These symmetry relations show the equivalence in the positions occupied by the elements r, a, d, and s, and of the positions occupied by the elements p, e, b, h, q, g, c, and f. These two sets of positions differ from each other and this is shown by the different way in which the $12j$ symbol degenerates with one element zero in either type of position:

$$\begin{Bmatrix} e & 0 & e & a & b & d & h \\ g & g & a & c & d & f & s \end{Bmatrix} = \begin{Bmatrix} a & b & e \\ c & d & f \\ g & h & s \end{Bmatrix} \div \{[e][g]\}^{\frac{1}{2}},$$

$$\begin{Bmatrix} 0 & e & a & b & d & h \\ q & g & c & d & f & f \end{Bmatrix} = \frac{(-1)^{a+b+c+d+e+f+2q}}{\{[e][f]\}^{\frac{1}{2}}} \begin{Bmatrix} b & c & q \\ g & e & a \end{Bmatrix} \begin{Bmatrix} h & f & q \\ c & b & d \end{Bmatrix}.$$

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The Scattering of Neutrons by Systems Containing Light Nuclei*

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The general expression for the slow-neutron cross section of a molecule is cast in a form which allows an explicit formulation of the assumption, that the duration of the collision is short compared to the natural periods of the molecule. It is shown that the assumption allows one to extend Placzek's results to molecules containing light nuclei, with only minor modifications. The limits of validity of the assumption are discussed, and the possibilities of exceptions are studied in detail on some examples.

1. INTRODUCTION

PLACZEK has recently[1] achieved considerable progress in the problem of evaluating the slow-neutron cross section of systems of nuclei, such as molecules or crystals. His results, however, are obtained under the assumption that the nuclei involved are heavy compared to the neutron. The following calculations are an attempt to remove this limitation.

It will appear that a rather different method is required for this purpose. In a broader sense, therefore, the present calculations may be offered as a contribution to the general technique for handling the scattering of a particle by a weakly bound system, when particles of comparable mass are involved.[2] The slow-neutron case here selected for study possesses, of course, some simplifying features (such as the constancy of the scattering length of each individual nucleus) the absence of which in other cases of interest may well restrict considerably the possibilities of the method here described.

In the following, the scattering system of nuclei will be referred to as a "molecule," although more complex systems may be implied. The reader is referred to Placzek's paper for all preliminaries; we shall borrow formulas and symbols from that paper without further explanation. We shall save some writing, however, by using units such that $\hbar=1$, and m (mass of the neutron) $=1$. This removes the need of a special symbol μ for the ratio M/m of nuclear mass to neutron mass.

The slow-neutron cross section σ of a molecule is in general a complicated function of the energy E_0 of the neutrons; in particular the slope of this function changes abruptly whenever E_0 attains the threshold for the excitation of a new level of the molecule. The results of Placzek indicate, however, that when E_0 becomes large compared to the level spacing Δ of the scattering system, those changes in slope become negligible, so that σ becomes a smooth function of E_0 which can be represented by means of simple asymptotic formulas.[3] For example in the case of a single nucleus, $\sigma(E_0)$ can be given as an expansion in falling powers of E_0, Eq. P(5.16).

In his argument, however, Placzek makes use of the fact that for a molecule composed of heavy nuclei the energy transfer is in general small (of the order M^{-1}) compared to the initial kinetic energy of the neutron. It is clear that this circumstance has a decisive role in preventing the excitation of any high level of the molecule from being felt in the total cross section until E_0 is well above the threshold for that particular level. Clearly this is a sufficient reason why no noticeable discontinuities in slope should occur. Placzek's calculations on heavy nuclei, therefore, offer no guarantee that a simple extension of his formulas to light nuclei is possible. This circumstance is strikingly illustrated

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[1] G. Placzek, Phys. Rev. **86**, 377 (1952). This paper will be referred to with the abbreviation P, for example, in quoting formulas, thus: Eq. P(5.16).
[2] We have in mind, in particular, the high energy problems mentioned in reference 5.
[3] See also A. M. L. Messiah, Phys. Rev. **84**, 204 (1951).

by the behavior of the cross section of a harmonically bound nucleus[4]; this case, because of its peculiar interest, will be again discussed in Sec. 4 of this paper.

In order to investigate the case of light nuclei it is necessary to perform the summation over the excited state b of the molecule, without first resorting to an expansion in powers of the fractional energy transfer, Eqs. P(2.10), P(3–4), P(3.5). This may be done by means of a "symbolic method,"[5] leading to Eq. (3) below. Our problem is to find a suitable expansion of this expression.

2. BASIC FORMULAS AND ASSUMPTIONS

The total neutron cross section of the molecule in the state a is given by P(1.1) based on Fermi's modified Born approximation. Notice that the summation over state b is unrestricted. An essential role in this expression is played by the operator F, which according to P(1.2) is a linear combination, with coefficients a_s, of exponential operators corresponding to the transfer of a momentum κ to the sth nucleus. Instead of $F_a{}^b$ for the matrix element P(1.4) we use the slightly more conventional notation F_{ba}. Using the Fourier representation of the δ function we write P(1.1) in the form

$$\sigma^{(a)}=(2\pi k_0)^{-1}\sum_b\int d\boldsymbol{\kappa}\int_{-\infty}^{+\infty}dt|F_{ba}|^2 \times\exp\{it(\tfrac{1}{2}\kappa^2-\boldsymbol{\kappa}\cdot\mathbf{k}_0+E_b-E_a)\}. \quad (1)$$

By means of the Hamiltonian operator P(7.1) we can write

$$e^{-itE_a}F_{ba}=(Fe^{-itH})_{ba}, \quad (2a)$$

$$e^{itE_b}(F_{ba})^*=(F^*e^{itH})_{ab}, \quad (2b)$$

F^* being the Hermitean conjugate of F. The summation over b is now simply a matrix multiplication, so that

$$\sigma^{(a)}=(2\pi k_0)^{-1}\int d\boldsymbol{\kappa}\int_{-\infty}^{+\infty}dtG_{aa}\exp[it(\tfrac{1}{2}\kappa^2-\boldsymbol{\kappa}\cdot\mathbf{k}_0)], \quad (3)$$

where G_{aa} is the expectation value in the state "a" of the operator

$$G=F^*e^{itH}Fe^{-itH}=F^*(0)F(t), \quad F(t)=e^{itH}Fe^{-itH}. \quad (4)$$

These expressions are deceptively simple, since they are exact, and hence contain implicitly all the possible intricacies of the problem. We shall reduce them to a more truly simple form, by means of an approximation valid for large values of the neutron momentum k_0.

Such an approximation suggests itself naturally, if one examines the expressions (3) and (4) more carefully. The expectation value G_{aa} can be recognized as a correlation function between momentum transfers $\boldsymbol{\kappa}$ (operator F) and $-\boldsymbol{\kappa}$ (operator F^*) applied t seconds apart from one another. At first sight it may seem surprising that such a time lag between two momentum transfers should play any role at all in a first-order Born calculation, which essentially expresses the idea that the collision is effected in a single elementary interaction. In fact the presence of two transfer operators in the formulas appears to be merely the trivial result of the circumstance that the amplitudes of the partial scattered waves have to be squared to yield cross sections. A different viewpoint will be taken, however, after due consideration of the so-called optical theorem, according to which the total cross section is also related linearly to the imaginary part of the forward elastic scattered wave.

For obvious reasons, when proceeding in this manner, the lowest-order cross section in the Born method is obtained from the second Born approximation to the elastic amplitude. Now this has a bearing on our question in two respects. First, if $\sigma^{(a)}$ is calculated in this way, one gets, we think, a better insight into the reason for the possibility of the transformation from (1) to (3). Secondly, the formula now appears connected with the following physical picture. The total cross section is a measure of the attenuation of the neutron's DeBroglie wave in crossing a space filled with molecules. The optical theorem merely expresses the fact that the attenuation is due to destructive interference of the incident wave with the secondary coherent waves emitted in the forward direction by each molecule. The second-order process leading to forward elastic scattering is the successive transfer to the molecule of two equal and opposite momenta, the two elementary interactions being now physically related parts of a single process; it is thus not surprising that the time interval between the two should appear explicitly in the formulas.

In the second Born approximation the two interactions mark the beginning and the end of the collision, and t may thus be properly viewed as the "collision time." The explicit appearance of this time in the formalism is perhaps the main advantage of Eq. (3). For it suggests at once an approximation based on the plausible physical idea that, for sufficiently large values of k_0, the duration of the collision must be short, and on the resultant assumption that large values of t do not give a significant contribution to the integral over t in Eq. (3). This specific assumption will be called for brevity the "short collision time approximation."

It is fitting to admit at this point, that having in Eq. (3) a complete mathematical statement of the problem, we should now supply, instead of a physical

[4] G. Placzek, Nuovo cimento (to be published). A brief qualitative statement of Placzek's result may be found in A. M. L. Messiah, J. phys. et radium **12**, 670 (1951).

[5] A. Akhiezer and I. Pomeranchuk, J. Phys. (U.S.S.R.) **11**, 167 (1947). My attention to this method was drawn in the course of conversations with Dr. Placzek and Dr. Chew. In particular I am indebted to Dr. Chew for showing me some unpublished calculations of his on the cross section of light nuclei for very energetic neutrons, following lines very similar to those in Sec. 3 of this paper.

plausibility argument, a formal proof that (3) has indeed the property postulated above. This, however, we are unable to do in a general manner. In fact we shall even find an interesting exception to the assumption, in the case of a harmonically and isotropically bound nucleus of mass $M=1$.

Nevertheless we believe that, apart from this rather unique exception, the assumption is fundamentally correct; the remaining part of this section will be devoted to a summary of all the arguments, besides physical plausibility, which can be brought forward in support of the assumption.

In Sec. 3 we shall examine the dependence on t of the integrand of (3) by means of an expansion valid from $t=0$ up to values large compared to E_0^{-1} but small compared to the natural periods of the molecule ($\sim\Delta^{-1}$ in Placzek's notation). Unfortunately this analysis tells us nothing about still larger values of t. Within the region examined, however, the short collision time assumption is fully confirmed. Indeed the integral over t converges rapidly as soon as $t\gg E_0^{-1}$.

The assumption receives further support from a study (Sec. 4) of the special case of a harmonically bound nucleus, which, because of its simplicity, lends itself to a detailed and rigorous treatment. Here an explicit analytical expression can be given for the integrand of (3), and the integration over $\varkappa$ can be carried out exactly. The remaining integration over t is then indeed found to possess the property postulated above, provided $M\neq 1$.

For an isotropic harmonic oscillator of mass $M=1$ the short collision time approximation breaks down, in the sense that, in addition to a small neighborhood of $t=0$ (which contributes the main term, i.e., the free n-p cross section, plus the "normal" terms in E_0^{-1}, E_0^{-3}, etc.), also small intervals around $t=\pm T$, $\pm 2T$, $\cdots$ (T being the oscillator's natural period) give significant contributions. This is just the kind of thing that the analysis of Sec. 3 could never reveal. Its significance for the general case thus requires careful consideration.

In addition it is noteworthy that the breakdown of the approximation for $M=1$ is directly connected (see Sec. 4) with the anomalous oscillatory behavior of the cross section, as a function of the energy, discovered by Placzek. This is indeed not very surprising; it is a well-known fact, often discussed, for example, in the theory of resonance cross sections, that rapid variations of a cross section, over a small interval ΔE, are associated with phenomena involving long collision times, namely $t\sim\Delta E^{-1}$ as required by complementarity.

We may legitimately ask what the nature of the process is, which leads to long collision times in the present case. It turns out that a quite simple and convincing answer is possible in terms of the ding-dong picture of formula (3) developed above in connection with the optical theorem. It is clear in fact that the collision time can be long if, and only if, the neutron is left with almost zero velocity after the first momentum transfer. This is precisely possible if $M=1$, in a head-on collision (notice that the nucleus is assumed to be in the ground state before the collision; therefore it has only a small initial velocity). After the first collision[6] the nucleus swings with a large amplitude; the second collision can occur either immediately, or after 1, 2, 3$\cdots$ periods, when the nucleus passes again near the initial position (where it left the neutron at rest) and with the right direction of motion to kick the neutron again in the forward direction.

This picture also explains in a very simple manner various other features of the problem. For example it clearly shows why already for $M=2$ the importance of the longer collision times is rapidly damped with increasing energy (Sec. 4). Going back to $M=1$, it shows why the Placzek oscillation phenomenon is strongly reduced (it appears only in terms of higher order than E_0^{-1}) if the oscillator is anisotropic (Appendix 2). In fact in this case the nucleus, after being kicked, will perform a Lissajous motion which does not bring it back to the origin until a condition $t\approx n_1T_1\approx n_2T_2\approx n_3T_3$ is satisfied, where T_1, T_2, T_3 are the three different periods, and $n_1n_2n_3$ are three integers. Clearly this makes a delayed second collision much less probable.

These intuitive considerations can now be extended to other cases, in order to show that the exception of the isotropic harmonic oscillator is rather unique. Consider for example an isotropic but slightly anharmonic oscillator. Even starting from the more conventional formula (1) it is possible to argue that the cross section at high energies will oscillate far less than in the exactly harmonic case. In the latter case, in fact, the large oscillation is obviously tied to the high degeneracy of the levels. If the oscillator is anharmonic this degeneracy is removed (only the $2l+1$ degeneracy due to angular momentum conservation is left) with the result that the levels are much more closely spaced.[7] Hence also the kinks in the cross section diagram which occur at each possible excitation energy will be more closely spaced with the result that the curve is much closer to a smooth function. Now reverting to our time-

[6] The first collision is represented by the first operator from the right, i.e., F, the second by F^*. For the sake of simplicity we are assuming in the text that the integral is over negative values of t only. This would give, apart from a factor i, the full forward scattered wave, instead of the imaginary part thereof.

[7] One can, of course, point out that not all levels can be easily excited in a collision. If the ground state is spread over a region of dimensions $\sim(M\omega)^{-\frac{1}{2}}$ and a momentum $\varkappa$ is transferred to the nucleus, only angular momenta up to $l_{\text{exc}}\sim\kappa(M\omega)^{-\frac{1}{2}}$ can be excited. On the other hand, treating the oscillator as nearly harmonic, the state of energy $\kappa^2/2M\approx n\omega$ contains angular momenta up to $l_{\max}\sim n$. Hence, $l_{\text{exc}}\sim l_{\max}{}^{\frac{1}{2}}$ apart from a numerical coefficient ~ 1. This means then, that while a level $n\omega$ of the harmonic oscillator splits into $n+1$ separate levels when the accidental degeneracy is removed by a small anharmonic term, only about $n^{\frac{1}{2}}$ of these appear as kinks in the $\sigma(E_0)$ function. While this is a considerable reduction, it still means that the amplitude of the oscillation decreases like $E_0^{-\frac{1}{2}}$, i.e., faster than the Doppler term.

dependent formalism, we have explained that the oscillations of the function are connected to the "long" collision times. Hence these must be relatively unimportant; our basic assumption must be essentially correct. In the double collision picture this can also be explained as follows. The difference between the harmonic and anharmonic case is that in the former case a wave packet always performs a strictly periodic motion; in the latter the wave packet undergoes the well-known diffusion phenomenon. Hence the probability that the nucleus hits again the neutron when it passes again near the initial position after one full oscillation is much reduced.

All of these arguments are admittedly only qualitative, but the gist of the matter seems to be that significant contributions from longer times (giving rise to "anomalous" asymptotic behaviors) may arise only for $M=1$. Furthermore, in the latter case, only for the isotropic harmonic oscillator does one find anomalies of the same order in $1/E_0$ as the Doppler term. In all other cases they are of a higher order. In the case of a molecule containing only heavy nuclei, moreover, we shall see that the approximation is exactly equivalent to the well-justified procedure of Placzek.

We now turn to the formal development of the preceding ideas, and in so doing we shall first examine (Secs. 3, 4) the "diagonal" terms in the cross section, i.e., the terms proportional to a_s^2 (see P, Sec. 7, Eq. P(7.13), etc.), postponing to Sec. 5 the discussion of the "nondiagonal" or "interference" terms, proportional to $a_{s'}\cdot a_s$ with $s'\neq s$. This separation is desirable not only for systematic reasons, but also and even more because the discussion is rather different in the two cases.

3. SINGLE NUCLEUS

For the sake of simplicity, we shall develop the treatment of a diagonal term for the example of a single nucleus bound by a fixed potential $V(r)$. The formula obtained is quite easily extended to the general case of a diagonal term, as is shown by the discussion in P; this point will be further elucidated at the end of this section.

Going back to Eqs. (3) and (4), and dropping the now useless index s and the summation sign from the definition P(1.2) of the operator F, we shall ask for an expansion of the integrand, which exhibits the existence of an effective collision time, much shorter than the natural periods of the "molecule."

To this end we must identify within the integrand the strongly time-dependent factor or factors that are responsible for the shortness of the collision.

An obvious factor of this kind is the exponential of Eq. (3) which oscillates with a frequency given by

$$\Delta E=\mathbf{k}_0\cdot\boldsymbol{\kappa}-\tfrac{1}{2}\kappa^2=\tfrac{1}{2}k_0^2-\tfrac{1}{2}(\mathbf{k}_0-\boldsymbol{\kappa})^2, \qquad (5)$$

which is of course the energy lost by the neutron if it transfers a momentum $\boldsymbol{\kappa}$ to the nucleus. At this stage, however, ΔE is not the energy transfer which actually occurs, but an indeterminate quantity depending on the integration variable $\boldsymbol{\kappa}$. Similarly at this stage ΔE is not yet equal to the energy gained by the molecule, $\Delta E'=E_b-E_a$, the ultimate equality between the two being imposed upon them by the integration over t.

The justification for regarding the exponential factor as strongly time dependent is provided by the estimates $|\boldsymbol{\kappa}|\sim k_0$, $\Delta E\sim E_0=\frac{1}{2}k_0^2$, valid in the region of $\boldsymbol{\kappa}$ space which effectively contributes to the integral.[8] A simple example to show that this strongly oscillating factor, after integration over $\boldsymbol{\kappa}$, can indeed give a time dependence implying a finite and short collision time is provided by the case of infinitely tight binding; it is then easy to see that $G_{aa}=$ constant. Integration over $\boldsymbol{\kappa}$ then leaves an expression proportional to

$$\int t^{-\frac{3}{2}}e^{-iE_0t}dt,$$

which is indeed convergent at infinity and clearly indicates a collision time of the order of E_0^{-1} (for the seeming divergence at $t=0$ see Sec. 4).

There are now cases in which G_{aa}, though not a constant, is a slow function of time and may be expanded in powers of t. The first term is then of the above type and gives the "bound" cross section $4\pi a^2$.[9] Furthermore, the successive terms reproduce the whole expansion in P exactly.[10] It is indeed quite obvious that the translation into our language of Placzek's assumption, that the energy transfer is $\ll E_0$, is the statement that the correlation function G_{aa} is weakly time dependent.

In the case of light nuclei, of course, the assumption fails, i.e., the exponential in (3) is not the only rapidly variable term. In particular the elementary example of a free nucleus at rest, for which one has, apart from a proportionality factor a^2,

$$G_{aa}\sim\exp(it\kappa^2/2M), \qquad (6)$$

clearly indicates that the two factors in (3), namely the exponential and G_{aa}, are on very much the same footing. In the case of a bound nucleus, the analogy is slightly obscured, simply because of the different behavior of the two energy transfers ΔE and $\Delta E'$; while

[8] In this consideration it is essential that, since a time dependence is under discussion, the integration over t has not been carried out. It is just for that reason that (contrary to a fairly common but slipshod formulation of the complementarity relationship for collisions) we cannot identify in general the ΔE that determines the time dependence (and hence the collision time according to the usual relation $t\sim\Delta E^{-1}$) with the actual energy transfer in the collision, or an average thereof. Clearly there is, for example, no reason why the collision time should become infinite when $M\to\infty$!

[9] More generally, for a molecule, the first term of the expansion of G_{aa} in powers of t gives Placzek's "static approximation," as one can see immediately.

[10] Again this is not hard to see, since an expansion of (4) in powers of t is simultaneously an expansion in powers of the molecular excitation energies E_b-E_a, which is the essence of Placzek's expansion.

the former is a unique function (5) of the momentum transfer $\boldsymbol{\kappa}$, the latter is not so, in general, so that G_{aa} is a weighted sum of exponentials $e^{it\Delta E'}$ with all allowed values of $\Delta E'$.

For a fast incident neutron, however, that is, therefore, for large momentum transfers, we know on physical grounds, and from various examples, that the weights are strongly in favor of values in the neighborhood of

$$\Delta E' \approx \kappa^2/2M, \tag{7}$$

i.e., the transfer to a free nucleus which appears in (6).

Thus a natural extension of our previous assumption suggests itself, namely, that G_{aa} is the product of the exponential in (6) times a slowly variable factor, which can be expanded in powers of t. It is also not difficult to make a rough guess about this latter factor. As we pointed out before, G, Eq. (4), is the product of two operators representing, respectively, momentum transfers $\boldsymbol{\kappa}$ and $-\boldsymbol{\kappa}$ to the nucleus but at different times, t seconds apart. The first and most obvious effect of this time lag is the appearance of a phase factor such as (6) due to the temporary increase in energy (7) produced by the first "kick." Another obvious effect, however, is that, owing to the first kick, the wave packet representing the nucleus will be set in motion and travel a distance $\approx \kappa t/M$ in the time interval between the kicks. Since after the application of the second kick (which restores the average velocity of the wave packet approximately to its original zero value) we must take the scalar product of the resultant wave function with the original state, we see that the displacement suffered by the wave packet in the time t will decrease the overlap integral by a factor roughly of the type

$$\exp(-\kappa^2 t^2/M^2D^2) = 1-\kappa^2 t^2/M^2D^2+\cdots, \tag{8}$$

if D represents the average dimensions of the wave packet. Just such a term will in fact appear in the more detailed calculations of the next two sections. And it is worth noting that if $\kappa \gg D^{-1}$, i.e., if the momentum transfer is large compared to the average momenta of the nuclei in the initial bound state, the factor (8) may be regarded as slowly variable compared to (6). This allows one to use the expanded form on the right-hand side of (8).

It is now convenient to isolate a factor like (6) from the time dependence of G. This may be done as follows. The momentum transfer operator $\exp(i\boldsymbol{\kappa}\cdot\mathbf{r})$ may be used to generate a unitary transformation of the Hamiltonian

$$H' = \exp(-i\boldsymbol{\kappa}\cdot\mathbf{r})H\exp(i\boldsymbol{\kappa}\cdot\mathbf{r}) = H+L+\tfrac{1}{2}M^{-1}\kappa^2, \tag{9}$$

where

$$L = M^{-1}(\boldsymbol{\kappa}\cdot\mathbf{p}). \tag{10}$$

The same unitary transformation will transform a function of H: $f(H)$ into $f(H')$. Since $F = a\exp(i\boldsymbol{\kappa}\cdot\mathbf{r})$, we see that (4) becomes

$$G = a^2 e^{itH'}e^{-itH} = a^2\exp(\tfrac{1}{2}it\kappa^2/M)e^{it(H+L)}e^{-itH}, \tag{11}$$

where our purpose is attained. Equation (3) becomes

$$\sigma^{(a)}/4\pi = (8\pi^2 k_0)^{-1}\int d\boldsymbol{\kappa}\int g_{aa}(\boldsymbol{\kappa},t)\exp[it\alpha(\boldsymbol{\kappa})]dt, \tag{12}$$

where

$$\begin{aligned}\alpha(\boldsymbol{\kappa}) &= \tfrac{1}{2}\kappa^2(1+M^{-1})-\boldsymbol{\kappa}\cdot\mathbf{k}_0 \\ &= \tfrac{1}{2}(1+M^{-1})\{(\mathbf{k}_r-\boldsymbol{\kappa})^2-k_r^2\}, \qquad (13)\\ \mathbf{k}_r &= \mathbf{k}_0 M/(M+1),\end{aligned}$$

and

$$g(\boldsymbol{\kappa},t) = a^2 e^{it(H+L)}e^{-itH}. \tag{14}$$

On the basis of previous considerations, we now expect (14) to be only weakly time dependent, compared to the exponential. In fact, if we neglect the time dependence of g altogether, integration over t gives $\delta[\alpha(\boldsymbol{\kappa})]$, which expresses energy conservation in a collision with a free nucleus at rest, an altogether reasonable first approximation.

We then proceed to expand:

$$g(\boldsymbol{\kappa},t) = \sum_{n=0}^{\infty}(it)^n g_n(\boldsymbol{\kappa})/n!, \tag{15}$$

where the coefficients are easily found[11] by means of the recursion formula and initial values:

$$\begin{aligned}g_{n+1} &= g_n L + n g_{n-1}[H,L] \\ &\quad +\tfrac{1}{2}n(n-1)g_{n-2}[H,[H,L]]+\cdots. \qquad (16)\\ g_0 &= a^2, \quad g_1 = a^2 L.\end{aligned}$$

Before using (15) and (16) in Eq. (12) we must calculate expectation values of these operators in the state a. Furthermore we shall assume that the scattering system is randomly oriented. If necessary, this may be achieved by means of an average over states, Eq. P(3.8). Such an average will be implied by the notation $\langle\cdots\rangle$. One then gets, with the abbreviation $\langle g_n(\kappa)\rangle = s_n \equiv s_n(\kappa^2)$,

$$\begin{aligned}&s_0/a^2 = a^2; \quad s_1/a^2 = \langle L\rangle = 0,\\ &s_2/a^2 = \langle L^2+[H,L]\rangle = \langle L^2\rangle = \kappa^2\langle p^2/3M^2\rangle = \tfrac{2}{3}(\kappa^2/M)\langle K\rangle,\\ &s_3/a^2 = (\kappa^2/6M^2)\langle\nabla^2 V\rangle = B_{\mathrm{Av}}\kappa^2/2M, \qquad (17)\\ &s_4/a^2 = \kappa^4\langle p^4/5M^4\rangle + (\kappa^2/3M^2)\langle(\nabla V)^2\rangle\\ &\qquad = (\kappa^2/M)^2\tfrac{4}{5}\langle K\rangle + (\kappa^2/M)C_{\mathrm{Av}}.\end{aligned}$$

These results include various simplifications; in the first place use is made of the fact that the expectation

[11] The easiest way to obtain (16) is to differentiate (14) thus: $dg/dt = ie^{it(H+L)}Le^{-itH} = igL(t)$, where $L(t) = e^{itH}Le^{-itH}$, and substitute (15) into the equation, using:

$$e^{itH}Le^{-itH} = L+it[H,L]+\tfrac{1}{2}(it)^2[H,[H,L]]+\cdots.$$

value, in a stationary state, of the time derivative $\dot{L}=i[H,L]$ vanishes. This applies also to $d^2L/dt^2=-[H,[H,L]]$ as well as to L itself, since $L=[H,\boldsymbol{\kappa}\cdot\mathbf{r}]$ is also a time derivative. These remarks give at once the results for g_1 and g_2. The latter, however, was also averaged over the direction of $\boldsymbol{\kappa}$, which is allowed for randomly oriented systems. The calculation of g_3 and g_4 is more involved, but similar. g_3, for instance, contains a term d^2L/dt^2, which cancels as explained above, a term L^3, which cancels when one averages over the direction of $\boldsymbol{\kappa}$, and a term $\dot{L}L+2L\dot{L}$, which can be reduced to $\frac{1}{2}[L,\dot{L}]$ by using $\langle L\dot{L}+\dot{L}L\rangle=0$. The evaluation of the commutator leads to the result above. g_4 is handled in a similar manner.

With the notation P(5.7), (5.8), (5.9) we can also write

$$\begin{aligned} &s_1/s_0=0; \qquad s_2/s_0=(4/3)K_{\text{Av}}y, \\ &s_3/s_0=B_{\text{Av}}y; \quad s_4/s_0=(16/5)(K^2)_{\text{Av}}y^2+2C_{\text{Av}}y. \end{aligned} \tag{18}$$

The expressions s_n play a similar role here as the expressions S_n in Eqs. P(3.9), (3.10), and (18) is similar to P(5.6), but simpler. The reason the first terms on the right-hand side of P(5.6) are missing in (18) is that those terms merely represent the effect of the reduced mass factor, as explained by Placzek, an effect which is here separately included once and for all exactly in the exponent $\alpha(\boldsymbol{\kappa})$, Eq. (13).

When the cross section (12) is averaged over a to produce isotropy (if necessary), and the Eqs. (15), (17), and (18) are used, the integration over t can be performed for each term. The nth term is, apart from a factor,

$$I_n=\int s_n(\kappa^2)\delta^{(n)}[\alpha(\boldsymbol{\kappa})]d\boldsymbol{\kappa}, \tag{19}$$

which, after a shift of the origin, $\boldsymbol{\kappa}=\mathbf{k}_r+\mathbf{q}$, may be integrated first over the solid angle $d\Omega_q$ (notice that the argument of the δ function does not depend on the direction of q) and then over q by means of n partial integrations. One gets

$$\begin{aligned} &I_n=(-1)^n[M/(M+1)]^{n+1}[(\partial/q\partial q)^n\Gamma_n(k_r,q)]_{q=k_r}, \\ &\Gamma_n(k_r,q)=q\int s_n(\kappa^2)d\Omega_q=(\pi/k_r)\int_{x^-}^{x^+}s_n(x)dx, \end{aligned} \tag{20}$$

with $x^{\pm}=(k_r\pm q)^2$.

Evaluating (20) explicitly up to $n=4$, and summing, with the appropriate factors, one gets a formula identical to P(3.11), apart from the following changes. (a) The right-hand side is multiplied with the reduced mass factor $[M/(M+1)]^2$. (b) The functions $S_n(\kappa^2)$ with the values P(5.2)(5.6) are replaced by the functions $s_n(\kappa^2)$, Eqs. (17), (18). (c) The parameters $u=4k_0^2$ and E_0 are replaced by $u_r=4k_r^2$, and $E_r=E_0M/(M+1)$.

The introduction of "relative" energy E_r and momentum k_r is of course to be expected in view of our approximation. Formula P(3.11) thus modified leads then, after trivial operations, to the result, in terms of the free cross section P(5.15):

$$\begin{aligned} \sigma/\sigma_{\text{free}}=1&+\tfrac{1}{3}K_{\text{Av}}M^{-1}E_0^{-1} \\ &-\tfrac{1}{3}\tfrac{2}{2}[(M+1)/M]^2C_{\text{Av}}M^{-1}E_0^{-3}+\cdots, \end{aligned} \tag{21}$$

which now takes the place of P(5.16).

The result is changed by so little that we may be justified in pointing out some differences which do not strike the eye. The first two terms are exactly the same as before; the only difference here is that they are not obtained by rearrangement and summation of a series of partial terms as in P(5.14); they come out exactly and at once, which is perhaps a slight methodical advantage. There is in both P(5.16) and (21) an invisible third term, of order E_0^{-2}, and proportional to B_{Av}; that the coefficient of this term cancels is established by Placzek's calculation only to the lowest order in M^{-1}; one could of course push the approximation further, but there is then no simple argument to predict the general structure of the term as a function of M. Equation (21) shows, however, that the term vanishes identically. The last term of (21), finally, differs from the corresponding term in P(5.16) because of the appearance of the inverse of the reduced mass factor. This means that Placzek's C term is proportional to the bound- rather than the free cross section. C_{Av}, see Eq. P(5.9), is proportional to the average square of the binding force. The result just mentioned is therefore physically plausible, but it could not have been inferred with certainty from an expansion in powers of M^{-1}.

We close this section with two more remarks. The first concerns another possible approximation method; it seems at first very tempting to use a "weak binding" approximation, expanding (14) in powers of the potential. The zero order then contains all terms of (15) obtained by neglecting systematically in (16) the commutator $[H,L]$ and commutators thereof. The result is both simple and physically plausible; it obviously describes the collision against a free nucleus, which is not initially at rest, but has instead a velocity distribution as found in the initial state. There the simplicity ends, however; already the next term looks rather complicated and not easily usable. It does not seem, therefore, that this approximation can be used to circumvent the difficulties of the "short collision time" method.

The second remark concerns the extension to a molecule containing several nuclei. We may use, of course, the discussion of P, Sec. 7, to separate the scattering into coherent and incoherent parts. The incoherent scattering is the sum of terms relating to individual nuclei, and for each of these terms a formula like (21) applies, or more precisely a formula which is related to (21) like P(7.8) to P(5.16), with the same change in the meaning of the symbol C. Finally, the formula can be extended to include the whole "diagonal"

term for a given nucleus simply by changing the value of the scattering length a_s.

4. ISOTROPIC OSCILLATOR

The main new result obtained in this section is to exhibit in detail the transition from the "normal" behavior of the asymptotic cross section of a heavy oscillator ($M\gg1$), Eqs. P(6.4) (6.8) (6.9) to the peculiar oscillating behavior discovered by Placzek[4] for the case of equal masses ($M=1$). This behavior may be described as follows: Writing the cross section in the form P(6.8) or, for $M=1$,

$$\sigma/\sigma_{\text{free}}=1+n_0^{-1}c(n_0), \tag{22}$$

where $n_0=E_0\omega^{-1}$ is the neutron energy measured in units of the oscillator's quantum, one would expect from the general formula P(6.9) that $c(n_0)\to\frac{1}{4}$ when $n_0\to\infty$. Placzek finds, instead, that $c(n_0)$ approaches asymptotically the periodic function of period one,

$$c_\infty(n_0)=1-\delta-\sum_{j=0}^{\infty}\Phi(x_j), \tag{23}$$

where $\delta=n_0-[n_0]$ is the fractional part of n_0, and $x_j=\sqrt{2}(j+\delta)^{\frac{1}{2}}$, while Φ is the error integral,

$$\Phi(x)=2\pi^{-\frac{1}{2}}\int_x^\infty \exp(-y^2)dy. \tag{24}$$

It is interesting to note that the function (23) has cusps at integer values of n_0. Thus the cusps which are present in the low-energy behavior of the cross section *vs* energy,[12] are also preserved in the asymptotic representation of the cross section.

The average of the function (23) over one period, however, is equal to $\frac{1}{4}$ and thus coincides with the constant limit expected from the general formula for $M>1$. This shows that if the cross section were measured with poor energy resolution ($\Delta E\gg\omega$) the asymptotic behavior would be found to be given by the general formula derived for $M>1$.

In principle, however, the oscillation of the $1/E_0$ term in the cross section for $M=1$ is observable, and the difference between the asymptotic behaviors in the cases $M=1$ and $M>1$ is quite real. On the other hand what one means by asymptotic behavior is partly a matter of definition. We shall see that the symbolic method leads to an asymptotic representation of the cross section by means of damped oscillations. The damping is zero for $M=1$ and increases with increasing M (as one might expect from a comparison of the $M=12$ and $M=\infty$ curves in P Fig. 1), so that for large M the function $c(n_0)$ very rapidly approaches a constant value. For $M>1$ but small, the asymptotic formula we shall give should be valid over a wider range of energies than the simple constant value $c(n_0)\sim\frac{1}{4}$.

In the case of a harmonic oscillator, the symbolic expression (3) can be transformed as follows. Having to do with a single nucleus, we omit the index s. In the ground state, or in any isotropic average over states, the expectation value of G must be independent of the direction of κ, which we may therefore choose to be the z axis, so that

$$F=ae^{i\kappa z}. \tag{25}$$

For a harmonic oscillator, one has:

$$e^{itH}ze^{-itH}\equiv z(t)=z\cos\omega t+\zeta\sin\omega t, \tag{26}$$

where ω is the proper frequency of the oscillator and ζ is, apart from a factor, the momentum associated to z. In fact,

$$[z,\zeta]=i(M\omega)^{-1}. \tag{27}$$

From (5), (25), and (26) one has:

$$\begin{aligned}&F(t)=ae^{i\kappa z(t)},\\ &G(t)=a^2e^{-i\kappa z}\exp(i\kappa z\cos\omega t+i\kappa\zeta\sin\omega t).\end{aligned} \tag{28}$$

This may be written with all the operators under a single exponential, remembering that if $[A,B]$ commutes with both A and B one has

$$e^Ae^B=e^{A+B+\frac{1}{2}[A,B]}=e^{A+B}e^{\frac{1}{2}[A,B]}. \tag{29}$$

In our case $[A,B]$ is a c number, and

$$\begin{aligned}G=a^2\exp\{&i(\kappa^2/2M\omega)\sin\omega t\}\\ &\times\exp\{-i\kappa z(1-\cos\omega t)+i\kappa\zeta\sin\omega t\}.\end{aligned} \tag{30}$$

Furthermore, it is easy to see that the expectation value in the ground state[13] of an operator $\exp(i\alpha z+i\beta\zeta)$ depends only on $\alpha^2+\beta^2$, and may thus be calculated more simply as the expectation value of $\exp\{i(\alpha^2+\beta^2)^{\frac{1}{2}}z\}$, which, in the ground state, is $\exp\{-(\alpha^2+\beta^2)/4M\omega\}$. One thus finds, after simple reductions,

$$G_{aa}=a^2\exp\{(\kappa^2/2M\omega)(e^{i\omega t}-1)\}, \tag{31}$$

which, if the exponent is expanded in powers of t, gives the expected behavior, Eqs. (7) and (8). A similar formula is obtained for a thermal distribution over the energy levels of the oscillator. For simplicity, however, we shall stick to the case of the ground state.

Inserting (31) into (3), and expressing σ in terms of the "bound" cross section $\sigma_b=4\pi a^2$ or later alternatively of the "free" cross section $\sigma_{\text{free}}=\sigma_bM^2/(M+1)^2$, we find

$$\begin{aligned}\sigma/\sigma_b=(8\pi^2k_0)^{-1}\int_{-\infty}^{+\infty}dt\int d\boldsymbol{\kappa}\exp\{&it(\tfrac{1}{2}\kappa^2-\mathbf{k}_0\cdot\boldsymbol{\kappa})\\ &-(\kappa^2/2M\omega)(1-e^{i\omega t})\}.\end{aligned} \tag{32}$$

[12] See, for example, E. Fermi, Ricerca sci. 7 (2), 13 (1936), and P, Fig. 1.

[13] Or more generally in an isotropic distribution over states.

We have assumed here that the $\varkappa$ and t integrations can be interchanged; if we first attribute to t a small positive imaginary part, the integral over $\varkappa$ becomes absolutely and uniformly convergent, and the interchange can be safely carried out.

Performing the $\varkappa$ integration and introducing a nondimensional time variable $\xi=\omega t$, and a nondimensional energy measure $n_0=k_0^2/2m\omega$ as before, and with the abbreviations

$$\rho\equiv\rho(\xi)=\xi^2\lambda(\xi),$$
$$\lambda\equiv\lambda(\xi)=[M^{-1}(1-e^{i\xi})-i\xi]^{-1}, \tag{33}$$

we find

$$\sigma/\sigma_b=\tfrac{1}{4}(\pi n_0)^{-\frac{1}{2}}\int_{-\infty}^{+\infty}\lambda^{\frac{3}{2}}e^{-n_0\rho}d\xi. \tag{34}$$

The integrand of (34) has singularities (branch points) where λ has poles or zeros. The only singularity on the real axis is at $\xi=0$, which according to a previous remark must be avoided by passing above it.[14]

For an asymptotic evaluation of (34) for large values of n_0, we can remark that any part of the integration path on which an inequality,

$$\mathrm{Re}(\rho)>c, \tag{35}$$

is satisfied, c being a positive constant, will give a negligible contribution, of the order e^{-cn_0}, to the integral. We may derive the greatest benefit from this, if we deform the path in such a way as to have (35) satisfied over as much of the path and with as large a value of c as is possible.

Now from (33) it is easy to see that $\mathrm{Re}(\rho)$ is positive over the whole real axis, except at the points $\xi=2\pi\nu$ ($\nu=0,\ \pm1,\ \pm2\cdots$) where it is zero. These points, therefore, must be examined more carefully.

Setting $\xi=2\pi\nu+\eta$, and expanding (33) in powers of η, one finds that, in the neighborhood of the real axis, the region where $\mathrm{Re}(\rho)>0$ has the structure represented by the shaded area in Figs. 1 and 2. We try to lay the path, as far as possible, within the shaded area; the place, where it must get out of it, is just above the origin. We may, however, deform the path in the manner indicated by the heavy line in the figures, so that the only part of the path where $\mathrm{Re}(\rho)<0$ is a small circular arc at the top of the loop around the origin.

It is best to divide the right-hand side of (34) into two parts, one I_p corresponding to the loop which leads—from a point ξ_i on the negative imaginary axis

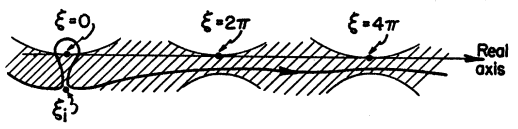

FIG. 1. Integration path for $M>1$.

[14] We shall assume that the complex ξ plane is cut along the negative imaginary axis, starting from the branch-point of $\lambda^{\frac{3}{2}}$ at $\xi=0$.

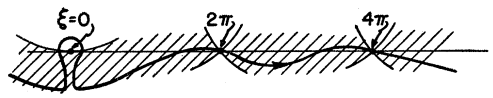

FIG. 2. Integration path for $M=1$.

—around the origin—back to the same point, and one I_h corresponding to the "horizontal" part of the path, which leads from $-\infty$ to the point ξ_i, and from ξ_i on the right-hand side of the imaginary axis[14] to $+\infty$.

We can choose the point ξ_i on the negative imaginary axis in such a way that the integrand is extremely small at ξ_i. We may choose, for instance, the point where ρ has a maximum along the negative imaginary axis. For $M\gg1$, $\xi_i\approx-i\ln M$ and the maximum value of ρ is also $\sim\ln M$, so that the exponential in the integrand has a very small value M^{-n_0}. As $M\to1$ the maximum value of ρ decreases; for $M=1$ one has $\xi_i=-2i$, and $\rho(\xi_i)=0.48$. Even with this value the exponential, $e^{-0.48n_0}$, is asymptotically negligible as soon as $n_0\gg1$.

If $M\gg1$ it can now be shown that the contribution I_h of the whole "horizontal path" is negligible. In fact, as M increases, the lower boundaries of the shaded area, indicated in Fig. 1, move downwards, the distance from the real axis being of the order of $\ln M$; the path can be laid in such a way that an inequality (35) is satisfied over the whole path, with a value of c of the order of $\ln M$. One then finds an upper limit to the integral along the horizontal path,

$$I_h<e^{-cn_0}\int|\lambda|^{\frac{3}{2}}d\xi\sim c_1e^{-cn_0}, \tag{36}$$

where c_1 is another constant. It should be noticed, to justify this, that $\lambda\sim|\xi|^{-1}$ when $\xi\to\pm\infty$, so that the integral in Eq. (36) is convergent. On the other hand, when M approaches unity the "necks" through which the path must pass become narrower and narrower, until they reduce, see Fig. 2, for $M=1$, to points, where $|e^{-n_0\rho}|=1$. The neighborhood of these points gives then a contribution to (34), which is not exponentially small compared to the main term; it yields, in fact, terms of order n_0^{-1}, and is responsible for the oscillatory behavior discovered by Placzek.

Now to the actual evaluation: Beginning with the loop integral, we notice that for $|\xi|\ll1$ the exponent $-n_0\rho\approx-in_0\xi M/(1+M)$, so that the exponential rapidly vanishes on the negative imaginary axis as soon as $|\xi|\gg n_0^{-1}$. After the substitution $\tau=-i\xi n_0M/(1+M)$, an expansion of ρ and $\lambda^{\frac{3}{2}}$ in powers of τ becomes simultaneously an expansion in powers of n_0^{-1}. Substituting into (34) and expanding the whole integrand with respect to n_0^{-1}, one then gets, apart from a factor, the expression

$$\int\tau^{-\frac{1}{2}}e^{\tau}[1+(Mn_0)^{-1}(\tfrac{3}{4}\tau+\tfrac{1}{2}\tau^2)$$
$$-(Mn_0)^{-2}\{\tfrac{1}{32}(8M-7)\tau^2-\tfrac{1}{24}(11-4M)\tau^3$$
$$-\tfrac{1}{8}\tau^4\}+\cdots]d\tau, \tag{37}$$

where the path runs in a loop around the origin from, and to, a point $\tau_i=-i\xi_i n_0 M/(1+M)$, which if $n_0\gg 1$ can be set $=-\infty$ without noticeable error. Using the integral representation of the reciprocal Γ function[15] one finds for the loop part:

$$I_l=(1+M^{-1})^{-2}\{1+(4Mn_0)^{-1}+0(n_0^{-3})\}. \quad (38)$$

Notice the reduced mass factor $(1+M^{-1})^{-2}\equiv\sigma_{\text{free}}/\sigma_b$; notice also that the coefficient of the n_0^{-2} term vanishes identically.

Turning now to I_h, we first assume $M=1$. Figure 2 clearly shows that the points $\xi=2\pi\nu$ ($\nu=\pm1, \pm2, \cdots$), are saddle-points for $\mathrm{Re}(\rho)$. This follows of course from the expansion already used, that is

$$\begin{aligned}&\rho(2\pi\nu+\eta)=\rho_\nu+\rho_\nu'\eta+\tfrac{1}{2}\rho_\nu''\eta^2+\cdots,\\ &\rho_\nu=2\pi i\nu, \quad \rho_\nu'=0, \quad \rho_\nu''=1+(i/\pi\nu).\end{aligned} \quad (39)$$

The inequality (35) can be satisfied everywhere on the path, excluding the neighborhood of the saddle-points. It is therefore sufficient to evaluate asymptotically the contribution $I_h(\nu)$ from a small interval around each saddle-point. Here we shall content ourselves with the lowest order term, which is proportional to n_0^{-1}. This, together with the corresponding term in (38), will yield the function $c_\infty(n_0)$.

The evaluation is based, of course, on the familiar reduction to a Gauss integral.

One has:

$$\exp(-n_0\rho)\approx\exp(-n_0\rho_\nu)\exp(-\tfrac{1}{2}n_0\rho_\nu''\eta^2),$$

which has a sharp Gaussian peak of width $n_0^{-\frac{1}{2}}$ at the saddle-point, provided the path crosses the saddle in the right direction.[16] To the lowest order in n_0^{-1} we are then allowed to replace $\lambda^{\frac{3}{2}}$ in the integral (34) by its value $\lambda_\nu^{\frac{3}{2}}$ at $\xi=2\pi\nu$, i.e., by $(i/2\pi\nu)^{\frac{3}{2}}$. Then, carrying out the Gauss integrals and remembering (34) and (38), we find that

$$\begin{aligned}\sigma/\sigma_b&\approx I_l+\sum_{\nu=1}^{\infty}(I_h^{(\nu)}+\text{cc})\\ &=I_l+\tfrac{1}{4}\sqrt{2}n_0^{-1}\sum_{\nu=1}^{\infty}\{\lambda_\nu^{\frac{3}{2}}(\rho_\nu'')^{-\frac{1}{2}}\exp(-n_0\rho_\nu)+\text{cc}\}. \quad (40)\end{aligned}$$

Using $M=1$ in Eq. (38) and the values (39), and expressing σ in terms of $\sigma_{\text{free}}=\frac{1}{4}\sigma_b$, we find, on comparison with (22),

$$c_\infty(n_0)=\tfrac{1}{4}+\sum_{\nu=1}^{\infty}(8\pi\nu)^{-1}\{(\pi\nu+i)^{-\frac{1}{2}}e^{-2\pi i\nu n_0+i\frac{3}{4}\pi}+\text{cc}\}. \quad (41)$$

We have now obtained two entirely different expressions (23) and (41) for the same function; but it is not difficult to verify by integration of (23) with a factor $\exp(2\pi i\nu\delta)$, that (41) is indeed the Fourier series for the function (23). The advantage of (23) is, of course, its much more rapid convergence.

We finally set ourselves the problem of bridging the gap between the two extreme cases $M=1$ and $M\gg1$. The preceding discussion clearly points the way. As long as $M>1$, it is always possible to say that $I_h\sim\exp(-cn_0)$, but $c\to0$ as $M\to1$, so that neglecting I_h entirely is not a good approximation. Looking at Fig. 1 we realize that there must be a saddle-point in the middle of each narrow "neck" of the shaded area. We can calculate I_h approximately by a saddle-point method, just as we did for $M=1$.

We obtain again (40), the only difference being in the values of I_l, and of the coefficients λ_ν, ρ_ν, ρ_ν''. The position of the saddle-points is quickly obtained as follows. The equation for a saddle-point ξ is $\rho'(\xi)=0$, which one can rewrite using (33),

$$e^{i\xi}=M\{1-2i\epsilon/(\xi+2i)\}, \quad (42)$$

where $\epsilon=1-M^{-1}<1$. Taking the logarithm on both sides, and designating ξ more specifically by ξ_ν, if ξ is the saddle-point which tends to $2\pi\nu$ when $M\to1$, we get

$$\xi_\nu=2\pi\nu-i\ln M-i\ln\{1-2i\epsilon(\xi_\nu+2i)^{-1}\}, \quad (43)$$

where the principal value of each logarithm is meant. From (43) it is easy to obtain an expansion in powers of $M-1$ or of ϵ, which converges rapidly if $(M-1)\ll1$. For the practically more interesting case: M equal a small integer, one can reach the goal more quickly by an iteration method. Starting from $\xi_\nu\approx2\pi\nu-i\ln M$ as an approximate value, one feeds this into the right-hand side of (43) and gets a better value, and so on.

Another usable expansion is one in falling powers of $2\pi\nu$:

$$\begin{aligned}&\xi_\nu=2\pi\nu-i\ln M+\sum_{n=1}^{\infty}a_n(2\pi\nu)^{-n},\\ &a_1=-2\epsilon, \quad a_2=-2i\epsilon(\ln M-2+\epsilon)\cdots.\end{aligned} \quad (44)$$

It is easy to see that (43) defines $\xi_\nu-2\pi\nu$ as an analytic function of $z=(2\pi\nu)^{-1}$ regarded as a complex variable, and that $z=0$ is not a singularity. Hence, (44) must have a nonzero radius of convergence and is in fact apparently quite usable down to $\nu=1$.

Knowing ξ_ν one can calculate the coefficients of the expansion (40). The most interesting one is the exponent ρ_ν. Using (42), (23) can be transformed into

$$\rho_\nu\equiv\rho(\xi_\nu)=i\xi_\nu(1+2i\xi_\nu^{-1})[1+i(2-\epsilon)\xi_\nu^{-1}]. \quad (45)$$

This too can be expanded for large ν:

$$\begin{aligned}\rho_\nu=i\{2\pi\nu-\epsilon^2(2\pi\nu)^{-1}+\cdots\}+\ln M-\epsilon\\ -\epsilon^2(2-\epsilon-\ln M)(2\pi\nu)^{-2}+\cdots,\end{aligned} \quad (46)$$

the error being of order $(2\pi\nu)^{-3}$.

[15] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (The McMillan Company, New York, 1946), fourth edition, Sec. 12.22.

[16] For example at an angle $-\frac{1}{2}\arctan(1/\pi\nu)$ to the real axis. According to (33) the exponent $-\frac{1}{2}n_0\rho_\nu''\eta^2$ is then real and negative. This is indicated in Fig. 2.

Some numerical values for the exponents ρ_ν are given in Table I. The most noteworthy feature, of course, is the nonvanishing real part of ρ_ν. Each term of the series (40) is a damped harmonic oscillation. The damping factor is only weakly dependent on ν, and is roughly $\exp\{-n_0(\ln M-\epsilon)\}$. Also, the imaginary part of ρ_ν is only slightly different from $2\pi\nu$, so that the series is almost harmonic. The amount of damping indicated by Table I is in good agreement, as far as a comparison is possible,[17] with the numerical results of Placzek, as displayed in P (Fig. 1).

Finally, it is noteworthy that even for M as low as 2, the damping is fairly rapid, the amplitude being reduced to $1/e$ when the energy increases by five oscillator quanta.

TABLE I. Values of ρ_ν.

$M=$	1	2	3	6	12
		(a) Real part of ρ_ν			
$\nu=1$	0	0.1880	0.4294	0.9694	1.598
2	0	0.1919	0.4313	0.9612	1.576
∞	0	0.1931	0.4320	0.9584	1.568
		(b) Imaginary part of ρ_ν divided by $2\pi\nu$			
$\nu=1$	1	0.9937	0.9888	0.9825	0.979
2	1	0.9984	0.9972	0.9956	0.995
∞	1	1	1	1	1

5. NONDIAGONAL TERMS

In the discussion of these terms we have to rely to an even larger extent than before on purely qualitative arguments, except in special examples. Furthermore it turns out that in the present instance the "short collision time" approximation is essentially equivalent to the "small energy transfer" approximation of Placzek, and does not lead to any improvement over his formulas. One useful result emerges from the following discussion, however, namely that as far as the nondiagonal terms are concerned, Placzek's formulas are not essentially tied to the condition $M\gg1$, a fact which is not obvious from the discussion given in P. Thus we may say that we have a suitable treatment for all cases.

If we pick in the operator (4) the interference term relative to, say, nuclei 1 and 2, that is, apart from a factor a_1a_2, the expression

$$G_{21}=f_2^*e^{itH}f_1e^{-itH},\quad f_s=\exp(i\boldsymbol{\kappa}\cdot\mathbf{r}_s),\tag{47}$$

the first problem is to find its time dependence. The discussion will be clearer if we first get rid of an obvious pitfall.

There is, of course, no analog to an interference term in the classical theory of impacts, and thus no *a priori* argument for a time dependence such as in (6), based on the classical energy momentum relation (7); to begin with, if $M_1\neq M_2$, we would not even know which mass to use in these equations. Nevertheless if we apply the transformation (9)(11) to (47), we get

$$G_{21}=f_2^*f_1\exp(it\kappa^2/2M_1)e^{it(H+L_1)}e^{-itH},\tag{48}$$

L_s being defined by (10) with M, and $\mathbf{p}$ replaced by M_s and $\mathbf{p}_s$. The first exponential in (48) represents a strong (if $M_1\sim1$) time dependence of the type we have no good reason to expect. Alternatively, we may obtain a similar factor involving M_2 instead of M_1, if we notice that $G_{aa}=G_{aa}^1$, where

$$G^1=e^{-itH}F^*e^{itH}F,\tag{49}$$

and transform accordingly, pushing F^* towards the right. The truth is, however, that the appearance of these strongly oscillating factors is without significance; they are canceled by compensating terms which occur in the expectation value of the remaining operators. More precisely we state that, if the time dependence of $\langle G_{21}\rangle$ is written as an exponential $\exp[if(t)]$, no linear term in t is present in the exponent.

This can be seen most simply by showing that the time derivative of $\langle G_{21}\rangle$ is zero at $t=0$. And this follows immediately from P(7.17). Since the point is of some importance, however, it will be further explained by an alternative derivation. We rewrite (47) in the form

$$G_{21}=\exp(-i\kappa z_2)\exp\{i\kappa z_1(t)\},\tag{50}$$

taking the z axis parallel to $\boldsymbol{\kappa}$. For comparison the diagonal term G_{11} can be similarly written, by replacing z_2 with z_1 in (50). For small values of t we expand in powers of t, neglecting terms of order t^2 or higher. Remembering (29) we obtain

$$\begin{aligned}G_{21}&\approx\exp(-i\kappa z_2)\exp(i\kappa z_1+it\kappa\dot z_1)\\&=\exp[i\kappa(z_1-z_2)+it\kappa\dot z_1],\end{aligned}\tag{51}$$

and similarly

$$\begin{aligned}G_{11}&\approx\exp(-i\kappa z_1)\exp(i\kappa z_1+it\kappa\dot z_1)\\&=\exp[it\kappa\dot z_1+\tfrac12 i\kappa^2M_1^{-1}t],\end{aligned}\tag{52}$$

where the main difference between the two operators is that the commutator term in (29) is zero for G_{21}, but not for G_{11}. It is just this term that gives the strong time dependent factor for G_{11}, but not for G_{21}. To complete this consideration, one has only to notice that under the assumption that the eigenfunction of state a is real (i.e., invariant against time reversal; this assumption is essential, and is also made in P) the expectation value of an operator $\exp(\alpha z+\beta p_z)$ is an even function of β. Hence the exponential operators in (51) do not contribute any linear exponent in t.

The cancellation of the strong linear term in G_{21} means that the first-order reduced mass correction does not apply to the interference terms, as pointed out in P. But for us it means, especially, that the transformation employed successfully in Sec. 3 is here not merely useless, but actually misleading. Under these circumstances it is more natural to expand the whole

[17] Owing to the omission of terms of order n_0^{-2}, our formula can only give a rough approximation for values of n_0 as low as those in P, Fig. 1.

G_{21} in powers of t, but then of course we are back with the "small energy transfer" approximation and no improvement over P is obtained. The question we want to discuss, however, is whether such an improvement is really necessary.

The absence of a large linear term is in itself no guarantee that the time dependence of G_{21} is weak. A strong time dependence could appear in higher powers of t in the expansion or at later times, when the expansion is of no help. The case of long times has been examined in detail in Appendix 3 for a special case. There one can see in (A13), for example, that when κ is large a strong time dependence can indeed appear for large t values. That turns out to be unimportant, however, for the simple reason that the value of G_{21} is at the same time quite negligible.

It is the latter circumstance that is decisive. Although in the general case this cannot be demonstrated as forcibly as in the special case of the appendix, we can at least show that quite improbable circumstances must occur for an exception to be possible.

Let us begin with the trivial case of two "independent" nuclei, for example two nuclei bound in a fixed external potential, but not interacting with each other, so that individual states can be assigned to each. In this well-known case the only coherent scattering is elastic; G_{21} is not time dependent at all; this is so, of course, because the two factors of the matrix element

$$M_b=(f_2^*)_{ab}(f_1)_{ba} \tag{53}$$

associated with the energy transfer E_b-E_a cannot both be $\neq 0$ unless $b=a$. Knowing this, we can see, furthermore, that the only nonzero matrix element M_a becomes negligible as soon as κ is large compared to the zero point momenta of 1 and 2 in the state a. This establishes our statement for this case.

Naturally, the example chosen is so special that its detailed features are of no special interest for the general case. If, for example, we add an interaction λV_{12} between the two particles, we expect to get the same result for the cross section in the limit $\lambda\to 0$; most of the detailed statements made above become invalid, however. In particular, it is necessary to remember the role of degeneracy in such a problem. Owing to degeneracy between levels of the unperturbed problem, even a weak interaction can lead to strong mixing of states, so that the matrix elements M_b for individual states can be strongly affected. It is no longer true, for example, that for κ large, every M_b must become necessarily small. (The reader will find it instructive to consider in detail the possible effects of mixing between states in which either one of the two particles is strongly excited, while the remaining one is left in the ground state.) On the other hand, a sum over states such as the sum in Eq. (1) possesses a well-known stability against perturbations, so that for small λ it will still be true that the contribution of large κ values to the nondiagonal term can be neglected.

In the above example, a significant departure from our general assumption could only occur if the interaction becomes so large as to cause large splittings amongst the original degenerate levels, or, in more physical language, if momentum is exchanged rapidly between the two particles, more precisely, so rapidly that a momentum exchange κ can occur during the short time available in a collision. If this necessary condition is examined more in detail, one finds that large κ values can only contribute if the energy E_0 of the incident neutron is smaller than an expression of the type of $(\partial^2 V/\partial x^2)D^2$, where V is the interaction and D the distance between the two particles. This expression again may be taken to be of the order of binding energies if the particles are close to one another in the molecule and even smaller otherwise.

Although this necessary condition is better than nothing, it is not very strong and we have some reason to think that much more stringent conditions must be met, so that in practice we may safely assume that large momentum transfers are negligible quite in general.

We shall try to show this by means of a semiclassical consideration based again on the time-dependent picture. Reverting to the form (4) of the operator G and using a configuration representation of the operator e^{itH}, we can write the expectation value of G_{21} in the state a in the form

$$\langle G_{21}\rangle=\int \psi_a^*(\mathbf{r}_1\mathbf{r}_2)\exp(-i\boldsymbol{\kappa}\cdot\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2\langle \mathbf{r}_1\mathbf{r}_2|e^{itH}|\mathbf{r}_1'\mathbf{r}_2'\rangle \times d\mathbf{r}_1' d\mathbf{r}_2'\exp(i\boldsymbol{\kappa}\cdot\mathbf{r}_1')\psi_a(\mathbf{r}_1'\mathbf{r}_2')e^{-itE_a}. \tag{54}$$

For simplicity only the coordinates of the two particles involved have been indicated explicitly, but if other particles are present, additional coordinates r_3, $\cdots$ and $r_3'\cdots$ would have to be written in at the left and right, respectively. The following argument would not be affected. Let us now consider a classical motion leading from positions $\mathbf{r}_1'$, $\mathbf{r}_2'$ at time t (it is convenient to fix our attention on the case $t<0$) to positions $\mathbf{r}_1$, $\mathbf{r}_2$ at time 0; let $S(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t)$ be the action integral for this motion. We now make the classical approximation

$$\langle \mathbf{r}_1\mathbf{r}_2|e^{itH}|\mathbf{r}_1'\mathbf{r}_2'\rangle=\exp\{iS(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_1'\mathbf{r}_2';t)\}, \tag{55}$$

neglecting a normalization factor, which would only complicate the formulas without much consequence. If a classical approximation is valid at all, the exponential on the right-hand side of (55) can be treated as a rapidly oscillating factor. We intend to discuss all the integrations in (3) and (54) (i.e., the integrations over $\boldsymbol{\kappa}$, t, $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_1'$, $\mathbf{r}_2'$) by means of the method of stationary phase. This is, of course, very crude, but since we only intend to ascertain the conditions under which a "large" result can be obtained, the approximation seems legitimate. We recall that

$$\partial S/\partial \mathbf{r}_i=\mathbf{p}_i,\quad \partial S/\partial \mathbf{r}_i'=-\mathbf{p}_i',\quad \partial S/\partial t=E, \tag{56}$$

where $\mathbf{p}_i$ and $\mathbf{p}_i'$ $(i=1, 2)$ are the final and initial momenta of the two particles and E is the energy in the classical motion envisaged above. We regard the momenta of 1 and 2 in state a as negligible, that is we treat ψ_a^* and ψ_a as slowly variable (we neglect their derivatives). Then writing the stationarity condition for the integrations (in the order mentioned above) we find

$$\mathbf{r}_2-\mathbf{r}_1'=-t(\mathbf{k}_0-\boldsymbol{\kappa}), \tag{57}$$

$$\tfrac{1}{2}\kappa^2-\boldsymbol{\kappa}\cdot\mathbf{k}_0+E=E_a, \tag{58}$$

$$\mathbf{p}_1=0, \quad \mathbf{p}_2=\boldsymbol{\kappa}; \quad \mathbf{p}_1'=\boldsymbol{\kappa}, \quad \mathbf{p}_2'=0. \tag{59}$$

In addition we must require, of course, that $\mathbf{r}_1\mathbf{r}_2$ and, respectively, $\mathbf{r}_1'\mathbf{r}_2'$ be in a region of configuration space where the wave function of the ground state is large. The meaning of these equations is obvious. They say that there must be a classical motion of 1 and 2 (and if necessary of the remaining nuclei) which starting from a probable[18] configuration $\mathbf{r}_1'\mathbf{r}_2'$, with momentum κ for nucleus 1 and zero momentum for nucleus 2, leads as a result of the interactions to probable[18] final positions $\mathbf{r}_1\mathbf{r}_2$ with momenta 0 and κ, respectively. Moreover, (58) is the energy conservation equation including the neutron, and (57) expresses the condition for the neutron to be able to travel, in the time $-t$, from position $\mathbf{r}_1'$ where it hits nucleus 1, to position $\mathbf{r}_2$ where it hits nucleus 2.

The result is thus by no means unexpected; in fact the above discussion is merely an explicit formalization of the intuitive considerations we have applied several times before. It will serve, perhaps, to show to what extent a classical description of the molecular motion is applicable to these essentially nonclassical interference terms.

If all this be granted, it will appear that (57) and (58) are additional requirements that will in general be hard to satisfy, even if the forces between 1 and 2 are strong enough to effect the momentum transfer that was discussed before, and is also exhibited in the conditions (59). While it is not true in general that the conditions are incompatible, they do turn out to be so, for example, in the case of the oscillator model of Appendix 3, where the conclusions reached have been checked by the direct quantum-mechanical calculation.

While it is not possible to state quite generally that the "classical" conditions (57) (58) (59) can never be satisfied, it seems reasonable to draw the following conclusions. The more complicated the system, the less likely it will be that the whole effect of a large blow applied to particle 1 can be undone by a counterblow applied simultaneously or at any other time, to a single other particle 2. Hence exceptions to the rule that large momentum transfers do not contribute significantly to interference terms will occur at most in very simple systems, like a diatomic molecule. Even so, they will play a role only under rather special conditions.

It follows then, that barring these special exceptions, and for neutrons satisfying the condition $E_0 \gg \Delta$, see P(2.3), the energy transfers effective in interference scattering will be $\ll E_0$, so that the approximation developed in P should be applicable, even to molecules containing very light nuclei. In particular the "static" approximation [first line of P(7.20)] should give an adequate representation of the cross section for most purposes.

Some comment is desirable, however, concerning the subsequent terms of Placzek's expansion, say, for instance, the 2nd and 3rd line of P(7.20). If our conclusions are correct, we should expect these terms to be small compared to the static approximation. Under the assumptions of P, the smallness of these terms is in fact warranted by the large mass of the nuclei, as for instance indicated by the factor $\mu_s\mu_{s'}$ in the last line of P(7.20). Such factors are of no help in our case. As pointed out in P, however, these terms are also small for other reasons, namely, because of factors $\sim\exp(-4E_0/M\omega)$, ω being a frequency of nuclear motion (Debye-Waller factors, etc.). Now as a rough rule of thumb, we may say the frequency ω varies with the mass as $M^{-\frac{1}{2}}$, so that the exponential varies $\sim\exp(-\alpha E_0/M^{\frac{1}{2}})$, α being roughly a constant. Thus this factor is actually much smaller for light nuclei and compensates for the absence of the mass denominators.

A different question, however, also arises. Namely, we may want to know not merely whether the second, third, $\cdots$ terms in the expansion are small, but also whether they effectively represent the error of the first, or static, approximation. This question is more difficult to answer in view of the energy dependence of the successive terms in P(7.20). Thus the first term is proportional to E_0^{-1}, while the second term and the terms in the second and third lines contain exponential factors of the type mentioned above. Proceeding further in the expansion, however, we would find the term $S_4'(0)$ in P(3.11) and other terms to be found later again yield simple reciprocal powers of E_0. Thus the series is definitely not an asymptotic expansion in the same sense as P(5.16) or (21). At very high energies we ought to leave out all exponential terms and keep the powers of E_0^{-1}; the series would then start as follows:

$$\sigma_{12}=4\pi a_1 a_2 k_0^{-2}\{\tfrac{1}{2}\langle r_{12}^{-2}\rangle_{\mathrm{Av}}-(1/96M_1M_2)E_0^{-2} \times\langle \mathrm{grad}_1 V\cdot\mathrm{grad}_2 V\rangle_{\mathrm{Av}}+\cdots\}. \tag{60}$$

For large masses and moderate energies, however, the terms thus thrown away are more important than the term added above.

For macroscopic bodies, such as crystals, there is in addition the question of the convergence of the sum over the indices s, s'. This question has been exhaustively discussed for the static approximation[19] but not

[18] Probable refers here to the space distribution in the ground state.

[19] Placzek, Nijboer, and Van Hove, Phys. Rev. **82**, 392 (1951).

for the second and third line of P(7.20). A provisional estimate we have made shows that no special difficulty is encountered, but we hope to come back to this question later.

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APPENDIX 1

Single Nucleus, Differential Cross Section

One can, by means of the method of Sec. 3, also calculate the differential cross section or the effective differential cross section. In the case of light nuclei this means, of course, lumping together final neutrons of widely different energy. The result is, therefore, somewhat less significant and will be discussed only briefly. In order to obtain the differential cross section we must go back to Eqs. (12) and (19) and introduce as an integration variable the final momentum of the neutron $\mathbf{k}=\mathbf{k}_0-\boldsymbol{\kappa}$ in place of $\boldsymbol{\kappa}$. Writing then $d\mathbf{k}=k^2dkd\Omega$ in place of $d\boldsymbol{\kappa}$ and performing the integral over k, but not over $d\Omega$ we obtain

$$k_0d\sigma/d\Omega=\sum_n(n!)^{-1}\int_0^\infty k^2s_n(\kappa^2)\delta^{(n)}(\alpha)dk, \qquad \text{(A1)}$$

where κ^2 and α are now functions of k:

$$2M\alpha=(1+M)k^2-2k_0k\cos\theta-(M-1)k_0^2,$$
$$\kappa^2=k_0^2-2k_0k\cos\theta+k^2.$$

Inserting (18) into (A1) one can calculate each term explicitly. We give the result in an abbreviated form. Introduce a variable $x=(k/k_0)-\cos\theta/(M+1)$ and the value x_0 corresponding to the value of k for which $\alpha=0$:

$$x_0=(M^2-\sin^2\theta)^{\frac{1}{2}}/(M+1). \qquad \text{(A2)}$$

Then, remembering that in Eq. (17), s_n is a function $s_n(u)$ of $u=\kappa^2$, write u as a function of x. This may be indicated explicitly by $u=k_0^2v_x$, where

$$v_x=1-2(k/k_0)\cos\theta+(k/k_0)^2$$
$$=[x-M\cos\theta/(M+1)]^2+\sin^2\theta. \qquad \text{(A3)}$$

Define functions

$$\phi_{n,m}(\theta)=(1+M^{-1})^{-n-1}\times\left[\left(\frac{\partial}{\partial x^2}\right)^n\left\{x^{-1}\left(x+\frac{\cos\theta}{M+1}\right)^2v_x{}^m\right\}\right]_{x=x_0}. \qquad \text{(A4)}$$

In particular,

$$\phi_{0,0}(\theta)=(1+M^{-1})^{-1}x_0{}^2[x_0-(1+M)^{-1}\cos\theta]^{-1}. \qquad \text{(A5)}$$

We can now write the first terms of the expansion of the differential cross section

$$a^{-2}d\sigma/d\Omega=\phi_{0,0}(\theta)+(2/3ME_0)K_{Av}\phi_{2,1}(\theta)-(B/6ME_0{}^2)\phi_{3,1}(\theta)+(2/15M^2E_0{}^2)\langle K^2\rangle_{Av}\phi_{4,2}(\theta)+(C/12ME_0{}^3)\phi_{4,1}(\theta)+\cdots. \qquad \text{(A6)}$$

The effective differential cross section can be similarly obtained if one adds a factor k_0/k to the integral in (A1). This leads to functions

$$\psi_{n,m}(\theta)=(1+M^{-1})^{-n-1}\times\left[\left(\frac{\partial}{\partial x^2}\right)^n\left\{x^{-1}\left(x+\frac{\cos\theta}{M+1}\right)v_x{}^m\right\}\right]_{x=x_0}. \qquad \text{(A7)}$$

To get $d\sigma_{\text{eff}}/d\Omega$, replace all ϕ's by ψ's in Eq. (A6), thus,

$$a^{-2}d\sigma_{\text{eff}}/d\Omega=\psi_{0,0}(\theta)+(2/3ME_0)K_{Av}\psi_{2,1}(\theta)+\cdots. \qquad \text{(A8)}$$

The formulas as written are not perhaps very explicit but the Eqs. (A5) to (A8) will give an explicit answer with a little work, but without difficulty, if needed.

One may wish to compare these formulas with P(5.19) and P(5.20). For this purpose bear in mind that the energy dependence in Eqs. (A6) and (A8) is given explicitly. And in fact one finds K_{Av} divided by E_0, B and $\langle K^2\rangle_{Av}$ divided by $E_0{}^2$, C divided by $E_0{}^3$ as expected.

On the other hand, the M dependence appears only in part. We have tried to write the ϕ and ψ functions so that they are of zero order in M, when M is large. Cancellations may occur, however, in the limit $M\to\infty$, so that a function may occasionally turn out to be of the order M^{-1} or even smaller. One verifies easily, for instance, that in the limit $M=\infty$, $\phi_{3,1}\to0$. Thus, the B term in Eq. (A6) is not of first order in M^{-1} as it seems to be, but higher, in agreement with P(5.19) where it appears to be of order M^{-2}. On the other hand, the $\psi_{3,1}$ function which multiplies B in the effective cross section does not vanish in the limit $M=\infty$, in agreement with the M dependence of the B term in P(5.20).

APPENDIX 2

Nonisotropic Oscillator

For simplicity we assume $M=1$ from the start, since this is the critical case. We assume that the oscillator has three different frequencies ω_1, ω_2, ω_3 along the Cartesian axes 1, 2 and 3. By an analysis completely

similar to that leading to (31), one finds

$$G_{aa}=a^2\prod_{j=1}^{3}\exp\{(\kappa_j^2/2\omega_j)(e^{i\omega_j t}-1)\},$$

and later, instead of (34),

$$\sigma/\sigma_b=\tfrac{1}{4}(\pi E_0)^{-\frac{1}{2}}\int_{-\infty}^{+\infty}dt\prod_{j=1}^{3}f_j(t), \tag{A9}$$

where

$$f_j(t)=(\omega_j\lambda_j)^{\frac{1}{2}}\exp(-t^2\omega_j k_j^2\lambda_j),$$
$$\lambda_j\equiv\lambda_j(t)=[1-e^{i\omega_j t}-i\omega_j t]^{-1},$$

$k_1k_2k_3$ being the components of the vector k_0. Leaving aside the neighborhood of $t=0$, which offers nothing essentially new, we examine the contribution from longer times. If a direction of k_0 is chosen at random, and E_0 is increased, it can be seen that the modulus of the integrand of (A9) goes to zero exponentially for any given $t\neq 0$ on the real axis. This is because the real parts of $f_1f_2f_3$ cannot be zero simultaneously if $\omega_1\neq\omega_2\neq\omega_3$ (barring the case $\omega_1:\omega_2:\omega_3=n_1:n_2:n_3$, where n_1, n_2, n_3 are three integers). However if k_0 is directed along one of the axes, then clearly the periodicity phenomenon of Sec. 4 reappears. Averaging the cross section over the direction of k_0, we see that "anomalous" terms will come from the neighborhood of the three axes.

Assume for example $k_1\approx k_0$, $k_2\ll k_0$, $k_3\ll k_0$. There are then saddle-points near the real axis; when k_2 and $k_3\to 0$ these saddle-points tend to $\omega_1 t=\pm 2\pi$, $\pm 4\pi$, $\cdots$. Writing for the saddle-point

$$t=2\pi\nu/\omega_1+\tau,$$

and expanding τ in powers of k_2 and k_3, we find

$$\omega_1\tau=k_0^{-2}(1+i/\pi\nu)^{-1}\{k_2^2A_2+k_3^2A_3\},$$

where

$$A_j=\xi_j\lambda_j(2-i\xi_j)(1+i\xi_j\lambda_j),$$
$$\xi_j=2\pi\nu\omega_j/\omega_1,\quad \lambda_j^{-1}=1-i\xi_j-e^{i\xi_j}.$$

The contribution of the saddle-point to the integral is again of the type of Eq. (40). Apart from less interesting factors, it is E_0^{-1} times an exponential of $-t^2\sum_j\omega_j k_j^2\lambda_j$ calculated at the saddle-point. Neglecting again higher order terms in k_2 and k_3, however, it is obvious that the exponent can be calculated at the "unperturbed" saddle-point $t=2\pi\nu/\omega_1$. The exponent is then found to be

$$-4\pi\nu E_0\omega_1^{-1}\{i+(k_2/k_0)^2\xi_2\lambda_2+(k_3/k_0)^2\xi_3\lambda_3\}.$$

Since λ_2 and λ_3 have a positive real part, the correction terms in k_2 and k_3 have, of course, the effect to introduce an exponential damping with increasing energy. The anomalous terms are thus only important when $k_2^2k_3^2\ll k_0^2$, more precisely within a solid angle of the order of ω_1/E_0. Averaging over the direction of the incident neutron, and including the similar contributions from the angular regions around axis 2 and 3, one finds that the anomalous term in the cross section is, roughly

$$(1/128)\textstyle\sum_\nu(\pi\nu)^{-5/2}(\omega_1/E_0)^2e^{-2\pi i\nu E_0/\omega_1},$$

plus two other similar terms in ω_2 and ω_3. For simplicity some factors of order of magnitude one, and some phase factors are omitted. This result shows that the anomalous oscillation does not entirely disappear from the asymptotic formula; however, two important differences emerge. First, the anomaly is removed from the E_0^{-1} correction, and shifted to a term of order E_0^{-2}; secondly, the numerical factors are such as to make the effect quite insignificant.

APPENDIX 3

Oscillator Model for Interference Terms

We consider a diatomic molecule of total mass $M=M_1+M_2$ with the potential energy

$$V(\mathbf{r})=\tfrac{1}{2}M_{12}\omega^2\mathbf{r}^2, \tag{A10}$$

where $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ and $M_{12}=M_1M_2/M$. This would be a tolerably good model for a molecule, were it not for the unrealistic feature, that the equilibrium position is at $r=0$. It does provide us, however, with a simple and exact illustration of some interesting points. In terms of the total and relative momenta: $\mathbf{P}=\mathbf{p}_1+\mathbf{p}_2$ and $\mathbf{p}=M^{-1}(M_2\mathbf{p}_1-M_1\mathbf{p}_2)$ the Hamiltonian of the molecule is

$$H=\tfrac{1}{2}(M^{-1}\mathbf{P}^2+M_{12}^{-1}\mathbf{p}^2)+V(\mathbf{r}).$$

It is an easy matter to evaluate the expectation value of the operator G, Eq. (4), for the ground state of the molecule. For simplicity let us consider only the non-diagonal term, $a_1a_2G_{21}$. The factors referring to the center of mass can be separated; one gets then easily:

$$\langle G_{21}\rangle=\exp(it\kappa^2/2M)\langle\exp(i\boldsymbol{\kappa}\cdot\mathbf{r}M_1/M)\times\exp[i\boldsymbol{\kappa}\cdot\mathbf{r}(t)M_2/M]\rangle, \tag{A11}$$

which is, so far, independent of the assumption (A10). With that assumption, however, we get

$$\mathbf{r}(t)=\mathbf{r}\cos\omega t+(M_{12}\omega)^{-1}\mathbf{p}\sin\omega t. \tag{A12}$$

A calculation similar to that of Sec. 4 then gives

$$\langle G_{12}\rangle=\exp\{-(\kappa^2/4M_{12}\omega)+(\kappa^2/2M\omega)(1+i\omega t-e^{i\omega t})\}. \tag{A13}$$

Before we proceed, we may notice various properties of (A13). For $t=0$ the expression is exponentially small for large κ, which, of course, illustrates the fact that when momenta $\boldsymbol{\kappa}$ and $-\boldsymbol{\kappa}$ are applied to two different nuclei, it is unlikely that the molecule will be left in the ground state. For small t, the exponent may be expanded, and the absence of a linear term may be verified.

For any real value of t, one has, furthermore,

$$|\langle G_{12}\rangle|\leq\exp\{-(\kappa^2/4M_{12}\omega)(M_1-M_2)^2M^{-2}\}. \tag{A14}$$

Thus if $M_1\neq M_2$, the molecule is not likely to be restored to the ground state, even if there is an arbitrary

time lag between the two momentum transfers. The equality sign in (A14), i.e., a maximum value for the matrix element, is obtained for $\omega t=\pm\pi$, $\pm 3\pi$, $\cdots$. This result, which recalls to mind the behavior of the diagonal matrix element in Sec. 4, is easily understood, since it is just after a half-period, or an odd multiple thereof, that the maximum momentum transfer from 1 to 2 has taken place.

If moreover $M_1=M_2$, the two nuclei will have completely interchanged their momenta, at the times indicated, so that both can be brought to rest by a counterblow $-\kappa$ applied to nucleus 2. In fact the absolute value of (A13) becomes, under these circumstances, equal to 1; one might think, therefore, that "long" times, of the order of the oscillator period, could give important contributions to the cross section, supplying us with a nondiagonal counterpart of the "anomalous" terms of Sec. 4. This is, however, not the case, no matter what values we choose for M_1 and M_2.

So far our discussion has only brought out the consequences of momentum conservation in the collisions and the initial and final values of the momenta. The subsequent integration over κ and t will produce the additional requirements of coincidence in space and energy conservation expressed by (57) and (58) of Sec. 5. Even without calculation one can see that those requirements cannot be fulfilled here. Initially the two nuclei are at rest and close to each other (neglecting the zero point motion); immediately after the first collision, nucleus 1 is moving rapidly with a momentum κ, which must be a value permissible in a free collision; nucleus 2 is at rest. Now when the second collision is supposed to occur, at a "favorable" time, say after a half-period, the two nuclei are again close together; hence the second collision can only occur if the velocity of the neutron after the first collision is equal to that of the center of mass. The reader can easily verify that this is incompatible with the condition $M_1=M_2$.

Now to the calculation. The integration over κ is trivial. Writing the cross section in the form $\sigma=4\pi\{a_1^2I_{11}+2a_1a_2I_{12}+a_2^2I_{22}\}$, and introducing the abbreviations $\xi=\omega t$, and

$$\lambda\equiv\lambda(\xi)=[(2M_{12})^{-1}-M^{-1}(1+i\xi-e^{i\xi})-i\xi]^{-1}, \quad \text{(A15)}$$

one finds

$$I_{12}=\tfrac{1}{4}(\pi n_0)^{-\frac{1}{2}}\int_{-\infty}^{+\infty}\lambda^{\frac{3}{2}}\exp(-n_0\xi^2\lambda)d\xi, \quad \text{(A16)}$$

i.e., an expression similar to (34), with a different function λ.

We must remember that (A16) includes the contribution of collisions with small momentum transfers. Thus it is not surprising that the integrand of (A16) is not now exponentially small for large energies n_0 in the neighborhood of time $\xi=0$. In fact, for small ξ, $\lambda\sim 2M_{12}$ and the contribution of small times to (A16) is

$$I_{12}\approx\tfrac{1}{4}(\pi n_0)^{\frac{1}{2}}(2M_{12})^{\frac{3}{2}}\int\exp(-2M_{12}n_0\xi^2)d\xi$$
$$=M_{12}\omega k_0^{-2}. \quad \text{(A17)}$$

Noticing that $\langle r_{12}^2\rangle=(2M_{12}\omega)^{-1}$, we recognize in (A17) the first and most important term of P(7.20). Other terms, of higher order in n_0^{-1}, can of course be obtained from the neighborhood of $\xi=0$ by a complete asymptotic expansion of the integral.

Leaving these terms aside, we now show that the remaining part of the integral, i.e., excluding the neighborhood of $\xi=0$, gives an exponentially small contribution (even for $M_1=M_2$). First, if $M_1\neq M_2$, and excluding a finite interval around the origin, it is easy to show that on the real axis an inequality like (35) is satisfied, which proves the statement. If $M_1=M_2$ we have to examine the neighborhood of the points $\xi=\pm\pi$, $\pm 3\pi$, $\cdots$ where the real part is equal to zero. One finds that at these points,

$$\frac{d}{d\xi}(\xi^2\lambda)=i\left(1+\frac{1}{M}\right)^{-2}\neq 0.$$

Hence, these points are not saddle points; if the integration path is deformed and caused to pass under the points $\xi=\pm(2n+1)\pi$, the inequality (35) can be re-established along the whole integration path, and the integral is thus $\sim\exp(-cn_0)$. This completes the proof of all our statements.