2}/\theta',\,\varphi')=k'^2\sin\theta'\cos\theta'.$$

Hence

$$S_3=(1/k')^2\int\int\delta(k_{x1}-k'_{x1})\delta(k_{x2}-k'_{x2}) \times\delta(k_{x3}-k'_{x3}-|2\pi\boldsymbol{\tau}-\mathbf{q}_f|)\,|\cos\theta'|^{-1}dk'_{x1}dk'_{x2}.$$

The first two δ functions yield $k'_{x1}=k_{x1}$ and $k'_{x2}=k_{x2}$ for a non-vanishing integrand. The consequent value of k'_{x3} is obtained through the condition of energy conservation:

$$(\hbar^2k'^2/2m_0)=(\hbar^2k^2/2m_0)-\hbar\omega_f. \tag{39}$$

Because of the equality of the first two components of $\mathbf{k}$ and $\mathbf{k}'$, this becomes

$$k'_{x3}=\pm(k^2_{x3}-2m_0\omega_f/\hbar)^{\frac{1}{2}}=\pm Z,$$

and

$$|\cos\theta'|=(|k'_{x3}|/k')=Z/k'.$$

Hence, finally,

$$S_3=\delta(k_{x3}\mp Z-|2\pi\boldsymbol{\tau}-\mathbf{q}_f|)/k'Z. \tag{40}$$

Next, $G_1^{f,\tau}$ is averaged over all directions of $\mathbf{k}$—a procedure physically equivalent to averaging over all crystal orientations, so that the result is the total polycrystal cross section for given k':

$$E_1^{f,\tau}=(1/4\pi)\int_0^{2\pi}d\varphi_k\int_0^{\pi}G_1^{f,\tau}\sin\theta_k d\theta_k,$$

where k, θ_k, φ_k are the polar coordinates of $\mathbf{k}$. From (37) and (40), we have

$$E_1^{f,\tau}=[\pi^2\hbar X/4km\omega_f(1-x_f)BN]\times[(2\pi\boldsymbol{\tau}-\mathbf{q}_f)\cdot\boldsymbol{\alpha}_f]^2\exp(-2W_f^{\tau})S_4,$$

where, after integration over φ_k,

$$S_4=\int_0^{\pi}\delta(k_{x3}\mp Z-|2\pi\boldsymbol{\tau}-\mathbf{q}_f|)Z^{-1}\sin\theta_k d\theta_k.$$

It can be shown that the argument of the δ function has the single root

$$k\cos\theta_k=(|2\pi\boldsymbol{\tau}-\mathbf{q}_f|^2+2m_0\omega_f/\hbar)/2|2\pi\boldsymbol{\tau}-\mathbf{q}_f|;$$

but since this solution is obtained through squaring the term preceded by $\mp$, it may pertain to either sign. It turns out that for one of the signs this solution always holds, for the other it is extraneous—which condition depends on whether $|2\pi\boldsymbol{\tau}-\mathbf{q}_f|^2$ is less than or greater than $2m_0\omega_f/\hbar$. (In the case of phonon absorption—i.e., where ω_f may be replaced by $-\omega_f$ in the conservation of energy and resulting formulae—it is for the plus sign alone that the above solution—with ω_f replaced by $-\omega_f$—holds.) That this solution gives no new condition is ascertained by the fact that it is derivable from the already imposed relation, $(\mathbf{k}-\mathbf{k}')=(2\pi\boldsymbol{\tau}-\mathbf{q}_f)$, if one uses the fact that

$$\mathbf{k}\cdot(2\pi\boldsymbol{\tau}-\mathbf{q}_f)=k|2\pi\boldsymbol{\tau}-\mathbf{q}_f|\cos\theta_k,$$

since the polar axis has been taken along the direction of $(2\pi\boldsymbol{\tau}-\mathbf{q}_f)$.

The ambiguity can be obviated by the change of variable:

$$z=k\cos\theta_k\mp(k^2\cos^2\theta_k-2m_0\omega_f/\hbar)^{\frac{1}{2}},$$

$$\frac{dz}{d\theta_k}=-k\sin\theta_k\pm\frac{k^2\cos\theta_k\sin\theta_k}{(k^2\cos^2\theta_k-2m_0\omega_f/\hbar)^{\frac{1}{2}}}$$

$$=\frac{\pm k\sin\theta_k}{(k^2\cos^2\theta_k-2m_0\omega_f/\hbar)^{\frac{1}{2}}}\times[k\cos\theta_k\mp(k^2\cos^2\theta_k-2m_0\omega_f/\hbar)^{\frac{1}{2}}]$$

$$=\frac{zk\sin\theta_k}{(k^2\cos^2\theta_k-2m_0\omega_f/\hbar)^{\frac{1}{2}}}=\frac{zk\sin\theta_k}{Z}.$$

Thus we have, finally,

$$S_4=(1/k)\int\delta(z-|2\pi\boldsymbol{\tau}-\mathbf{q}_f|)(dz/z)=[k|2\pi\boldsymbol{\tau}-\mathbf{q}_f|]^{-1}, \tag{41}$$

so that

$$E_1^{f,\tau}=[\pi^2\hbar X/4k^2m\omega_f(1-x_f)BN|2\pi\boldsymbol{\tau}-\mathbf{q}_f|]\times[(2\pi\boldsymbol{\tau}-\mathbf{q}_f)\cdot\boldsymbol{\alpha}_f]^2\exp(-2W_f^{\tau}). \tag{42}$$

Carrying through the same procedure in the case of phonon absorption by the neutron, we obtain the result expected directly from (35):

$$E_{-1}^{f,\tau}=x_fE_1^{f,\tau}. \tag{43}$$

Now (42) represents the total polycrystalline scattering cross section for excitation of the fth oscillator, (43) for absorption of energy from the fth oscillator. To obtain a physically measurable quantity, it is necessary to sum (42) and (43) over all f—for each $\mathbf{q}_f$, over the three directions of polarization and the two (γ and μ) oscillators, and then over all of $\mathbf{q}$ space (the restriction to *half* of $\mathbf{q}$ space having been removed at (34))—and then to add the results. Also, summation over suitable $\boldsymbol{\tau}$ must be carried out. The suitable values of $\boldsymbol{\tau}$ and the corresponding ranges of $\mathbf{q}$ (the index f is no longer required) are ascertained by the conditions

$$\mathbf{k}-\mathbf{k}'=2\pi\boldsymbol{\tau}-\mathbf{q} \tag{44}$$

and conservation of energy, (39). For phonon

absorption, the latter is replaced by setting $-\omega$ for ω, so that the general condition for energy conservation is

$$k'^2 = k^2 \pm 2m_0\omega/\hbar. \tag{45}$$

From (44) we find, upon squaring, the condition for the cosine of the angle between $\mathbf{k}$ and $(2\pi\boldsymbol{\tau}-\mathbf{q})$ to be less than unity:

$$\frac{k^2-k'^2+|2\pi\boldsymbol{\tau}-\mathbf{q}|^2}{2k|2\pi\boldsymbol{\tau}-\mathbf{q}|}\leqslant 1,$$

or

$$(|2\pi\boldsymbol{\tau}-\mathbf{q}|-k)^2-k'^2\leqslant 0.$$

This inequality is satisfied if and only if

$$k'-k\leqslant|2\pi\boldsymbol{\tau}-\mathbf{q}|\leqslant k+k',$$

a result significant for phonon absorption, where $k'\geqslant k$. The condition that the cosine of the angle between $\mathbf{k}'$ and $(\mathbf{q}-2\pi\boldsymbol{\tau})$ be less than unity yields the corresponding result applicable to phonon absorption: The sign of the left-hand member of the above inequality is reversed. Thus the general restriction for all first-order inelastic processes is

$$|k-k'|\leqslant|2\pi\boldsymbol{\tau}-\mathbf{q}|\leqslant k+k'. \tag{46}$$

The previous introduction of an average sound velocity renders summation of $E_1^{f,\tau}$ over the three directions of polarization quite a simple matter. Since for a given $\mathbf{q}$ the three $\boldsymbol{\alpha}_f$ are unit orthogonal vectors, the sum over them gives, from (42),

$$E_1'^{\tau}=[\pi^2\hbar X/2k^2m\omega(1-x)BN]\times|2\pi\boldsymbol{\tau}-\mathbf{q}|\exp(-2W^{\tau}), \tag{47}$$

where the prime of $E_1'^{\tau}$ indicates that summations over the three directions of polarization and the two oscillators (γ and μ) have been carried out for the particular $\mathbf{q}$.

In summing (47) over all points of $\mathbf{q}$ space, we again integrate after multiplying the summand by the factor

$$[N/(2\pi)^3]dq_1dq_2dq_3=[N/(2\pi)^3]Bq^2\sin\theta_q dq d\theta_q d\varphi_q, \tag{48}$$

whereby the relation (22) has been written in polar coordinates. Instead, however, of integrating over the angle θ_q, we introduce the variable λ, where

$$|2\pi\boldsymbol{\tau}-\mathbf{q}|=2\pi\tau+\lambda q\quad(-1\leqslant\lambda\leqslant 1). \tag{49}$$

For $\tau\neq 0$ (the case $\tau=0$ is handled separately later), it can be shown that for simple, body-centered and face-centered cubic lattices $2\pi\tau>q_0$, so that the substitution (49) is valid for these structures at least. If the direction of $\boldsymbol{\tau}$ is taken to be that of $\theta_q=0$, then (49) becomes on squaring

$$4\pi^2\tau^2+q^2-4\pi\tau q\cos\theta_q=4\pi^2\tau^2+4\pi\tau q\lambda+q^2\lambda^2,$$

whence

$$\sin\theta_q d\theta_q=(2\pi\tau+\lambda q)d\lambda/2\pi\tau.$$

Therefore, finally, the total inelastic cross section (for phonon emission) is given by

$$E_1^{\tau}=(X\hbar/32\pi^2k^2m\tau)\times\int\int\int\frac{(2\pi\tau+\lambda q)^2\exp(-2W^{\tau})}{\omega(1-x)}q^2dqd\lambda d\varphi_q.$$

As variable of integration, λ takes on all values between -1 and $+1$ consistent with (46), which through (49) now reads:

$$|k-k'|\leqslant 2\pi\tau+\lambda q\leqslant k+k'. \tag{50}$$

Also, for given τ, q is limited to those values consistent with conservation of energy, the above inequalities, and $q\leqslant q_0$. Integration over φ_q merely yields a factor of 2π.

We employ an approximation to the first mean value theorem of the integral calculus by replacing the factor, $\exp(-2W^{\tau})$, by its value for $\lambda=0$, and thereby remove it to the left of the signs of integration; W^{τ} is therefore the same as W_0^{τ}, given by (30). Upon integration over φ_q and λ, then,

$$E_1^{\tau}=(X\hbar/16\pi k^2m\tau)\exp(-2W_0^{\tau})\times\int[4\pi^2\tau^2\lambda+2\pi\tau q\lambda^2+(1/3)q^2\lambda^3]_{\lambda_1}^{\lambda_2}\frac{q^2dq}{\omega(1-x)}, \tag{51}$$

where λ_1, λ_2 are the limits of integration over λ. They are functions of τ and q, consistent with both (50) and $-1\leqslant\lambda_1\leqslant\lambda_2\leqslant 1$.

In order to evaluate the integral over q, we appeal once more to the Debye approximation—namely, $\omega=cq$, where c is the constant sound velocity. By letting $\beta=\hbar\omega/k_0T$, whence x

$=\exp(-\hbar\omega/k_0T)=\exp(-\beta)$, we at length obtain

$$E^{\tau}_{\pm 1}=(\hbar X k_0^2T^2/16\pi\tau\hbar^2k^2mc^3)\exp(-2W_0^{\tau})\times\{4\pi^2\tau^2K_1^{\pm 1}+(2\pi\tau k_0T/\hbar c)K_2^{\pm 1}+(1/3)(k_0T/\hbar c)^2K_3^{\pm 1}\},\quad(52)$$

where

$$\begin{cases}K_{\nu}^{+1}=\int(\lambda_2{}^{\nu}-\lambda_1{}^{\nu})\beta^{\nu}\{[\exp(\beta)-1]^{-1}+1\}d\beta & \text{(phonon emission)}\\ K_{\nu}^{-1}=\int(\lambda_2{}^{\nu}-\lambda_1{}^{\nu})\beta^{\nu}[\exp(\beta)-1]^{-1}d\beta & \text{(phonon absorption)},\end{cases}\quad(53)$$

for $\nu=1, 2, 3$.

In order to interpret (50) to obtain the limits of integration in (53) as well as the choices of λ_1 and λ_2, we must rewrite the energy conservation condition (45) in terms of the Debye approximation:

$$k'^2=k^2\pm 2m_0cq/\hbar.\quad(54)$$

The lower limit is in general zero; all limits which differ from zero are inversely proportional to T. (For, $\beta=\hbar cq/k_0T$, and the limits are determined through restrictions upon q alone.) If the upper limit for q is just q_0, then the upper limit for β is Θ/T, since $\hbar cq_0/k_0=\Theta$, the Debye temperature of the scatterer. For phonon emission, the highest possible value for q is clearly $(\hbar k^2/2m_0c)$, by (54); the corresponding limit for β is $(\hbar^2k^2/2m_0k_0T)=(T_0/T)$, where T_0 is the neutron temperature. A convenient aid to obtaining the limits and values of λ_1 and λ_2 will be indicated in the final section of the paper.

C. The Case $\tau=0$

We now investigate the possibility of inelastic scattering for $\tau=0$. For phonon emission, by (46) and (54),

$$k^2-2qk+q^2\leqslant k'^2=k^2-2m_0cq/\hbar,$$

whence

$$\hbar q+2m_0(c-v)\leqslant 0,$$

where $v=(\hbar k/m_0)$ is the incident neutron velocity. Hence, for neutrons of velocity less than the sound velocity in the scattering substance, single phonon emission cannot occur at all for $\tau=0$. For faster neutrons, $(v>c)$, only oscillators for which $q\leqslant 2m_0(v-c)/\hbar$ may participate.

For phonon absorption, (46) and (54) give

$$k^2+2kq+q^2\geqslant k'^2=k^2+2m_0cq/\hbar,$$

whence

$$\hbar q\geqslant 2m_0(c-v).$$

These results, obtained in similar fashion by Wick,[7] are only approximate in that they rest upon the Debye approximation for the frequency spectrum.

For $\tau=0$, the transformation (49) is neither valid nor necessary. We employ (48) directly to obtain

$$E^{0}_{\pm 1}=(\hbar X/4k^2m)\times\int[x^{(1\mp 1)/2}\exp(-2W^0)/\omega(1-x)]q^3dq,\quad(55)$$

where

$$W^0=(3\hbar^2q^2/2mk_0\Theta)\{(1/4)+(T/\Theta)^2Q_1(\Theta/T)\},$$

and the limits are given through $|k-k'|\leqslant q\leqslant k+k'$. The evaluation of this integral may be carried out numerically for those specific problems in which consideration of $\tau=0$ is required.

(It turns out that for Fe scattering 300-degree neutrons, the conditions necessary are not satisfied, so that $\tau=0$ does not enter into the computation carried out for this work.)

D. Recapitulation

The total inelastic cross section is obtained, finally, by summing the expression $E^{\tau}_{in}=E^{\tau}_1+E^{\tau}_{-1}$, (52) and (55), over all suitable values of τ:

$$E_{in}=\textstyle\sum_{\tau}E^{\tau}_{in}.\quad(56)$$

The suitability of a particular τ depends upon the consistency of its absolute value τ with the inequalities (50) for any simultaneously permissible λ and q. Also, there are possible restrictions upon the values of τ imposed by the crystal structure of the scattering substance. For example, as we shall see later, a body-centered cubic lattice requires that $(a\tau)^2$, where (a) is the lattice constant, be an even integer. For a simple cubic structure there is no such restriction.

[7] G. C. Wick. Physik. Zeits. **38**, 403 (1937).

III. COMPARISON WITH X-RAY PROBLEM

From (54) we see that in the limit $m_0 \ll (\hbar k^2/2cq_0) = (\hbar^2 k^2/2k_0\Theta)$—which is equivalent to $\Theta \ll T_0$, the neutron temperature—we have $k=k'$. In this limit, therefore, we should expect that our results should apply to the scattering of x-rays as well, provided that isotropy of scattering is assumed. Insofar as the mathematical treatment is concerned, setting $k=k'$ through $m_0=0$ merely means lifting the restrictions on the limits of integration in K_ν—*viz.*, the limits are always 0 and (Θ/T), while $\lambda_1=-\lambda_2=-1$. This comes about through the weakening of the condition (50) to read $2\pi\tau+\lambda q \leqslant 2k$. (It is clear, then, that for values of τ so large that $2\pi\tau+q_0>2k$, there are still restrictions on the values of the upper limits and of λ_2. But it is not necessary to consider such special cases here; they would of course apply to x-rays as well.) For the sake of simplicity, only the term in (52) involving $K_1^{\pm 1}$ is considered; but the following comparison is valid even if the smaller term in $K_3^{\pm 1}$ is taken into account. (Since $\lambda_1=-\lambda_2=-1$, $K_2^{\pm 1}=0$.)

From (52), (53), and (25), under the conditions of the preceding paragraph,

$$E_{in}^{\tau}=E_1^{\tau}+E_{-1}^{\tau}=(X\pi k_0^2T^2\tau/\hbar c^3k^2m) \times\exp(-2W_0\tau)\{Q_1(\Theta/T)+(1/4)(\Theta/T)^2\}.$$

Since there is no comparable formula for x-rays readily available, it is necessary to develop further the work of Zachariasen,[3] beginning with his Eq. (15), which we rewrite in the notation of the present work:

$$J_2=(X/4\pi)\exp(-2W_0\tau)(2\pi\tau)^2(B/m) \times\int_0^{q_0}\frac{Q}{\omega^2}\prod_{i=1}^{3}\frac{\sin^2[g_i(k_i-k_i'+q_i)/2]}{\sin^2[(k_i-k_i'+q_i)/2]}\frac{4\pi q^2}{(2\pi)^3}dq.$$

Here we have written the angular independent $(X/4\pi)$ for the non-isotropic Sf^2. Also, $(\mathbf{k}-\mathbf{k}')^2$ has been replaced by the equivalent $(2\pi\tau-\mathbf{q})^2$; the subsequent negligence of $\mathbf{q}$ compared with $2\pi\tau$ is equivalent in one case to ignoring of the K_3 term, while in $\exp(-2W_0\tau)$ it corresponds with the use of the mean value theorem in the present work to reach the result (51). The frequency ν is replaced by $(\omega/2\pi)$, while the volume element dv is substituted for by $[4\pi q^2dq/(2\pi)^3]$—integration over a sphere of radius q_0 thus replacing the integral over rectangular variables. An average sound velocity has been adopted, so that the sum $\sum_j \gamma_j^2=1$ is carried out. In terms of ω,

$$Q=\hbar\omega[\exp(\hbar\omega/k_0T)-1]^{-1}+\tfrac{1}{2}\hbar\omega.$$

Reducing Zachariasen's formula to the single atom by dividing by N, we obtain

$$(J_2/N)=(4\pi^2X/m)\exp(-2W_0\tau) \times\int_0^{q_0}(Q/\omega^2)\delta(\mathbf{k}-\mathbf{k}'+\mathbf{q}-2\pi\tau)q^2dq,$$

where use has been made of (27) to replace the sine-squared ratios. Instead of integrating over q immediately, we perform the angle integrations over all directions of $\mathbf{k}$ and $\mathbf{k}'$ to obtain the total polycrystal cross section. These integrations of the function $\delta(\mathbf{k}-\mathbf{k}'+\mathbf{q}-2\pi\tau)$ have already been carried out above—(38) to (41). The result for the x-ray inelastic polycrystal cross section per atom (again with negligence of $\mathbf{q}$ compared with $2\pi\tau$) is then

$$(J_3/N)=(X\pi\tau/mk^2) \times\exp(-2W_0\tau)\int_0^{q_0}(Q/\omega^2)q^2dq.$$

Using $\omega=cq$, and introducing $\beta=\hbar cq/k_0T$, we finally arrive at the expected result:

$$(J_3/N)=(X\pi k_0^2T^2\tau/\hbar c^3k^2m)\exp(-2W_0\tau) \times\{Q_1(\Theta/T)+(1/4)(\Theta/T)^2\}.$$

This is precisely the result directly above for E_{in}, and thus provides the desired check with the x-ray theory as developed by Zachariasen.

(Even though, on the one hand, the term in K_3 has been dropped and, on the other, $\mathbf{q}$ has been neglected in comparison with $2\pi\tau$, the check is still perfect. Detailed comparison with the steps leading to (52) readily verifies the equivalence of these negligences, and consequently the exactness of the agreement.)

IV. RESULTS FOR LOW TEMPERATURES

For $T\ll\Theta$ and $T\ll T_0=(\hbar^2k^2/2mk_0)$, both, the upper limit of integration in K_ν, (53), is large

compared with unity. Since the term of the integrand involving $[\exp(\beta)-1]^{-1}$ is close to zero for $\beta\gg 1$, the upper limit may be replaced by infinity for such small values of T. For the term not involving the exponential, which appears in K_ν^1 only, the limit must remain finite. [Actually, the criterion for the smallness of T varies with τ since the limits of integration depend strongly on this parameter through (50).] Also, for T small, it is only the range of small q—$q<k_0T/\hbar c$—which contributes appreciably to the result from the exponential part of the integrand. For sufficiently small q, the restrictions upon λ through (50) drop out, so that $\lambda_1=-\lambda_2=-1$. Comparison of (53) with (25) shows that for this case $K_1^{-1}=2Q_1(\infty)$ and $K_1^1=2Q_1(\infty)+\int(\lambda_2-\lambda_1)\beta d\beta$. For the term in K_ν^1 not involving the exponential, this simplification cannot be made. For $T\ll\Theta$, W_0^τ is simplified by setting $Q_1(\infty)(=\pi^2/6)$ for $Q_1(\Theta/T)$, (25).

Because the term of K_ν^1 does not involve the exponential, it is not possible to perform a complete simplification for T small. One can, however, glean some general qualitative points of interest from the preceding results. Of course, for $T=0$ phonon absorption must vanish, as the factor T^2 in (52) shows, since the integrals K_ν^{-1} converge for $T=0$. In the case of phonon emission, however, since the integral K_ν^1 contains a term which diverges as $T^{-\nu-1}$, inspection of (52) reveals a non-vanishing cross section at absolute zero. For, although at $T=0$ the lattice has no energy to give to the neutron, it is still possible for an elastic vibration to be excited by the impact of the incident neutron.

For $T\ll\Theta$, $T\ll T_0$, both, the most significant term, aside from that which is non-vanishing at $T=0$, is proportional to T^2. This quadratic term turns out to be directly evaluable, so long as the condition

$$(3\pi^2\hbar^2\tau^2/mk_0\Theta)\ll 1 \qquad (57)$$

is met. From the remarks of the preceding paragraphs, it is seen that for low temperatures

$$E_{in}^\tau=E_1^\tau+E_{-1}^\tau=C_2(\pi Xk_0^2\tau/4\hbar c^3k^2m)\times\{4Q_1(\infty)T^2+C_1-C_1(12\pi^2\hbar^2\tau^2/mk_0\Theta)\times(T/\Theta)^2Q_1(\infty)\}, \qquad (58)$$

where

$$C_1=T^2\int(\lambda_2-\lambda_1)\beta d\beta+(k_0T^3/2\pi\tau\hbar c)\int(\lambda_2^2-\lambda_1^2)\beta^2d\beta+(T^4/3)(k_0/2\pi\tau\hbar c)^2\int(\lambda_2^3-\lambda_1^3)\beta^3d\beta,$$

$$C_2=\exp(-3\hbar^2\pi^2\tau^2/mk_0\Theta);$$

$\exp(-2W_0^\tau)$ has been replaced by the first two terms of its expansion. Now, the highest possible value of C_1 is attained for $\lambda_1=-\lambda_2=-1$ and when the limits of integration are zero and (Θ/T). This maximum is then

$$C_1=\Theta^2\{1+\tfrac{1}{2}(k_0\Theta/2\pi\tau\hbar c)^2\}.$$

It can be shown that the second term in brackets is at most of the order of magnitude unity; so that $C_1=\Theta^2$ is a satisfactory order of magnitude approximation. The value of the last term in brackets in (58) is therefore, to order of magnitude, $(12\pi^2\hbar^2\tau^2/mk_0\Theta)Q_1(\infty)T^2$. If (57) is fulfilled, then this term is negligible compared with the first in brackets, and (58) becomes:

$$E_{in}^\tau=C_2(\pi Xk_0^2\tau Q_1(\infty)/\hbar c^3k^2m)T^2+C_3, \qquad (59)$$

where

$$C_3=C_1C_2(\pi Xk_0^2\tau/4\hbar c^3k^2m).$$

It is interesting to compare this result with the corresponding quantity for elastic scattering. Expansion of the exponential in (31) to two terms and use of the fact that $\Theta=(\hbar cq_0/k_0)=(\hbar c/k_0)(6\pi^2/B)^{\frac{1}{3}}$, by (23), gives

$$E_{el}^\tau=C_4-C_2(\pi Xk_0^2\tau Q_1(\infty)/\hbar c^3k^2m)T^2 \qquad (C_4=\text{constant}).$$

With (59), this gives the noteworthy result that for low T [and (57)], the total (elastic plus inelastic) cross section is temperature independent.

Now the values of ω contributing appreciably to the integral $Q_1(\infty)$ are small—the smaller, the smaller T. Since it is this integral which provides the term in T^2, we need to consider processes involving only low frequency oscillators in the consideration of this term. For finite temperatures these are on the average excited to high quantum states to render their energies to the order of k_0T. For high quantum numbers—

whereby the separation of energy levels is small compared with k_0T—it should be possible to give the problem a classical treatment. We should expect, therefore, to find a classical description of the constancy of total scattering with temperature, under the assumption (57), for low temperatures.

Since for low frequency oscillators $\mathbf{k}-\mathbf{k}'=2\pi\boldsymbol{\tau}$ approximately, $4\pi^2\hbar^2\tau^2$ is essentially the square of the neutron's momentum change in being scattered. If we consider now a classical collision between a neutron and a free scattering nucleus, $4\pi^2\hbar^2\tau^2$ is therefore the square of the scatterer's momentum change. Also, $mk_0\Theta$ is of the order of the square of the momentum of the scattering nucleus. Condition (57) holds, therefore, so long as the motion of the scatterer is hardly disturbed by the impact of the neutron. This condition obtains if and only if the scatterer mass is large compared with that of the neutron. Since we have required that $T\ll T_0$, or that the probable neutron energy change be small compared with the incident neutron energy, it is necessary also that the scatterer velocity be small compared with the incident particle velocity. Otherwise, the neutron would experience a considerable "Doppler shift" in velocity and therefore undergo an appreciable energy change.

Thus the classical picture is the following: Light, rapid particles are scattered by heavy, slowly moving centers. All processes, in general, involve an interchange, however small, of energy; but owing to the relative mass and velocity magnitudes, the scattering (total for all energy changes) is just what it would be for neutrons scattered by immovable centers at rest. The more strongly are (57) and $T\ll T_0$ fulfilled, the more closely does the total scattering approach the "rigid scattering." This is equivalent to our quantum-mechanical limiting result.

V. RESULTS FOR HIGH TEMPERATURES

For $T\gg T_0$, $T\gg\Theta$, both, then the integrals are simplified somewhat by dint of the fact that $\beta\ll 1$ over the range of integration, and $\exp(\beta)$ may be replaced by $(1+\beta+\beta^2/2)$. Thus we have, by (53),

$$K_\nu^{\pm 1}=\int(\lambda_2{}^\nu-\lambda_1{}^\nu)(\beta^{\nu-1}\pm\beta^\nu/2)d\beta$$

to this approximation and with use of $(1+z)^{-1}=1-z$ for $z\ll 1$. As for the factor $\exp(-2W_0{}^\tau)$, for large T, $Q_1(\Theta/T)\cong(\Theta/T)+(1/4)(\Theta/T)^2$, so that, according to (30),

$$W_0{}^\tau\cong(6\pi^2\hbar^2\tau^2/mk_0\Theta)(T/\Theta).$$

It is thus clear that for large T the cross section $E_{\pm 1}^\tau$ varies as $(aT\pm b)\exp(-\alpha T)$, where a, b, α are constants. (This fact is hardly evidence that the inelastic scattering cross section vanishes at very high temperatures; for temperatures too high, the entire mathematical treatment breaks down, since the assumption of harmonically bound nuclei in a crystal is no longer valid.)

The particular asymptotic expressions for both high and low T are employed in the computation carried out at the end of this work.

VI. NUMERICAL EVALUATION

The remainder of the work is devoted to the computation of the inelastic cross section per nucleus for 300-degree neutrons scattered by polycrystalline iron at temperatures up to 1000°K. The slight change in lattice constant with temperature is neglected in the computation.

A description of the positions of the cubic body-centered lattice points—the structure exhibited by iron through 1000°K—in terms of the basic vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ must be such that the position vector $\boldsymbol{\sigma}=\sigma_1\mathbf{a}_1+\sigma_2\mathbf{a}_2+\sigma_3\mathbf{a}_3$ of the $\boldsymbol{\sigma}$th lattice point bear only integer components σ_1, σ_2, σ_3. Also, every integer triple σ_1, σ_2, σ_3 $(0\leqslant\sigma_i\leqslant g_i)$ should denote the position of one and only one lattice point. These requirements follow from the work of Section II. If $\mathbf{i}_{x_1}$, $\mathbf{i}_{x_2}$, $\mathbf{i}_{x_3}$ are three mutually orthogonal dimensionless unit vectors, then the following triple $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ satisfies the required conditions for the body-centered cubic lattice:

$$\mathbf{a}_1=a\mathbf{i}_{x_1},\quad \mathbf{a}_2=a\mathbf{i}_{x_2},\quad \mathbf{a}_3=(a/2)(\mathbf{i}_{x_1}+\mathbf{i}_{x_2}+\mathbf{i}_{x_3}),$$

where (a) is the lattice constant.

The reciprocal lattice is defined generally by the system of basic vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$, where

$$\mathbf{b}_1=\mathbf{a}_2\times\mathbf{a}_3/D,\quad \mathbf{b}_2=\mathbf{a}_3\times\mathbf{a}_1/D,\quad \mathbf{b}_3=\mathbf{a}_1\times\mathbf{a}_2/D;\qquad D=(\mathbf{a}_1\times\mathbf{a}_2)\cdot\mathbf{a}_3. \tag{60}$$

For the present choice of $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, we find

$$\mathbf{b}_1=(1/a)(\mathbf{i}_{x_1}-\mathbf{i}_{x_3}),\quad \mathbf{b}_2=(1/a)(\mathbf{i}_{x_2}-\mathbf{i}_{x_3}),\quad \mathbf{b}_3=(2/a)\mathbf{i}_{x_3}.$$

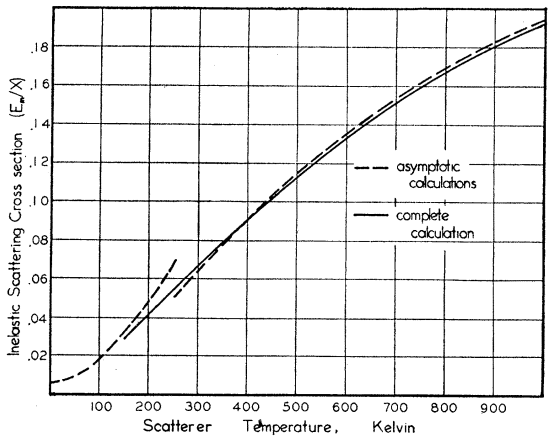

FIG. 1. Inelastic scattering cross section *vs.* temperature of scattering crystal.

A vector $\boldsymbol{\tau}$ having components τ_1, τ_2, τ_3 in the reciprocal lattice system is written:

$$\boldsymbol{\tau}=\tau_1\mathbf{b}_1+\tau_2\mathbf{b}_2+\tau_3\mathbf{b}_3=(\tau_1/a)(\mathbf{i}_{x1}-\mathbf{i}_{x3})+(\tau_2/a)(\mathbf{i}_{x2}-\mathbf{i}_{x3})+(2\tau_3/a)\mathbf{i}_{x3}.$$

This gives the relation between the Cartesian and reciprocal lattice (covariant) components of a vector:

$$\tau_{x1}=\tau_1/a,\quad \tau_{x2}=\tau_2/a,\quad \tau_{x3}=(1/a)(2\tau_3-\tau_1-\tau_2).$$

From here, the Jacobian of the transformation from the Cartesian to the reciprocal lattice system is found to be $(2/a^3)$. Consequently, its reciprocal, defined by (22), is $B=(a^3/2)$; whence, according to (23), $q_0=(12\pi^2)^{\frac{1}{3}}/a$.

Also, the magnitude of a vector $\boldsymbol{\tau}$ in terms of its reciprocal lattice components is clearly given through

$$a^2\tau^2=\tau_1^2+\tau_2^2+(2\tau_3-\tau_1-\tau_2)^2. \qquad (61)$$

Clearly, for integer triples τ_1, τ_2, τ_3 we must have $a^2\tau^2$ an even number. Hence in summation over $\boldsymbol{\tau}$, as in (56), (32), only those $\boldsymbol{\tau}$ for which $a^2\tau^2$ is even are summed over. (Physically, this means a destructive interference between the two simple cubic lattices making up the body-centered lattice, for "Bragg reflections" at "Miller planes" for which $a^2\tau^2$—the sum of the squares of the Miller indices—is odd.)

It is noticed for the special case of a body-centered lattice, the Jacobian B is equal to the volume per nucleus, here $a^3/2$. It is possible to show that this result is perfectly general provided that the basic lattice vector system is chosen with the "one-to-one" restriction imposed here. In this event, $(\mathbf{a}_1\times\mathbf{a}_2)\cdot\mathbf{a}_3$ is the volume per nucleus. By direct substitution through (60), we find that $(\mathbf{b}_1\times\mathbf{b}_2)\cdot\mathbf{b}_3=[(\mathbf{a}_1\times\mathbf{a}_2)\cdot\mathbf{a}_3]^{-1}$, the number of nuclei per unit volume. Now if we write the expansion of $\mathbf{b}_i$ in terms of the unit Cartesian vectors as $\mathbf{b}_i=\sum_j\beta_{ij}\mathbf{i}_{xj}$, then $\boldsymbol{\tau}=\sum_i\tau_i\mathbf{b}_i=\sum_{ij}\tau_i\beta_{ij}\mathbf{i}_{xj}$. Hence $\tau_{xj}=\sum_i\tau_i\beta_{ij}$; the Jacobian of this transformation is the determinant whose elements are the coefficients β_{ij}. This is clearly equal to $(\mathbf{b}_1\times\mathbf{b}_2)\cdot\mathbf{b}_3$, from the definition of the β_{ij}. Since this determinant is the reciprocal of the earlier defined B, we have $B=(\mathbf{a}_1\times\mathbf{a}_2)\cdot\mathbf{a}_3$, whence the theorem is proved.

The numerical work can be greatly simplified through consideration of the expression (51) for E_1^{τ}. Even for $q=q_0$, the term $(1/3)q^2\lambda^3$ can be shown to be small compared with $4\pi^2\tau^2\lambda$. First, since $-1\leqslant\lambda\leqslant 1$, $|\lambda|^3\leqslant|\lambda|$. For $\tau\neq 0$, the smallest employed value of τ^2 [by the considerations just following (61) above] is $(2/a^2)$. Therefore, $4\pi^2\tau^2\geqslant(8\pi^2/a^2)=79/a^2$. On the other hand, $q_0^2=(12\pi^2)^{\frac{1}{3}}/a^2=24/a^2$, so that $(1/3)q^2\leqslant 8/a^2$. Hence it is quite reasonable to neglect the term involving $K_3^{\pm 1}$ in (52) compared with that containing $K_1^{\pm 1}$. The larger τ—and the lower T—the better the approximation; in the present work the error thus involved is much less than 10 percent, since an appreciable contribution to the results comes from values of τ^2 a number of times as large as $(2/a^2)$. Similarly, the term involving $K_2^{\pm 1}$ is neglected, since for the most part $(\lambda_2^2-\lambda_1^2)=0$. Thus simplified, the expression for $E_{\pm 1}^{\tau}$ becomes

$$E_{\pm 1}^{\tau}=X[\pi a(a\tau)k_0^2T^2/4\hbar m(ak)^2c^3]\times\exp(-2W_0\tau)K_1^{\pm 1},$$

where, for sake of convenience, the reciprocal lengths k and τ have been introduced as multiples of $(1/a)$.

The author has, with great benefit, plotted the curves $|k\pm k'|$ as functions of q—all, by (54), parabolic arcs. There is one plot for each of phonon emission and phonon absorption, each done in units of $(1/a)$. On the same plots were drawn the lines $2\pi\tau\pm q$ for all permissible values of τ. This leads to a simple graphical interpretation of the inequalities (50): The double (λ, q)

integration is performed over that portion of a "$\lambda-q$ plane" consisting of the area common to the region between the two parabolic arcs $|k\pm k'|$ and that between the two straight lines $2\pi\tau\pm q$—and to the left of $q=q_0$—for each value of τ. The lines $2\pi\tau\pm q$, when "integration boundaries," are the curves $\lambda=\pm 1$. If the parabolic arc $|k\pm k'|$ is an integration boundary, then it corresponds to the curve $\lambda=(|k\pm k'|-2\pi\tau)/q$. Intersections between the straight lines and the parabolic arcs provide ready information as to the limits of the q integrations (and therefore of those over β), and as to when one changes from one to another of the values of λ_1 and λ_2. The q values of these intersections are obtained exactly by the solution of four quadratic equations—$2\pi\tau\pm q=|k\pm k'|$—but their meanings are most readily interpreted through the graphs.

Whenever an integration boundary is supplied by a parabolic arc, the latter has been replaced by a suitably chosen tangent straight line. Since the integrations are carried out numerically, replacing of the parabolic arcs by straight line segments serves the great advantage of omission of the temperature T from explicit appearance in the integrands. Thus only single tabulations, good for all T, need to be carried out; the temperature appears only in the limits of integration. The only integrals so required are

$$Q_1(z)=\int_0^z \beta[\exp(\beta)-1]^{-1}d\beta,$$

$$Q_0(z)=\int^z\{[\exp(\beta)-1]^{-1}+1\}d\beta = \log[\exp(z)-1];$$

in addition are required

$$\int_0^z \beta\{[\exp(\beta)-1]^{-1}+1\}d\beta=Q_1(z)+z^2/2,$$

$$\int^z[\exp(\beta)-1]^{-1}d\beta=Q_0(z)-z.$$

In the high temperature approximation consistent with Section V, we have for $z\ll 1$

$$Q_1(z)=z-(z^2/4);\quad Q_0=\log z+(z/2)-(z^2/8).$$

The constants from which the computations spring follow: $\hbar=1.056\times10^{-27}$ erg sec., $k_0=1.38\times10^{-16}$ erg deg.$^{-1}$, $m_0=1.66\times10^{-24}$ g, $m=9.22\times10^{-23}$ g, $a=2.90\times10^{-8}$ cm, $\Theta=453$°K, $\omega_0=(k_0\Theta/\hbar)=5.93\times10^{13}$ sec.$^{-1}$, $q_0=[(12\pi^2)^{\frac{1}{3}}/a]=1.69\times10^{8}$ cm^{-1}, $c=(\omega_0/q_0)=3.50\times10^{5}$ cm sec.$^{-1}$, $T_0=300$°K, $v=(2k_0T_0/m_0)^{\frac{1}{2}}=2.23\times10^{5}$ cm sec.$^{-1}$, $k=(m_0v/\hbar)=3.51\times10^{8}$ cm^{-1}, $aq_0=4.91$, $(\hbar k^2a/2m_0c)=3.24$, $ak=10.18$.

The results of the computation may be grasped most readily from the accompanying graphs (Fig. 1). From 0.6 percent of the free elastic cross section, at absolute zero, the inelastic cross section rises steadily to 19.2 percent, at 1000°K. Between 150°K and 400°K, the increase of the inelastic cross section is essentially linear, but at higher temperatures the slope exhibits a steady decrease.

Use of the low temperature approximation given earlier produces the stated parabolic rise from $T=0$; extension of the approximate curve to 250°K shows good agreement with the rigorously computed curve at 150°K, but at higher temperatures the deviation becomes appreciable. Since the low temperature expression is valid for $T\ll T_0$,—here 300°K—the beginning of deviation at 150°K is to be expected.

The asymptotic expression valid for high temperatures gives agreement at 1000°K to about the computational accuracy of the work—about 1 percent of the result. Although the approximation made is valid only for $T\gg\Theta$,—453°K for Fe—the asymptotic expression gives an accurate result even below 400°K; the deviation at 250°K is only about 8 percent of the result. This low temperature agreement is merely fortuitous, however; it arises from the compensating effects of the errors committed in the

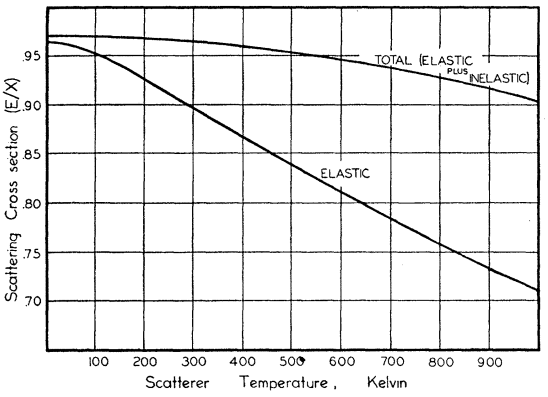

FIG. 2. Comparison of total and elastic scattering cross sections.

approximation. Although there is no *a priori* assurance of the over-all reliability of the high temperature expression in general, one is led to expect a suitable computational result for any given case by means of a plausible interpolation between the low and high temperature curves.

The elastic and total (elastic plus inelastic) scattering cross sections are plotted in Fig. 2. Since $(3\pi^2\hbar^2\tau^2/mk_0\Theta)\ll 1$ here ($\leqq .007a^2\tau^2$), the predicted constancy of the total cross section at low temperatures is clearly exhibited. The constancy is strict up to 150°K; but even up to 400°K, the entire variation (a monotonic decrease) is no more than a percent. At 1000°K, the value has decreased to 90 percent of the free elastic cross section, from the maximum of 97 percent at absolute zero. Such a variation should be readily detected by a reasonably sensitive experiment.

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The Evolution of Contracting Stars

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By use of the method of successive homology transformations in conjunction with Bialobjeski-Eddington's formula, it is possible to predict the changes of radii and luminosities of massive stars in different stages of their hydrogen and contractive evolution. It is shown that at a certain stage of contraction the star must reach the maximum of its luminosity, and it is calculated that for the star masses of 5, 10, 20, and 40 suns the maximum luminosities are 1×10^5, 4×10^5, 1×10^6, and 4×10^6 suns, respectively. In the later contractive stages total luminosity of the star remains constant whereas its visual luminosity rapidly decreases because of the shift of energy into the ultraviolet part of the spectrum. It is to be expected that for such high values of the (luminosity)/(mass) ratio, radiation pressure becomes strong enough to eject stellar atmospheres into the surrounding space, and it is shown that the ejection will actually take place if the force of gravity on the stellar surface will be somewhat reduced by the centrifugal force due to axial rotation. It is also shown that under the conditions existing in the ejective atmospheres of Wolf-Rayet stars, radiation pressure is primarily due to the light scattering by free electrons. In discussing the motion of the ejected gases, it may be necessary to assume that their original velocity of about 2000 km/sec. can be considerably reduced by the gravitational action of the star. If this is the case, gaseous envelopes which will form around Wolf-Rayet stars in the course of several centuries will possess properties very similar to those of the planetary nebulae. This would indicate a close evolutionary relationship between these two classes of celestial objects. An alternate evolutionary road of a massive star consists in the formation of an energy-producing shell, which will take place in all cases where the convective currents due to axial rotation are not fast enough to secure homogeneity of stellar matter. It is indicated that the growth of such shells will probably lead to the formation of an extensive atmosphere which offers certain possibilities for the interpretation of the so-called red giant stars as intermediate evolutionary stages between the stars of the main sequence and the Wolf-Rayet stars. In conclusion the problem of stellar collapse, which is expected to take place towards the end of contractive evolution, is discussed in some detail.

1. INTRODUCTION

IT is generally accepted at present that during the largest part of their evolutionary life stars receive their energy supply from thermonuclear reactions in which hydrogen is being transformed into helium through the "catalytic" action of