# The Scattering of Neutrons by Systems of Heavy Nuclei*†

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It is shown that the scattering of neutrons by a system of heavy nuclei may, for neutron energies that are large compared with the level separation of the system, be described in terms of averages of simple two-particle operators over the initial state. Expressions are derived for the total and differential cross sections and for the first few moments of the energy transfer. The expression for the cross section can be explicitly evaluated even for complicated scattering systems and leads to an accurate representation of the energy dependence of the nuclear scattering. The results are applied to the problem of the detection of small electronic contributions to the cross section.

## 1. INTRODUCTION

WE consider the collision of a neutron of mass $m$, energy $E_0$, wave vector $\mathbf{k}_0$, and wave number $k_0$ with a system of $N$ nuclei—such as a molecule, a gas, a liquid, or a crystal—in the state "$a$" of energy $E_a$. The standard Born approximation[1] leads to the scattering cross section,

$$\sigma^{(a)}=\frac{2}{k_0}\sum_b\int|(F(\boldsymbol{\kappa}))_a{}^b|^2\delta\left\{\kappa^2-2\mathbf{k}_0\cdot\boldsymbol{\kappa}+\frac{2m}{\hbar^2}(E_b-E_a)\right\}d\boldsymbol{\kappa}. \quad (1.1)$$

The summation extends over all states of the nuclear system, and the integration variable $\mathbf{k}$ is the momentum transferred to the system, divided by $\hbar$. The delta-function expresses conservation of energy and the scattering amplitude $F(\boldsymbol{\kappa})$ is given by

$$F(\boldsymbol{\kappa})=\sum_{s=1}^{N}a_s\exp(i\boldsymbol{\kappa}\cdot\mathbf{r}_s). \quad (1.2)$$

Here $\mathbf{r}_s$ is the position vector of nucleus $s$ and $a_s$ its scattering length.

The scattering lengths will be taken to be independent of $E_0$ and $\boldsymbol{\kappa}$ in the energy region considered, they may, however, depend on the nuclear spin variables. For nuclei without spin the scattering length $a_s$ is simply related to the scattering cross section $\sigma_s$ of the bound nucleus by

$$\sigma_s=4\pi a_s^2, \quad (1.3)$$

and the matrix element of the scattering amplitude may here be written

$$F_a{}^b=\int\psi_b{}^*(\mathbf{r}_1,\cdots\mathbf{r}_N)F\psi_a(\mathbf{r}_1,\cdots\mathbf{r}_N)d\mathbf{r}_1\cdots d\mathbf{r}_N, \quad (1.4)$$

where the $\psi$'s are the eigenfunctions of the Hamiltonian $H$ of the motion of the nuclei in the field of the interatomic forces.

For nuclei with spin, (1.3) and (1.4) have to be modified which will be taken care of in Sec. 7.

The straightforward evaluation of (1.1) requires detailed knowledge of the eigenfunctions of all accessible states. It is therefore possible for the very simplest cases only, and even there it becomes progressively more laborious with increasing neutron energy. In the following it will be shown, however, that for systems of heavy nuclei the cross section may be expressed in terms of averages of simple operators over the initial state as soon as the neutron energy is large compared to the level separation of the system.

## 2. GENERAL CONSIDERATIONS

In the limit of infinite neutron energy, (1.1) goes over into[2]

$$\sigma_\infty{}^{(a)}=\sum_s\left(1+\frac{m}{M_s}\right)^{-2}\sigma_s, \quad (2.1)$$

where $M_s$ is the mass of nucleus $s$. We shall have to determine, in particular, the behavior of the cross section on the approach to this limit. While certain general statements in regard to this problem may be made on the basis of the classical particle picture,[3] their application to the case of heavy nuclei would appear to be of limited practical use without a closer investigation. This may be seen as follows. In classical mechanics the collision—in our case of contact interaction—takes place instantaneously and the energy dependence of the cross section is determined by the momentum distribution of the scattering particles. The cross section of a system under the influence of forces will thus be equal to that of a free system with the same momentum distribution. A necessary condition for the description of the collision in classical particle terms requires that the collision time $\hbar/E_t$, where $E_t$ is the classical energy transfer, be short compared to the periods of the

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[1] For the justification of the use of the Born approximation in the treatment of this problem see E. Fermi, Ricerca sci. 7, 13 (1936); G. Breit, Phys. Rev. 71, 215 (1947).

[2] E. Fermi, Ricerca sci. 7, 13 (1936).

[3] G. Placzek, Phys. Rev. 75, 1295 (1949); and as quoted in reference 7.

system. Accordingly, the energy transfer $(m/M)E_0$ has to be large compared to the level separation of the system, and thus

$$E_0 \gg (M/m)\Delta, \tag{2.2}$$

where $\Delta$ is the level separation. Indeed, one can see immediately that unless condition (2.2) is satisfied the energy distribution of the scattered neutrons must differ appreciably from the classical energy distribution.

For heavy nuclei (2.2) becomes extremely restrictive and we shall therefore attempt to study the collision under the much less restrictive condition,

$$E_0 \gg \Delta. \tag{2.3}$$

For this purpose we start from the static approximation which results from neglecting the energy changes associated with the transition of the system. It is obtained by omitting the last term in the delta-function in (1.1). The summation over $b$ can then be carried out immediately by closure so that (1.1) goes over into

$$\sigma^{(a)} = \frac{2}{k_0}\int (F^*(\boldsymbol{\kappa})F(\boldsymbol{\kappa}))_a{}^a \delta(\kappa^2 - 2\mathbf{k}_0\cdot\boldsymbol{\kappa})d\boldsymbol{\kappa}$$

$$= \int (|F(\mathbf{k}_0 - k_0\boldsymbol{\Omega})|^2)_a{}^a d\Omega, \tag{2.4}$$

where $\boldsymbol{\Omega}$ is a unit vector. Equation (2.4) represents the average of the cross section of a system, consisting of nuclei fixed in definite positions, over the configurations of the initial state of the real system. It may thus be referred to as the static approximation. This approximation forms the basis of the theory of x-ray scattering by molecules, crystals, and liquids.[4]

The cross section (2.4) has to be well distinguished from the elastic cross section (or more precisely, the cross section for scattering without change of quantum state) which from (1.1) is given by

$$\sigma_{el}{}^{(a)} = (2/k_0)\int |(F(\boldsymbol{\kappa}))_a{}^a|^2 \delta(\kappa^2 - 2\mathbf{k}_0\cdot\boldsymbol{\kappa})d\boldsymbol{\kappa}$$

$$= \int |(F(\mathbf{k}_0 - k_0\boldsymbol{\Omega}))_a{}^a|^2 d\Omega. \tag{2.5}$$

In the literature the cross section is frequently divided into an elastic and inelastic part and the energy dependence of each part is discussed separately. It is clear from (2.4) that in the static approximation this separation is an unnecessary complication which has to be avoided as far as possible. This situation will be shown later to hold also in higher approximations.

For systems consisting of one nucleus only, the static approximation leads to a constant cross section. Since here $|F|^2 = a_s{}^2$, we have from (2.4)

$$\sigma^{(a)} = \sigma_s. \tag{2.4a}$$

For systems consisting of several nuclei the evaluation of (2.4) involves the probability distribution of internuclear distances in the initial state (pair density). In the limit of infinite neutron energy the cross section (2.4) reduces here to

$$\sigma_\infty{}^{(a)} = \sum_s \sigma_s, \tag{2.6}$$

which differs from the correct result (2.1) by the absence of the reduced mass factors.

It will now be our problem to establish the exact conditions of validity of the static approximation which neglects the energy changes and to improve it by taking account of the energy changes. We shall limit ourselves to systems of random orientation. This will contribute to brevity and the generalization of the results to oriented systems such as single crystals will become quite obvious in the course of the treatment.

For systems of random orientation we may average the delta-function in (1.1) over all directions of $\mathbf{k}_0$, whereby (1.1) goes over into

$$\sigma^{(a)} = \frac{1}{2k_0{}^2}\sum_b{}^{E_b<E_0+E_a} \int_{a,b} |F_a{}^b(\boldsymbol{\kappa})|^2 \frac{d\boldsymbol{\kappa}}{\kappa}, \tag{2.7}$$

where the subscript $a, b$ under the integral sign indicates that the integration extends over a region in $\boldsymbol{\kappa}$-space bounded by the spheres of radius $k_0 + k_{ab}$ and $|k_0 - k_{ab}|$ with

$$k_{ab}{}^2 = 2mh^{-2}(E_0 + E_a - E_b). \tag{2.8}$$

Introducing the average $\phi_{ab}(\kappa^2)$ of the square of the matrix element over all directions of $\boldsymbol{\kappa}$

$$\phi_{ab}(\kappa^2) = (1/4\pi)\int |F_a{}^b(\boldsymbol{\kappa})|^2 d\Omega_\kappa \tag{2.9}$$

and putting

$$(E_b - E_a)/E_0 = x_{ab}, \tag{2.10}$$

we may write (2.7)

$$\sigma^{(a)} = \frac{\pi}{k_0{}^2}\sum_b{}^{x_{ab}<1} \int_{k_0{}^2\{1-(1-x_{ab})^{\frac{1}{2}}\}^2}^{k_0{}^2\{1+(1-x_{ab})^{\frac{1}{2}}\}^2} \phi_{ab}(\kappa^2)d\kappa^2. \tag{2.11}$$

If in this expression the quantities $x_{ab}$ are neglected throughout, which implies also the replacement of the restricted sum over $b$ by an unrestricted one, it goes over into

$$\sigma^{(a)} = \frac{\pi}{k_0{}^2}\int_0^{4k_0{}^2} (\sum_b \phi_{ab}(\kappa^2))d\kappa^2$$

$$= \frac{1}{4k_0{}^2}\int_0^{4k_0{}^2} d\kappa^2 \int (|F(\boldsymbol{\kappa})|^2)_a{}^a d\Omega_\kappa, \tag{2.12}$$

[4] See the review article by M. Born in Reports of Progress of Physics 9, 294 (1943).

which is the result of the static approximation (2.7), averaged over all directions of $\mathbf{k}_0$.

The expression (2.11) has a form suitable for taking the energy exchanges into account. For heavy nuclei, owing to the difficulty of large energy transfers between light and heavy particles, the quantities $x_{ab}$ will be small for all transitions with appreciable matrix element, provided the neutron energy is large compared to the level spacing and the neutron velocity large compared to the average nuclear velocities. If these conditions—the latter of which only implies a very weak limitation on the admissible degree of initial excitation of the system—are satisfied, we may therefore expand the integrals in (2.11) in powers of $x_{ab}$ and replace the restricted sum by an unrestricted one. This method will be carried out in the following sections. With appropriate changes it is also applicable to the treatment of other problems. For the scattering of x-rays by atoms, in particular, it leads to certain modifications of hitherto accepted results.[5]

## 3. AN EXPRESSION FOR THE CROSS SECTION IN TERMS OF AVERAGES OVER THE INITIAL STATE

With the notations $u=4k^2$, $t=\kappa^2$, (2.11) may be written

$$\sigma^{(a)}=\sum_b \sigma_{ab} \tag{3.1}$$

$$\sigma_{ab}=(\sigma_{ab})_+-(\sigma_{ab})_- \tag{3.2}$$

$$(\sigma_{ab})_\pm=\frac{4\pi}{u}\int_0^{t_\pm}\phi_{ab}(t)dt \tag{3.3}$$

$$t_\pm=(u/4)\{1\pm(1-x_{ab})^{\frac{1}{2}}\}^2.$$

The expansion of $(\sigma_{ab})_+$ in powers of $x_{ab}$ is obtained by expanding the integral in powers of $u-t_+$ and expressing this quantity by its expansion in powers of $x_{ab}$

$$u-t_+=\frac{ux_{ab}}{2}\left\{1+\frac{x_{ab}}{8}+\frac{x_{ab}^2}{16}+\frac{5}{128}x_{ab}^3+\cdots\right\}. \tag{3.4}$$

This yields[6]

$$\begin{aligned}\frac{(\sigma_{ab})_+}{4\pi}=&\frac{1}{u}\int_0^u\phi(t)dt-\frac{x}{2}\phi(u)+\frac{x^2}{16}\{-\phi(u)+2u\phi'(u)\}\\&+\frac{x^3}{32}\{-\phi(u)+u\phi'(u)-\tfrac{2}{3}u^2\phi''(u)\}\\&+\frac{x^4}{512}\{-10\phi(u)+9u\phi'(u)\\&\qquad-4u^2\phi''(u)+(4/3)u^3\phi'''(u)\}.\end{aligned} \tag{3.5}$$

To expand $(\sigma_{ab})_-$, we expand $\phi$ in powers of $t$, integrate and expand $t_-$ in powers of $x$

$$t_-=\tfrac{1}{16}ux^2(1+\tfrac{1}{2}x+\cdots). \tag{3.6}$$

Noting that $\phi_{ab}(0)=0$ for $a\neq b$ and $x_{ab}=0$ for $a=b$, we obtain

$$\frac{(\sigma_{ab})_-}{4\pi}=\frac{x^4}{512}u\phi'(u)+O(x^5). \tag{3.7}$$

The lower limit of the integrals in (2.11) thus gives rise to a fourth-order correction only.

The quantities $\sigma_{ab}$ have now to be summed over $b$. At the same time we may average the cross section over the initial states of the system. Putting

$$\sigma=\sum_a \gamma_a\sigma^{(a)}, \tag{3.8}$$

where $\gamma_a$ is the probability of finding the system in state "$a$" before the collision and introducing sums $S_n$ by

$$S_n(t)=\sum_a \gamma_a S_n{}^{(a)}(t) \tag{3.9}$$

$$S_n{}^{(a)}(t)=\sum_b^{E_b<E_0+E_a}(E_b-E_a)^n\phi_{ab}(t), \tag{3.10}$$

we obtain for the cross section from (3.1), (3.2), (3.5), (3.7)–(3.10)

$$\begin{aligned}\frac{\sigma}{4\pi}=&\frac{1}{u}\int_0^u S_0(t)dt-\frac{1}{2E_0}S_1(u)+\frac{1}{16E_0^2}\{-S_2(u)+2uS_2'(u)\}\\&+\frac{1}{32E_0^3}\{-S_3(u)+uS_3'(u)-\tfrac{2}{3}u^2S_3''(u)\}\\&+\frac{1}{512E_0^4}\{-10S_4(u)+u(9S_4'(u)-S_4'(0))\\&\qquad-4u^2S_4''(u)+(4/3)u^3S_4'''(u)\}.\end{aligned} \tag{3.11}$$

We now have to discuss the quantities $S_n$. With (2.9) we may write (3.10)

$$\begin{aligned}&S_n{}^{(a)}(\kappa^2)\\&\quad=\frac{1}{4\pi}\int d\Omega_\kappa\sum_b^{E_b<E_0+E_a}(E_b-E_a)^n|(F(\boldsymbol{\kappa}))_a{}^b|^2.\end{aligned} \tag{3.12}$$

For freely orientable systems such as molecules, the averaging over the directions of $\boldsymbol{\kappa}$ is superfluous since the sum over $b$ will here depend on the magnitude of $\boldsymbol{\kappa}$ only. For systems showing the type of random orientation present in polycrystals, however, this averaging process is necessary.

Expressing $E_b-E_a$ as the diagonal element of the operator $H-E_a$

$$E_b-E_a=(H-E_a)_b{}^b$$

[5] G. Placzek, Bull. Am. Phys. Soc. **27**, No. 1, 13 (1952).

[6] In order to save indices, we write in the following $x$ for $x_{ab}$ and $\phi$ for $\phi_{ab}$.

and neglecting the limitation of the sum in (3.12), we obtain by closure

$$\sum_b (E_b-E_a)^n |F_a{}^b|^2=\sum_b (F^*)_b{}^a(\{H-E_a\}^n)_b{}^b F_a{}^b$$
$$=(F^*\{H-E_a\}^n F)_a{}^a. \qquad (3.13)$$

From the argument given at the end of the preceding section it may be concluded that under the conditions stated there the error committed by closure will be quite negligible for heavy nuclei and small $n$. In Sec. VI this will also be shown in somewhat greater detail for a specific example. Combining (3.9), (3.12), and (3.13) we obtain finally

$$S_n(\kappa^2)=\langle F^*(\boldsymbol{\kappa})(H-E_a)^n F(\boldsymbol{\kappa})\rangle_{\text{Av}}, \qquad (3.14)$$

where the average is to be taken (1) over the configuuration of state "$a$," (2) over the distribution of states "$a$" initially present in the system, and (3) if necessary, over the directions of $\boldsymbol{\kappa}$. The first two averaging processes can sometimes be combined in the customary way by the use of transformation theory.

With the help of the relation,

$$\langle (H-E_a)O\rangle_{\text{Av}}=\langle O(H-E_a)\rangle_{\text{Av}}=0,$$

where $O$ is a time-independent operator, (3.14) may be expressed in various ways. A convenient form is

$$\begin{aligned} S_0&=(F^*F)_{\text{Av}}\\ S_1&=(F^*[HF])_{\text{Av}}\\ S_2&=([F^*H][HF])_{\text{Av}}\\ S_3&=([F^*H][H[HF]])_{\text{Av}}\\ S_4&=([H[HF^*]][H[HF]])_{\text{Av}}, \end{aligned} \qquad (3.15)$$

where $[AB]$ is the commutator of the operators $A$ and $B$. The evaluation of (3.15) will be carried out in Secs. V and VII.

The quantities $S_n$ admit a simple physical interpretation. If a momentum $\hbar\kappa$ is imparted to the system, the average energy transfer accompanying this momentum transfer is given by $S_1(\kappa^2)/S_0(\kappa^2)$ and the $n$-th moment of the energy transfer by $S_n(\kappa^2)/S_0(\kappa^2)$. This will be used later in connection with the comparison of classical and quantum-mechanical results. The moments so defined are of course different from the moments of the energy transfer occurring in an actual collision. The latter are given by

$$\langle E^l\rangle_{\text{Av}}=\sum_a \gamma_a \sum_b (E_b-E_a)^l \sigma_{ab}/\sigma \qquad (3.16)$$

and may be expressed in terms of the quantities $S_n$ and their derivatives by noting that the denominator of (3.16) is given by (3.11) while the numerator results from (3.11) by simply replacing $S_n$ by $S_{n+l}$. The moments (3.16) which are thus, for small $n$, obtainable by our method, are also simply related to the moments of the energy distribution of the scattered neutrons, given by $\langle (E_0-E)^l\rangle_{\text{Av}}$.

## 4. THE DIFFERENTIAL CROSS SECTION

The treatment of the preceding section can be extended to the differential cross section. The differential cross section associated with the transition $a\rightarrow b$ is given by

$$d\sigma_{ab}/d\Omega=(1-x_{ab})^{\frac{1}{2}}\phi_{ab}(\kappa_{ab}{}^2). \qquad (4.1)$$

The factor $(1-x_{ab})^{\frac{1}{2}}$ represents the ratio of the velocities of scattered and incoming neutron and $\kappa_{ab}{}^2$ is determined by the relation,

$$\boldsymbol{\kappa}_{ab}=\mathbf{k}_0-k_0(1-x_{ab})^{\frac{1}{2}}\boldsymbol{\Omega}, \qquad (4.2)$$

where $\boldsymbol{\Omega}$ is a unit vector in the direction of scattering.

For scattering without energy change (4.2) goes over into

$$\boldsymbol{\kappa}_0=\mathbf{k}_0-k_0\boldsymbol{\Omega}. \qquad (4.3)$$

$\kappa_0{}^2$ is related to the cosine $\mu_0$ of the scattering angle by

$$\mu_0=1-\kappa_0{}^2/2k_0{}^2.$$

From (4.2) and (4.3) we have

$$\kappa_{ab}{}^2=k_0{}^2(1-x)^{\frac{1}{2}}+k^2(1-(1-x)^{\frac{1}{2}})^2. \qquad (4.4)$$

One now expands $\phi_{ab}(\kappa_{ab}{}^2)$ in powers of $\kappa_{ab}{}^2-\kappa_0{}^2$ and substitutes

$$\kappa_0{}^2-\kappa_{ab}{}^2=\tfrac{1}{2}\kappa_0{}^2 x_{ab}$$
$$+\tfrac{1}{4}(\tfrac{1}{2}\kappa_0{}^2-k^2)x_{ab}{}^2(1+\tfrac{1}{2}x_{ab}+\tfrac{5}{16}x_{ab}{}^2+\cdots).$$

Inserting the resulting expansion for $\phi$ as well as the expansion of $(1-x_{ab})^{\frac{1}{2}}$ into (4.1), one obtains, after summation over $b$ and averaging over $a$, the following result, where again $u=4k_0{}^2$, the scattering angle is measured by

$$t=\kappa_0{}^2=\tfrac{1}{2}u(1-\mu_0)=u\sin^2(\theta/2) \qquad (4.5)$$

and $S_n$ stands for $S_n(t)$

$$\frac{d\sigma}{d\Omega}=S_0-\frac{1}{2E_0}\{S_1+tS_1'\}$$
$$-\frac{1}{16E_0{}^2}\{2S_2-(2t+u)S_2'-2t^2S_2''\}$$
$$-\frac{1}{32E_0{}^3}\{2S_3-2tS_3'+tuS_3''+\tfrac{2}{3}t^3S_3'''\}$$
$$-\frac{1}{512E_0{}^4}\{20S_4-2(10t-u)S_4'+(4t^2+4tu-u^2)S_4''$$
$$+4t^2(\tfrac{2}{3}t-u)S_4'''-(4/3)t^4S_4''''\}. \qquad (4.6)$$

As a check we integrate this expression over $d\Omega$. For this and other purposes it is convenient to write it in

the form,

$$\frac{d\sigma}{d\Omega}=S_0-\frac{1}{2E_0}\frac{\partial}{\partial t}tS_1+\frac{1}{16E^2}\frac{\partial}{\partial t}\{(u-2t)S_2+2t^2S_2'\}$$
$$+\frac{1}{32E_0^3}\frac{\partial}{\partial t}\{(u-2t)(S_3-tS_3')-\tfrac{2}{3}t^3S_3''\}$$
$$+\frac{1}{512E_0^4}\frac{\partial}{\partial t}\{(u-2t)(10S_4+(u-10t)S_4'$$
$$+4t^2S_4'')+(4/3)t^4S_4'''\}. \quad (4.7)$$

Introducing (4.7) into

$$\frac{\sigma}{4\pi}=\frac{1}{2}\int_{-1}^{1}\frac{d\sigma}{d\Omega}d\mu_0=\frac{1}{u}\int_0^u\frac{d\sigma}{d\Omega}dt \quad (4.8)$$

one immediately obtains (3.11).

Under actual experimental conditions, the measured differential cross section will depend on the variation of the detector sensitivity with energy. We shall concern ourselves with a $1/v$ detector. In this case the partial differential cross sections have to be multiplied by the ratio of the velocities of incident and scattered neutron before the summation over $b$. This will just compensate the factor $(1-x_{ab})^{\frac{1}{2}}$ in (4.1). It can be shown that the omission of this factor exempts the factors of $S_n$, $S_n'$, $S_n''$, etc. in (4.7) from the operation $\partial/\partial t$. We find thus for the effective differential cross section measured by a $1/v$-detector

$$\left(\frac{d\sigma}{\partial\Omega}\right)_{\text{eff}}=S_0-\frac{tS_1'}{2E_0}+\frac{1}{16E_0^2}\{(u-2t)S_2'+2t^2S_2''\}$$
$$+\frac{1}{32E_0^3}\{(u-2t)(S_3'-tS_3'')-\tfrac{2}{3}t^3S_3'''\}$$
$$+\frac{1}{512E_0^4}\{(u-2t)(10S_4'+(u-10t)S_4''$$
$$+4t^2S_4''')+(4/3)t^4S_4''''\}. \quad (4.9)$$

## 5. SINGLE NUCLEUS

We take as the scattering system a single nucleus in the potential $V(\mathbf{r})$. The scattering amplitude is here given by a single term,

$$F=a_s\exp(iPz/\hbar), \quad (5.1)$$

where $P=\hbar\kappa$ is the momentum transferred to the nucleus and $z$ the component of $\mathbf{r}$ in the direction of $\mathbf{P}$. From (5.1) and (3.15) we have

$$S_0=a_s^2. \quad (5.2)$$

With the Hamiltonian

$$H=p^2/2M+V(\mathbf{r}), \quad (5.3)$$

one obtains for the commutation relations:

$$[HF]=\frac{P}{M}F(\tfrac{1}{2}P+p_z) \quad (5.4)$$

$$[H[HF]]=\frac{P}{M}F\left\{-\frac{\hbar}{i}\frac{\partial V}{\partial z}+\frac{P}{M}(\tfrac{1}{2}P+p_z)^2\right\}, \quad (5.5)$$

where $p_z$ is the component of the momentum of the nucleus in the direction of $\mathbf{P}$.

The expressions (5.4) and (5.5) are now introduced into (3.15). Integration by parts with real eigenfunctions and subsequent averaging over the directions of $\boldsymbol{\kappa}$ (i.e. $\mathbf{P}$) yields

$$\begin{aligned}&S_1/S_0=y\\&S_2/S_0=y^2+(4/3)K_{Av}y\\&S_3/S_0=y^3+4K_{Av}y^2+B_{Av}y\\&S_4/S_0=y^4+8K_{Av}y^3+4(\tfrac{4}{5}\langle K^2\rangle_{Av}+B_{Av})y^2+2C_{Av}y,\end{aligned} \quad (5.6)$$

where

$$y=\hbar^2\kappa^2/2M=P^2/2M. \quad (5.7)$$

$K$ is the kinetic energy of the nucleus and

$$B=\tfrac{1}{3}(\hbar^2/M)\nabla^2V \quad (5.8)$$

$$C=\tfrac{1}{3}(\hbar^2/M)(\text{grad}V)^2. \quad (5.9)$$

It is instructive to compare the expressions (5.6) with their classical value. In classical mechanics the energy transfer accompanying the instantaneous transfer of momentum $\mathbf{P}$ to a particle of momentum $\mathbf{p}$ moving in the potential $V(\mathbf{r})$ is independent of the potential and given by

$$E=(1/2M)\{P^2+2\mathbf{P}\cdot\mathbf{p}\}. \quad (5.10)$$

Averaging the $n$th power of (5.10) over the momentum distribution and over the directions of $\mathbf{P}$ one obtains

$$S_n/S_0=\frac{1}{n+1}\sum_{l=0}^{[n/2]}4^l\binom{n+1}{2l+1}\langle K^l\rangle_{Av}y^{n-l}, \quad (5.11)$$

where $[n/2]$ stands for the largest integer smaller than or equal to $n/2$. Comparison with (5.6) shows that (5.6) is represented by (5.11) plus additional terms which depend on the potential and which appear for $n>2$ only.

We are now ready for the evaluation of the cross section. Observing that the value $y_0$ of $y$ corresponding to $\kappa^2=u=4k_0^2$ is

$$y_0=4E_0/\mu \quad (5.12)$$

where $\mu=m/M$, we obtain from (3.11), (5.2), (1.3), and (5.6)

$$\frac{\sigma}{\sigma_s}=1-\frac{2}{\mu}+\frac{1}{\mu^2}\left(3+\frac{1}{3}\frac{\mu K_{Av}}{E_0}\right)-\frac{1}{\mu^3}\left(4+\frac{2}{3}\frac{\mu K_{Av}}{E_0}\right)$$
$$+\frac{1}{\mu^4}\left\{5+\frac{\mu K_{Av}}{E_0}-\frac{1}{32}\frac{\mu^3C_{Av}}{E_0^3}\right\}+\cdots. \quad (5.13)$$

The terms containing $\langle K^2\rangle_{Av}$ and $B_{Av}$ have canceled; one-half of the term containing $C_{Av}$ is contributed by the term $uS_4'(0)$ which arises from the lower limit of the integral in (2.11) and the other half by the terms $S_4(u)$ and $uS_4'(u)$. The terms starting with $1/\mu^n$ represent the terms containing $S_n$ and its derivatives in (3.11). The expansion of the partial cross section $\sigma_{ab}$ in powers of $x_{ab}$ is thus found to lead to an expansion of the cross section $\sigma$ in powers of $1/\mu$, where the characteristic energies of the system are measured in terms of $E_0/\mu$. It is, however, important to observe that the quantities $K_{Av}/\mu^{-1}E_0$ and $C_{Av}/(\mu^{-1}E_0)^3$—the former of which represents the square of the ratio of the momenta of nucleus and neutron—may be large. The terms of (5.13) have therefore to be rearranged, by writing

$$\frac{\sigma}{\sigma_s}=\left(1-\frac{2}{\mu}+\frac{3}{\mu^2}-\frac{4}{\mu^3}+\frac{5}{\mu^4}\right)+\frac{1}{3}\frac{K_{Av}}{E_0}\left(1-\frac{2}{\mu}+\frac{3}{\mu^2}\right)-\frac{1}{32}\frac{C_{Av}}{\mu E_0^3}. \quad (5.14)$$

Here the first term represents the reduced mass effect, mentioned in Secs. I and II, the second term, of the order of the square of the velocity ratio, the Doppler effect and the third term the effect of the potential.

Introducing the cross section of the free nucleus at rest by

$$\sigma_{\text{free}}=\sigma_s(1+1/\mu)^{-2}, \quad (5.15)$$

we have thus

$$\sigma/\sigma_{\text{free}}=1+\tfrac{1}{3}K_{Av}/\mu E_0-\tfrac{1}{32}C_{Av}/\mu E_0^3. \quad (5.16)$$

The cross section is thus approximately equal to the cross section of the free nucleus with the same momentum distribution and the direct effect of the binding manifests itself only in the last term, which decreases as $E_0^{-3}$.

For the average energy transfer one obtains from (3.16) by replacing, in (3.11), $S_n$ by $S_{n+1}$

$$(E_t)_{Av}=\frac{2}{\mu}\left\{E_0\left(\frac{\mu}{\mu+1}\right)^2-\frac{4}{3}K_{Av}\left(1-\frac{17}{4\mu}+\cdots\right)+\frac{B_{Av}}{8E_0}\left(1-\frac{8}{3\mu}+\cdots\right)-\frac{4}{15}\frac{\langle K^2\rangle_{Av}}{\mu E_0}(1+O(1/\mu))\right\}. \quad (5.17)$$

In the higher moments of the energy transfer the direct influence of the binding becomes rapidly more important at low neutron energy. Here a potential term is appreciable in the second moment and leading in the third moment. The energy dependence of these higher moments shows how these quantum effects disappear as the neutron energy increases to a value large compared to $\mu$ times the level separation, as can be studied in detail on the basis of the data for an oscillator given in Sec. VI.

For the differential cross section one finds from (5.6) and (4.7)

$$\frac{4\pi}{\sigma_s}\frac{d\sigma}{d\Omega}=1-\frac{4}{\mu}+\frac{1}{\mu^2}\left(2\beta+6\beta^2+\frac{\mu}{3}\frac{K_{Av}}{E_0}\right)-\frac{4}{\mu^3}\beta\left\{3\beta+\frac{\mu K_{Av}}{E_0}(1-\beta)\right\}+\frac{2}{\mu^4}\left\{\beta^2(3+10\beta-5\beta^2)+\frac{3\mu K_{Av}}{E_0}\beta(1-\beta)+\frac{\mu^2 D}{8E_0^2}(1-6\beta+6\beta^2)+\frac{\mu^3 C_{Av}}{64E_0^3}\right\} \quad (5.18)$$

where

$$\beta=\sin^2(\theta/2)$$

and

$$D=\tfrac{4}{5}\langle K^2\rangle_{Av}+B_{Av}.$$

Rearranging terms and introducing (5.15), one has from (5.18)

$$\frac{d\sigma}{d\Omega}=\frac{\sigma_{\text{free}}}{4\pi}\left(1+\frac{1}{\mu}\left\{2\cos\theta+\frac{K_{Av}}{3E_0}-\frac{C_{Av}}{32E_0^3}+\cdots\right\}+\frac{1}{\mu^2}P_2(\cos\theta)\left\{1+\frac{2}{3}\frac{K_{Av}}{E_0}+\frac{\langle K^2\rangle_{Av}+(5/4)B_{Av}}{5E_0^2}+\cdots\right\}+\frac{1}{\mu^3}P_2(\cos\theta)\left\{\frac{K_{Av}}{3E_0}+\cdots\right\}+\frac{1}{\mu^4}\left\{\frac{(5\cos^2\theta-1)(1-\cos^2\theta)}{8}+\cdots\right\}\right). \quad (5.19)$$

Equation (5.19) contains two terms depending on the potential which are again small and the remainder is identical with the differential scattering cross section of a free nucleus with the same momentum distribution. Solving the latter problem in the usual way by transforming from center-of-mass to laboratory system and expanding the result in powers of the velocity ratio and the coefficients of this expansion in powers of $1/\mu$, one indeed finds again (5.19) except for the two potential terms.

The relative order of the various terms in (5.19) depends on the neutron energy and the degree of excitation of the system. For high excitation and low neutron energy, for example, it will not be consistent to carry the last two terms of (5.19) since under these conditions they will be smaller than terms which would arise if the original expansion (5.18) were carried to higher order than the fourth. Nevertheless, however, the terms contained in (5.19) are more than amply sufficient for an accurate representation of the differential cross section of heavy nuclei at all neutron energies satisfying the conditions stated at the end of Sec. II.

The effective differential cross section, obtained in the same way as (5.19), turns out to be

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{eff}}=1+\frac{1}{\mu}\Big\{1+\cos\theta\Big(1+\frac{K_{\text{Av}}}{3E_0}+\frac{B_{\text{Av}}}{8E_0^2}+\frac{5C_{\text{Av}}}{32E_0^3}+\cdots\Big)\Big\}+\frac{\cos\theta}{\mu^2}\Big\{1+\frac{2K_{\text{Av}}}{3E_0}+\frac{B_{\text{Av}}+(2/5)\langle K^2\rangle_{\text{Av}}}{2E_0^2}+\cdots\Big\}+\frac{\cos\theta}{2\mu^3}\Big\{\sin^2\theta+(11-9\cos^2\theta)\frac{K_{\text{Av}}}{3E_0}+\cdots\Big\}+\frac{\cos\theta}{2\mu^4}\{\sin^2\theta+\cdots\}. \quad (5.20)$$

From the results of this section it appears that, while the collision is describable in terms of the classical particle picture only if the neutron energy $E_0$ is large compared to $\mu$ times the level separation $\Delta$, the quantum characteristics of the collision will, in the energy region $\Delta\ll E_0\ll\mu\Delta$, manifest themselves primarily in the energy distribution of the scattered neutrons. The higher moments of the energy transfer show a strong explicit dependence on the binding potential. In the cross section and the differential cross sections, on the other hand, this dependence is much less pronounced and the binding affects these quantities mainly through its influence on the nuclear momentum distribution.

## 6. ISOTROPIC OSCILLATOR

As an example we consider a three-dimensional isotropic harmonic oscillator of frequency $\omega$ at a temperature $T$. For this system one finds easily

$$\begin{aligned} K_{\text{Av}}&=\tfrac{3}{2}T_{\text{eff}} & B&=(\hbar\omega)^2\\ \langle K^2\rangle_{\text{Av}}&=(15/4)T_{\text{eff}}^2 & C_{\text{Av}}&=\tfrac{2}{3}BK_{\text{Av}}=(\hbar\omega)^2T_{\text{eff}}, \end{aligned} \quad (6.1)$$

where the effective temperature $T_{\text{eff}}$ is related to the temperature $T$ by

$$T_{\text{eff}}/T=(\hbar\omega/2T)\coth(\hbar\omega/2T). \quad (6.2)$$

For (5.16) we have thus for the cross section

$$\frac{\sigma}{\sigma_{\text{free}}}=1+\frac{T_{\text{eff}}}{2\mu E_0}\Big\{1-\frac{1}{16}\Big(\frac{\hbar\omega}{E_0}\Big)^2\Big\}. \quad (6.3)$$

The corresponding expressions for the differential cross sections and the moments of the energy transfer follow directly by insertion of (6.1) into the general formulas of the preceding section and will thus not be written down here.

For $T=0$, (6.3) goes over into

$$\frac{\sigma}{\sigma_{\text{free}}}=1+\frac{1}{4\mu n_0}\Big(1-\frac{1}{16n_0^2}\Big), \quad (6.4)$$

where $n_0=E_0/\hbar\omega$.

The asymptotic expression (6.4), valid for large $n_0$, may now be compared with the exact one. The transition probabilities are given by[2]

$$\phi_{0n}(\kappa^2)=a_s^{2}\xi^n\exp(-\xi)/n! \quad (6.5)$$

$$\xi=\hbar\kappa^2/2M\omega=P^2/2M\hbar\omega=y/\hbar\omega. \quad (6.5a)$$

Introduction of (6.5) into (3.1)–(3.3) yields

$$\frac{\sigma}{\sigma_{\text{free}}}=\frac{(\mu+1)^2}{4\mu n_0}\sum_{n=0}^{[n_0]}\{\Pi_n(\xi_n^{(-)})-\Pi_n(\xi_n^{(+)})\}, \quad (6.6)$$

where

$$\xi_n^{(\pm)}=(2/\mu)\{n_0-\tfrac{1}{2}n\pm[n_0(n_0-n)]^{\frac{1}{2}}\}$$

$$\Pi_n(x)=\frac{1}{n!}\int_x^\infty\xi^ne^{-\xi}d\xi=e^{-x}\sum_{l=0}^{n}\frac{x^l}{l!}$$

$$=1-\frac{x^{n+1}e^{-x}}{(n+1)!}\sum_{m=0}^{\infty}\frac{(n+1)!}{(n+m+1)!}xm. \quad (6.7)$$

Since for large $\mu$ the variation of the cross section with energy is a small effect, it is convenient to write the cross section in the form,

$$\frac{\sigma}{\sigma_{\text{free}}}=1+\frac{c(n_0)}{\mu n_0} \quad (6.8)$$

and discuss $c(n_0)$ rather than $\sigma$.

From (6.4) we have then

$$c(n_0)=\tfrac{1}{4}\{1-1/(4n_0)^2\} \quad (6.9)$$

while from (6.6)

$$c(n_0)=-\mu n_0+\frac{(\mu+1)^2}{2}\sum_{n=0}^{[n_0]}\{\Pi_n(\xi_n^{-})-\Pi_n(\xi_n^{+})\}. \quad (6.10)$$

Numerical comparison of these two expressions (see Fig. 1) shows, that for $\mu=12$ their difference becomes negligible at $n_0\approx4.2$ and in the limit of large $\mu$ already at $n_0\approx2$. Analytically, this may be seen as follows: Expanding (6.10) in powers of $1/\mu$,

$$c=c_0+c_1/\mu+c_2/\mu^2+\cdots, \quad (6.11)$$

one finds

$$c_0=\begin{cases}(2n_0-1)(n_0(n_0-1))^{\frac{1}{2}}-2n_0(n_0-1) & \text{for } n_0>1\\ 2n_0(1-n_0) & \text{for } n_0<1.\end{cases} \quad (6.12)$$

By expansion in powers of $1/n_0$, (6.12) goes over into (6.9). The quantities $c_n/\mu^n$ contribute asymptotically only to terms of higher order than (6.9) but reach their asymptotic form for $n_0\gg n$ only. Consequently, the deviations of (6.10) from (6.9) will extend to higher and higher $n_0$ as $\mu$ decreases. For $\mu=1$, $c(n_0)$ becomes, for large $n_0$, a periodic function of $n_0$, with period 1 and average $\frac{1}{4}$.[3,7]

[7] A. Messiah, J. phys. et radium **12**, 670 (1951).

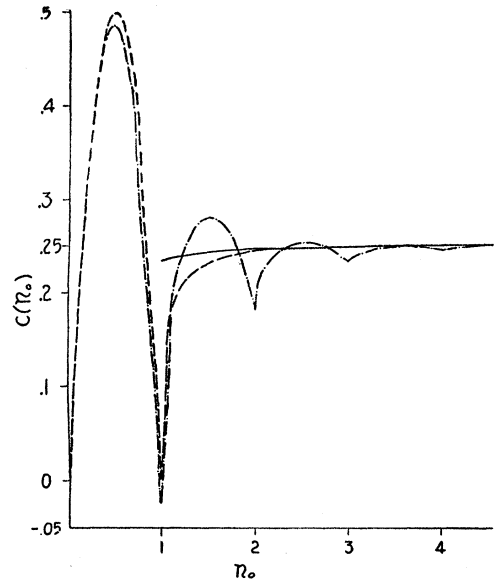


FIG. 1. The coefficient $c(n_0)$ in Eq. (6.8) for the cross section of isotropic oscillator at zero temperature; ———— asymptotic, Eq. (6.9); -·-·-·-·-·- $\mu=12$, Eq. (6.10); — — — — — $\mu=\infty$, Eq. (6.12).

It may also be noted that for the ground state of the oscillator the sums $S_l$ can be evaluated explicitly. From (6.5) and (3.10) we have for the restricted sums

$$S_l(\xi, n_0)=a_s^2 e^{-\xi}\sum_n^{[n_0]}(n^l/n!)\xi^n, \tag{6.13}$$

where $\xi$ is related to $\kappa^2$ and $y$ by (6.5a).

For $l=0$ (6.13) becomes with (6.7)

$$S_0(\xi, n_0)=a_s^2\Pi_{[n_0]}(\xi). \tag{6.14}$$

$S_l$ may be expressed in terms of $S_0$ by decomposing $n^l$ into binomial coefficients. In this way one finds

$$\begin{aligned}
S_1(\xi, n_0)&=\xi S_0(\xi, n_0-1)\\
S_2(\xi, n_0)&=\xi^2 S_0(\xi, n_0-2)+\xi S_0(\xi, n_0-1)\\
S_3(\xi, n_0)&=\xi^3 S_0(\xi, n_0-3)+3\xi^2 S_0(\xi, n_0-2)+\xi S_0(\xi, n_0-1)\\
S_4(\xi, n_0)&=\xi^4 S_0(\xi, n_0-4)+6\xi^3 S_0(\xi, n_0-3)\\
&\quad+7\xi^2 S_0(\xi, n_0-2)+\xi S_0(\xi, n_0-1).
\end{aligned} \tag{6.15}$$

If $S_0(\xi, n_0-j)$ is replaced by $S_0(\xi, \infty)=a_s^2$, (6.15) goes over into (5.6) which can also be checked by introducing (6.1) into (5.6). The derivatives of $S_l$ with respect to $\xi$ may also be expressed in terms of $S_0$ with the aid of the relation,

$$\xi S_l'=S_{l+1}-\xi S_0. \tag{6.16}$$

From (6.14) we have for the relative error in $S_0$ caused by the closure approximation

$$\delta_0=\frac{S_0(\xi, \infty)-S_0(\xi, n_0)}{S_0(\xi, \infty)}=1-\Pi_{[n_0]}(4\beta n_0/\mu), \tag{6.17}$$

where

$$\beta=\kappa^2/4k_0^2=\mu\xi/4n_0<1.$$

If $4\beta/\mu$ is small compared to one, which for large $\mu$ will be true for all values of $\beta$, (6.17) goes over into

$$\delta_0=\frac{1}{[n_0]+1)!}\left(\frac{4\beta n_0}{\mu}\right)^{[n_0]+1}\exp(-4\beta n_0/\mu). \tag{6.18}$$

For large $n_0$ we have, expressing $[n_0]$ by

$$[n_0]=n_0-1+\epsilon,$$

where $\epsilon$ varies between 0 and 1 and using Stirlings' formula,

$$\delta_0=(2\pi n_0)^{-\frac{1}{2}}(4\beta/\mu)^{\epsilon}\{(4\beta/\mu)\exp(1-4\beta/\mu)\}^{n_0}. \tag{6.19}$$

If $\mu$ is large, $\delta_0$ will thus decrease exponentially with increasing energy for all values of $\beta$.

If $4\beta/\mu$ is no longer small, we have to revert to the original expression (6.17). From the integral representation of $\Pi$ it is then seen that for $4\beta/\mu\geq 1$, $\delta_0$ does not vanish for large $n_0$, but tends to the limit $\frac{1}{2}$. A more detailed analysis, taking compensation effects into account, shows, however, that the closure correction to $c(n_0)$ decreases for all $\mu>1$ as $\exp(-\alpha n_0)$ where

$$\alpha=-q-\log(1-q),\quad q=[(\mu-1)/(\mu+1)]^2. \tag{6.20}$$

For $1-q\ll 1$, $\alpha=\log(4/\mu)-1$,

for $q\ll 1$, $\alpha=\frac{1}{2}[(\mu-1)/(\mu+1)]^4$.

## 7. SEVERAL NUCLEI

We now have to generalize the results of Sec. V to a system of $N$ nuclei with the Hamiltonian

$$H=V(\mathbf{r}_1, \mathbf{r}_2, \cdots\mathbf{r}_N)+\textstyle\sum_s p_s^2/2M_s. \tag{7.1}$$

At this stage it becomes necessary to consider the spin dependence of the scattering lengths. For a nucleus of spin $j_s$, the scattering length is given by[8]

$$\begin{aligned}
a_s=\frac{1}{2j_s+1}\{&(j_s+1)a_s^{(+)}+j_s a_s^{(-)}\\
&+2(\boldsymbol{\alpha}_n\cdot\boldsymbol{\alpha}_s)(a_s^{(+)}-a_s^{(-)})\}.
\end{aligned} \tag{7.2}$$

$a_s^{(+)}$ and $a_s^{(-)}$ are the scattering length associated with scattering processes leading to final states of the system nucleus plus neutron with spin $j_s+\frac{1}{2}$ and $j_s-\frac{1}{2}$, respectively, and $\boldsymbol{\alpha}_s$ and $\boldsymbol{\alpha}_n$ are the Pauli spin operators for nucleus and neutron.

Averaging over the orientations of the neutron spin, we have, with

$$\langle\boldsymbol{\alpha}_n\cdot\boldsymbol{\alpha}_s\rangle_{Av}=0;\quad\langle(\boldsymbol{\alpha}_n\cdot\boldsymbol{\alpha}_s)^2\rangle_{Av}=\tfrac{1}{4}j_s(j_s+1), \tag{7.3}$$

for the scattering cross section of the bound nucleus

$$\frac{\sigma_s}{4\pi}=\langle a_s^2\rangle_{Av}=\frac{1}{2j_s+1}\{(j_s+1)(a_s^{(+)})^2+j_s(a_s^{(-)})^2\}. \tag{7.4}$$

The definition of the matrix element (1.4) has now to be modified by inclusion of the spin coordinates. If the spins of different nuclei are not correlated—and this excludes homoeonuclear molecules at low temperatures, the averaging of (3.12) over position and spin coordinates may be carried out independently. As a consequence, the product $a_s a_{s'}$ has to be replaced by

$$\langle a_s a_{s'}\rangle_{Av}=\begin{cases}\langle a_s\rangle_{Av}\langle a_{s'}\rangle_{Av}=a_s^{(c)}a_{s'}^{(c)} & \text{for } s'\neq s\\ \langle a_s^2\rangle_{Av}=\sigma_s/4\pi & \text{for } s'=s,\end{cases} \tag{7.5}$$

where the coherent scattering length $a_s^{(c)}$ is defined by

$$a_s^{(c)}=\langle a_s\rangle_{Av}=\frac{1}{2j_s+1}\{(j_s+1)a_s^{(+)}+j_s a_s^{(-)}\} \tag{7.6}$$

and $\langle a_s^2\rangle_{Av}$ is given by (7.4).

[8] M. Hamermesh and J. Schwinger, Phys. Rev. **69**, 145 (1945).

The cross section (1.1) and the differential cross sections may then be written as a sum of two parts which are usually denoted as the coherent and the incoherent cross section. The coherent cross section is obtained by replacing $a_s$ with $a_s^{(c)}$ throughout, while in the incoherent cross section the product terms with $s' \neq s$ are omitted and $a_s^2$ is replaced by

$$\langle a_s^2\rangle_{Av} - (\langle a_s\rangle_{Av})^2 = \frac{j_s(j_s+1)}{2j_s+1}(a_s^{(+)} - a_s^{(-)})^2.$$

The expressions of Sec. V for the total and the differential cross sections of a system containing a single nucleus will thus directly represent the incoherent cross section of a system of several nuclei with uncorrelated spins, if $\sigma_{\text{free}}$ is replaced by the incoherent cross section $\sigma_{fs}^{(i)}$ of a free nucleus at rest

$$\sigma_{fs}^{(i)} = 4\pi\left(\frac{\mu_s}{\mu_s+1}\right)^2 \frac{j_s(j_s+1)}{2j_s+1}(a_s^{(+)} - a_s^{(-)})^2. \quad (7.7)$$

The averages entering these expressions are then to be taken for nucleus $s$ and, in particular, the differentiations in the definitions (5.8) and (5.9) of $B$ and $C$ with respect to the coordinates of nucleus $s$. For the total incoherent scattering cross section we have thus

$$\sigma^{(i)} = \sum_s \sigma_{fs}^{(i)}\left\{1 + \frac{1}{3}\frac{\langle K_s\rangle_{Av}}{\mu_s E_0} - \frac{1}{32}\frac{\langle C_s\rangle_{Av}}{\mu_s E_0^3}\right\}. \quad (7.8)$$

As an example let us consider a Debye crystal containing a single type of nuclei. One has then

$$\begin{aligned} K_{Av} &= \frac{36T^4}{\Theta^3}\int_0^{\Theta/2T} x^3 \coth x\,dx \\ B_{Av} &= \tfrac{3}{5}\Theta^2 \\ C_{Av} &= \frac{96T^6}{\Theta^3}\int_0^{\Theta/2T} x^5 \coth x\,dx \\ \langle K^2\rangle_{Av} &= (5/3)(K_{Av})^2, \end{aligned} \quad (7.9)$$

where $\Theta$ is the Debye temperature.

For $T \ll \Theta$

$$\begin{aligned} K_{Av} &= \frac{9}{16}\Theta\left\{1 + \frac{8}{15}\left(\frac{\pi T}{\Theta}\right)^4\right\} \\ C_{Av} &= \frac{1}{4}\Theta^3\left\{1 + \frac{32}{21}\left(\frac{\pi T}{\Theta}\right)^6\right\} \end{aligned} \quad (7.10)$$

for $T \gg \Theta$

$$\begin{aligned} K_{Av} &= \frac{3}{2}T\left\{1 + \frac{1}{20}\left(\frac{\Theta}{T}\right)^2\right\} \\ C_{Av} &= \frac{3}{5}T\Theta^2\left\{1 + \frac{5}{84}\left(\frac{\Theta}{T}\right)^2\right\}. \end{aligned} \quad (7.11)$$

The incoherent cross section per nucleus becomes then

$$\frac{\sigma^{(i)}}{\sigma_{\text{free}}^{(i)}} = 1 + \frac{K_{Av}}{3\mu E_0}\left\{1 - \frac{\nu}{24}\left(\frac{\Theta}{E_0}\right)^2\right\}. \quad (7.12)$$

The coefficient $\nu$ depends but little on the temperature; it decreases from $\nu=1$ for $T \ll \Theta$ to $\nu = 9/10$ for $T \gg \Theta$. For heavy nuclei (7.12) will hold as soon as the neutron energy is slightly larger than the Debye temperature. In the effective differential cross section the direct binding effect is somewhat larger as a result of the presence, in the first line at (5.20), of the term containing $B_{Av}$ which at low temperatures and $E_0 = 2\Theta$ amounts to twenty percent of the Doppler term.[9]

Returning now to the general problem it will be convenient to abandon the customary division of the cross section into a coherent and an incoherent part. Instead, we shall distinguish between diagonal terms ($s=s'$) and interference terms ($s \neq s'$). The diagonal terms are represented by the results of Sec. V,[10] so that we only have to calculate the interference terms. For this purpose we express the quantities $S_n$ by

$$S_n = \sum_s \langle a_s^2\rangle_{Av} G_n^{(ss)} + \sum{}'_{ss'} a_s^{(c)} a_{s'}^{(c)} G_n^{(ss')}. \quad (7.13)$$

$G_n^{(ss)}$ is given by (5.6). For $G_n^{(ss')}$ we have from (3.12) with the notation

$$\begin{aligned} f_s &= \exp(i\boldsymbol{\kappa}\cdot\mathbf{r}_s) = \exp(iPz_s/\hbar), \\ G_0^{(ss')} &= \langle f_{s'}^* f_s\rangle_{Av} = \left\langle \frac{\sin\kappa r_{ss'}}{\kappa r_{ss'}}\right\rangle_{Av} \\ G_1^{(ss')} &= \langle f_{s'}^*[Hf_s]\rangle_{Av} \\ G_2^{(ss')} &= \langle [f_{s'}^* H][Hf_s]\rangle_{Av} \\ G_3^{(ss')} &= \langle [f_{s'}^* H][H[Hf_s]]\rangle_{Av}. \end{aligned} \quad (7.14)$$

[9] The statements made so far on the basis of the usual theory of neutron scattering by crystals [J. M. Cassels, *Progress in Nuclear Physics*, Vol. I (edited by O. R. Frisch, London-New York, 1950)] about the behavior of the cross section at high energies are either entirely erroneous because of inconsistent approximations [R. Weinstock, Phys. Rev. **65**, 1 (1944); R. J. Finkelstein, Phys. Rev. **72**, 907 (1947)], or very incomplete. [A. Akhiezer and I. Pomeranchuk, J. Phys. (U.S.S.R.) **11**, 167 (1947); D. A. Kleinman, thesis, Brown University (1951).] Akhiezer and Pomeranchuk have given an integral representation of the cross section. From its discussion they conclude that the neutron energy, at which the direct binding effects in the cross section become negligible, is determined by a condition which is essentially identical with Eq. (2.2) rather than (2.3) and which is therefore much too restrictive. Furthermore, their treatment leads to the same energy dependence for coherent and incoherent cross section at high energy. Actually, however, the derivatives of these two quantities with respect to the energy have opposite sign at high energy. The evaluation of the asymptotic interference term (7.21) for crystals [Placzek, Nijboer, and Van Hove, Phys. Rev. **82**, 392 (1951)] shows that this term, which has negative sign, is for heavy nuclei of considerably larger size than the Doppler term. At high energy therefore the coherent cross section increases with increasing energy, in contrast to the incoherent cross section which decreases with increasing energy.

[10] Adding the diagonal terms of the coherent cross section to the expressions (7.8) for the incoherent cross section is equivalent to replacing $\sigma_{fs}^{(i)}$ by the total free cross section $\sigma_{fs}$.

The commutation relations of $f_s$ with the Hamiltonian (7.1) are identical with (5.4)–(5.5),

$$[Hf_s]=\frac{P}{M_s}f_s(\tfrac{1}{2}P+p_{sz}) \tag{7.15}$$

$$[H[Hf_s]]=\frac{P}{M_s}f_s\left\{-\frac{h}{i}\frac{\partial V}{\partial z_s}+\frac{P}{M_s}(\tfrac{1}{2}P+p_{sz})^2\right\}. \tag{7.16}$$

With the aid of the relation

$$\langle f_sf_{s'}{}^*(\tfrac{1}{2}P+p_{sz})\rangle_{\text{Av}}=\langle f_sf_{s'}{}^*(\tfrac{1}{2}P-p_{s'z})\rangle_{\text{Av}}=0 \quad \text{for} \quad s\neq s'$$

obtained through integration by parts, one finds from (7.14) and (7.15):

$$G_1{}^{(ss')}=0 \tag{7.17}$$

$$G_2{}^{(ss')}=\frac{P^4}{4M_sM_{s'}}G_0{}^{(ss')}+\frac{\hbar^2}{M_sM_{s'}}\langle\exp(i\boldsymbol{\kappa}\cdot\mathbf{r}_{ss'})(\mathbf{p}_s\cdot\boldsymbol{\kappa})(\mathbf{p}_{s'}\cdot\boldsymbol{\kappa})\rangle_{\text{Av}}. \tag{7.18}$$

From (7.17) it follows that the first-order reduced mass correction does not apply to the interference terms. The second term in (7.18) is the analog of the Doppler term encountered previously and represents an effect caused by the correlation of the momenta of different nuclei. In classical statistics there is no such correlation and the term will thus vanish at high temperatures.

In a diatomic molecule, for example, the translational momenta of the two nuclei are fully correlated and the momenta of relative motion fully anticorrelated. At high temperatures, when the relative motion is fully excited, these two effects cancel out while at low temperatures the negative correlation prevails. The result of the evaluation of the term for a particular case will be given in the discussion of the cross sections; now let us just consider the average of the product of the momenta alone.

Expressing the momenta $\mathbf{p}_1$ and $\mathbf{p}_2$ of the nuclei in a diatomic molecule by the momentum $\mathbf{p}_c$ of the center of gravity and the momentum $\mathbf{p}$ of relative motion, we have

$$\mathbf{p}_1=\frac{M_1}{M_1+M_2}\mathbf{p}_c+\mathbf{p}, \quad \mathbf{p}_2=\frac{M_2}{M_1+M_2}\mathbf{p}_c-\mathbf{p},$$

$$(\mathbf{p}_1\cdot\mathbf{p}_2)_{\text{Av}}=\frac{M_1M_2}{(M_1+M_2)^2}\langle p_c{}^2\rangle_{\text{Av}}-\langle p^2\rangle_{\text{Av}}=2M_r(E_t-E_i),$$

where $E_t$ and $E_i$ are the average kinetic energies of translation and internal motion. At high temperatures $E_i=E_t=\frac{3}{2}T$; at low temperatures, $T\ll\hbar\omega$, $E_t-E_i=-\hbar\omega/4+T/2$ or $-\hbar\omega/4+3T/2$ according to whether the temperature is large or small compared to the rotational quanta.

For $G_3$ one finds

$$G_3{}^{(ss')}=\frac{P^2}{M_s}G_2{}^{(ss')}+\frac{P^2}{M_sM_{s'}}\left\langle f_sf_{s'}{}^*\left\{\frac{\hbar^2}{2}\frac{\partial^2V}{\partial z_s\partial z_{s'}}+\frac{P}{M_s}p_{sz}{}^2(p_{s'z}-\tfrac{1}{2}P)\right\}\right\rangle_{\text{Av}}. \tag{7.19}$$

The expression for $G_4$ is longer and will not be given here. The discussion of the higher approximations in the preceding sections was necessary mainly to gain clear insight into the structure of the theory. This having been achieved we can limit ourselves, in the discussion of the interference effects, to the terms represented by $S_0$, $S_1$, and $S_2$. In this approximation one finds from (3.11) for the contribution of the interference terms to the cross section

$$\sigma_{\text{int}}=8\pi\sum_{s,s'}^{s'<s}a_s{}^{(c)}a_{s'}{}^{(c)}\left\{\frac{1}{2k_0{}^2}\left\langle\frac{1}{r_{ss'}{}^2}\right\rangle_{\text{Av}}-\frac{1}{2k_0{}^2}\left\langle\frac{\cos2k_0r_{ss'}}{r_{ss'}{}^2}\right\rangle_{\text{Av}}+\frac{\langle 2k_0z_{ss'}\sin2k_0z_{ss'}v_{sz}v_{s'z}\rangle_{\text{Av}}}{v_0{}^2}+\frac{1}{\mu_s\mu_{s'}}\left\langle\frac{\sin2k_0r_{ss'}}{2k_0r_{ss'}}+\cos2k_0r_{ss'}\right\rangle_{\text{Av}}\right\}. \tag{7.20}$$

Here $v_0$ denotes the neutron velocity, and $v_{sz}$ and $v_{s'z}$ components of the nuclear velocities; $z_{ss'}$ stands for $\mathbf{r}_{ss'}\cdot\mathbf{k}_0/k_0$ and $v_{sz}$ for $\mathbf{v}_s\cdot\mathbf{k}_0/k_0$. It will of course be kept in mind that the quantities $v_{sz}$ and $v_{s'z}$ do not commute with $z_{ss'}$. The first two terms in (7.20) represent the static approximation and the rest the corrections resulting from $G_2$. At high temperatures the third term vanishes. For short neutron wavelength all the terms except the first one are not only rapidly fluctuating but also their magnitude goes to zero with decreasing wavelength.[11] The cross section is then represented by

$$\sigma_{\text{int}}=\frac{4\pi}{k_0{}^2}\sum_{s,s'}^{s'<s}a_s{}^{(c)}a_{s'}{}^{(c)}\langle r_{ss'}{}^{-2}\rangle_{\text{Av}}. \tag{7.21}$$

The wavelength at which (7.20) goes over into (7.21) depends upon the nature of the scattering system and its determination requires rather careful considerations.[12]

Introducing (7.13) and (7.18) into (4.7) or (4.9), one obtains simple but somewhat lengthy expressions for the contribution of the interference terms to the differential cross section. In an abbreviated form they may be written as follows:

$$\left(\frac{d\sigma_{\text{int}}}{d\Omega}\right)_{\text{eff}}=\varphi_0+\left\{(1-2\beta)\frac{\partial}{\partial\beta}+2\beta^2\frac{\partial^2}{\partial\beta^2}\right\}(\beta\varphi_1+\beta^2\varphi_2) \tag{7.22}$$

$$\frac{d\sigma_{\text{int}}}{d\Omega}=\left(\frac{d\sigma_{\text{int}}}{d\Omega}\right)_{\text{eff}}+2\left(-1+2\beta\frac{\partial}{\partial\beta}\right)(\beta\varphi_1+\beta^2\varphi_2), \tag{7.23}$$

[11] This also holds for systems with long-range order; see reference 12.

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

where $\beta=\sin^2\frac{1}{2}\theta$. The quantities $\varphi_n$ are functions of $\kappa_0^2=4k_0^2\beta$

$$\varphi_0=2\sum_{s,s'}^{s'<s} a_s^{(c)}a_{s'}^{(c)}\left\langle\frac{\sin\kappa_0 r_{ss'}}{\kappa_0 r_{ss'}}\right\rangle_{\text{Av}}$$

$$\varphi_1=2\sum_{s,s'}^{s'<s} a_s^{(c)}a_{s'}^{(c)}\langle\cos\kappa_0 z_{ss'}v_{sz}v_{s'z}\rangle_{\text{Av}}/v_0^2$$

$$\varphi_2=2\sum_{s,s'}^{s'<s}\frac{a_s^{(c)}}{\mu_s}\frac{a_{s'}^{(c)}}{\mu_{s'}}\left\langle\frac{\sin\kappa_0 r_{ss'}}{\kappa_0 r_{ss'}}\right\rangle_{\text{Av}}.$$

For a diatomic molecule the differential cross sections may be expressed in terms of functions simply related to the error function of complex argument; if, in particular, the effective wavelength $1/\kappa_0$ is large compared to the vibrational amplitude the evaluation of $\varphi_0$ and $\varphi_2$ is trivial and for $\varphi_1$ one then finds for temperatures large compared to the rotational quanta

$$\varphi_1=2a_1^{(c)}a_2^{(c)}\langle(\cos\kappa_0 z_{12})v_{1z}v_{2z}\rangle_{\text{Av}}/v_0^2=$$
$$-a_1^{(c)}a_2^{(c)}\frac{(E_{\text{vib}}-T)}{3(\mu_1+\mu_2)E_0}\left(\frac{\pi}{2\kappa_0 r_0}\right)^{\frac{1}{2}}$$
$$\times\{J_{1/2}(\kappa_0 r_0)-2J_{5/2}(\kappa_0 r_0)\}. \quad (7.24)$$

Here $r_0$ is the equilibrium distance of the nuclei and $E_{\text{vib}}$ the average total vibrational energy. (7.24) provides a simple example for the structure of momentum correlation term. For $T\gg\hbar\omega$, $E_{\text{vib}}-T=0$ and $\varphi_1$ vanishes.

### 8. APPLICATIONS

The isolation of small electronic contributions to the scattering cross section, which may be caused by ordinary magnetic effects,[13,14] scattering by spin waves[15] and the spin-independent interaction between neutron and electron[16,14] requires a very precise theoretical determination of the dependence of the nuclear scattering on neutron energy or scattering angle. Off hand this may seem too pretentious a task if the scattering system is as complex as in the transmission experiments of Rainwater, Rabi, and Havens on liquid bismuth.[17] On the basis of the results derived above, however, it can be approached with reasonable assurance. The characteristic temperature of liquid Bi, corresponding to the Debye temperature of a solid, is of the order of 100 degrees abs. The expressions (5.16) and (7.20) for the cross section will thus be valid for neutron energies large compared to $10^{-2}$ ev. Since $\mu=209$, the last term in (7.20), which is quadratic in the mass ratio, may be neglected. Since the melting temperature is 544 degrees abs and thus large compared to the characteristic temperature, the effect of the correlation of the momenta, given by the third term in (7.20) disappears, while in the second term of (5.16) $K_{\text{Av}}=3T/2$. With a slight modification[18,12] of the first two terms of (7.20) which is equivalent to neglecting deflections by an angle $k_0^2d^2$, where $d$ is of the order of the total linear dimensions of the scattering system, the scattering cross section per nucleus is thus given by

$$\sigma=\sigma_{\text{free}}\left\{1+\frac{T}{2\mu E_0}\left(1-\frac{C_{\text{Av}}}{16TE_0^2}\right)\right\}$$
$$-\sigma_{\text{coh}}\frac{2\pi}{k_0^2}\int_0^\infty(1-\cos 2k_0 r)\{\rho-g(r)\}dr. \quad (8.1)$$

Here $\sigma_{\text{free}}$ is, as before, the total scattering cross section of the free nucleus at rest and $\sigma_{\text{coh}}=4\pi(a_s^{(c)})^2$ the coherent cross section of the bound nucleus; $g(r)$ is the density at distance $r$ from a given nucleus and $\rho$ the ordinary density. The evaluation of the interference term in (8.1) has been carried out by Placzek, Nijboer, and Van Hove.[12] The third term in (8.1) depends on the average square of the force acting on the nucleus which cannot be calculated precisely for a liquid. Even the crudest estimates, however, are sufficient to show that at the relevant neutron energies this term cannot amount to more than a fraction of the Doppler term.

The discussion of the electronic contributions to the cross section has, in part, been given previously.[14,16] For an isolated rare gas atom paramagnetic scattering is absent and diamagnetic scattering negligible.[14] For liquid bismuth, on the other hand, the ordinary magnetic effects are hardly accessible to a satisfactory theoretical analysis. Although they do not interfere with the nuclear scattering the possibility that they might be of relevant size can by no means be excluded *a priori*. Since they are entirely caused by the outer electrons, however, their energy dependence will differ from that of the contribution of the spin-independent neutron-electron interaction which comes from all the electrons. The energy dependence of the latter has been calculated on the basis of the ordinary form factor.[16] Its isolation would thus seem to require a study of the variation with energy of the difference between the observed cross section and (8.1).

Among other applications of results derived here, the problem of the energy dependence and angular distribution of neutron scattering by heavy molecules might in particular be mentioned. The theory in the form developed here is valid for neutron energies large compared to the vibrational quanta, while many of the

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experiments[19,20] carried out so far concern neutron energies large compared to the rotational but small compared to the vibrational quanta. In order to extend the theory to this region the Hamiltonian (7.1) is replaced by the Hamiltonian of a rigid molecule. The results for the diagonal terms obtained in this way agree for high temperatures with the semiclassical mass tensor approximation[21] and differ from it for low temperatures to which it is not directly applicable. In addition one obtains the interference terms which are not given by the mass tensor approximation and which are particularly important for the angular distribution. The discussion of these results and their comparison with the experiments and with the approximation of Alcock and Hurst[20] will be given in a separate paper.

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# Triton Binding Energy by a Randomized Net-Point Method*

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A numerical procedure is investigated for solving Schrödinger's equation for a system of particles. A net-point analysis is applied directly to the integral equation equivalent to Schrödinger's equation. A unique feature is the introduction of the concept of a "randomized" net of points. This is designed to cope with the problem of obtaining adequate covering of the space when many dimensions are involved.

The method is applied to the problem of finding the binding energy of the triton with the assumption of central forces. The result obtained for an exponential potential as determined by the most recent low energy scattering data is approximately 10 percent too deep. It may be concluded that more effective repulsion must be introduced into the "equivalent central potential" to bring about agreement with experiment.

## I. THE RANDOMIZED NET-POINT PROCEDURE

A NUMERICAL net-point procedure for solving Schrödinger's equation has been investigated with special regard towards finding the lowest (ground state) eigenvalue for a system of three (or more) particles. The spin-free time independent Schrödinger equation for a system of particles may generally be written as

$$(\Delta-k^2)\psi=V\psi \tag{1}$$

and can be transformed into an equivalent integral equation by means of the appropriate Green's function $G(P, Q)$. Thus,

$$\lambda\psi(P)=-\int dQG(P, Q)V(Q)\psi(Q), \tag{2}$$

where $P$ is a point in an arbitrary $n$-dimensional space. If $V$ is an attractive well, than the largest eigenvalue $\lambda_0$ corresponds to the binding energy of the system. The integral may be replaced by a sum over a discrete set of $N$ points $P_i$ yielding

$$\lambda\psi(P_i)=\sum_{j=1}^{N}\Delta Q_jG(P_i, Q_j)V(Q_j)\psi(Q_j), \tag{3}$$

where $\Delta Q_j$ is the volume element associated with the point $Q_j$.

Because the number of dimensions $n$ may in general become large, the following unique manner of selecting the points $P_i$ was introduced: Consider the set of $N$ equally spaced points in each dimension. From each such set, choose a point at random; the aggregate of $n$ of these taken together constitutes a single point $P_i$ in $n$-dimensional space. This process is repeated with the remaining points until they are all exhausted. The final result is a set of $N$ points in $n$-dimensional space.

The purpose of this mode of selection is to afford some compromise between the desires of having the points $P_i$ equally spaced throughout the volume and of having the points randomly distributed throughout the volume. The latter desideratum is suggested by a random sampling procedure (Monte Carlo) for evaluating a multi-dimensional integral. It should be noted that the prescribed procedure selects points which are equally probable from the random sampling point of view. An advantage of randomly spacing the points is that it maximizes the number of coordinates chosen in each dimension.

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