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SCATTERING THEORY IN THE IMPULSE APPROXIMATION

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A new formulation of the impulse approximation method is presented which differs from the original one by greater simplicity (the cross section for the scattering of an incident particle by a complex system is represented in the form of a certain average over its initial state; the cross section for the transition of the system to a given final state is described under certain additional assumptions by a formula which is a generalization of the Fermi pseudopotential method to the case of arbitrary pair interactions). The general method is used to calculate the resonance (Breit-Wigner) scattering of neutrons by chemically bound atoms in the case of sufficiently broad resonances.

1. INTRODUCTION

THE impulse approximation which was first introduced in the papers by Chew et al[1-2], who applied it to the problem of the collision of fast nucleons with nuclei, is based on the following assumptions about the nature of the interaction between the incident particle (treated as structureless) with a complex system of bound particles.

First, it is assumed that the effective radius of interaction of the incident particle with the particles of the scattering system A is much smaller than the average distance R between them: $A \ll R$, while the interaction itself between the incident particle and one of the particles of the system in the region A is considerably stronger than the interaction between the particles of the system, i.e., the potential V for the interaction between the scattered particle and the complex system may be regarded as a pair interaction, i.e., $V = \sum_{\nu=1}^{N} V_\nu(\mathbf{r}_\nu - \mathbf{r})$ (N is the number of particles in the system, $\mathbf{r}_\nu$ are their coordinates, $\mathbf{r}$ are the coordinates of the incident particle). Such a situation, obviously, occurs, in particular, if the energy of the incident particle is so great that the latter can approach the particles of the system so that the separation distances become very small.

The second assumption consists of supposing that the time characterizing the pair interaction τ is so small that the interaction between the bound particles does not have time to manifest itself significantly, i.e., $\tau \ll 1/\omega$ ($1/\omega$ is the time needed for a significant change in the state of the system).

These considerations enable us to represent the probability amplitude A_{fi} for the transition of the scattering system from the state Φ_i into the state Φ_f in the following manner[1]:

$$A_{fi}^{imp} = -\frac{m}{2\pi h^2}\int \Phi_f^*(\xi)\, e^{-i\mathbf{k}'\mathbf{r}} V(\mathbf{r}, \xi)\, \Psi_i^{imp}\, d\mathbf{r}\, d\xi, \quad (1)$$

where m is the mass of the incident particle, k′ is the wave number for the incident particle in the final state, ξ are the coordinates of the scattering system;

$$\Psi_i^{imp} = \psi_{\mathbf{kq}}\, G(\mathbf{q})\, d\mathbf{q},$$

$\psi_{\mathbf{kq}}$ is the wave function describing the scattering of the incident particle with momentum $h\mathbf{k}$ by a free particle of the system having momentum $h\mathbf{q}$, $G(\mathbf{q})$ is the wave function of the scattering system in the impulse approximation. The superiority of the impulse approximation over the Born approximation consists, evidently, in rigorously taking into account the form of the pair interaction V_ν (in the sense that no assumption is made about it having to be small).

The present paper consists of a further development of the method of impulse approximation in two directions.

1. An expression is obtained for the differential cross section for the scattering of an incident particle into a certain angular range $d\omega$ and a certain energy range $d\epsilon$ in terms of an average over the initial state of the scattering system Φ_i:

$$d^2\sigma/d\varepsilon d o = \langle \Phi_i, T^{imp}\Phi_i\rangle,$$

where T^{imp} is a certain combination of operators

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[1] For the sake of simplicity we consider scattering by only a single particle of the system.

which involves the Hamiltonian of the system H and the amplitudes for the pair scattering. This result is obtained by summing over all the states of the system by means of a method analogous to that utilized by Zemach and Glauber[3]. Thus, in order to obtain $d^2\sigma/d\epsilon\, do$ it turns out to be possible to avoid explicit use of the wave functions for the final states Φ_f.

2. For the case when the amplitudes for pair scattering vary but little within the limits of the momentum spread of the particles of the scattering system it turns out to be possible to represent the quantities A_{fi}^{imp} in an even simpler form than (1), viz., in the form of the Born approximation with a certain altered potential defined in terms of the amplitudes for pair scattering. Thus, the Fermi pseudopotential method can be generalized, provided the conditions for the applicability of the impulse approximation are satisfied, to pair interactions of arbitrary type.

2. GENERAL FORMULATION OF THE IMPULSE-APPROXIMATION METHOD

In subsequent discussion we shall employ the apparatus of the formal scattering theory in accordance with which the probability for the transition of a scattering system per unit time is given by the following expression (in subsequent development we use the system of units in which h = 1):

$$P_{fi} = 2\pi\,|T_{fi}|^2\,\delta\,(\varepsilon_i - \varepsilon_f + k^2/2m - k'^2/2m), \tag{2}$$

where

$$T_{fi} = (\Psi_f T \Psi_i), \qquad \Psi_f = e^{i\mathbf{k}'\mathbf{r}}\Phi_f, \qquad \Psi_i = e^{i\mathbf{k}\mathbf{r}}\Phi_i \tag{3}$$

and the scattering operator T is defined by the equation

$$T = V + V\,(E - H' + i\eta)^{-1}\,V, \qquad H' = K + U + V, \tag{4}$$

K is the operator for the kinetic energy of all the N+1 particles, U is the energy of interaction of N particles of the system, η is an adiabatic parameter which is made to go to zero in all the final formulas.

In accordance with the basic assumptions of the impulse approximation the operator T may be represented in the form of the following expansion:

$$T = T_0 + T_1 + T_2 + \ldots; \qquad T_0 = \sum_{\nu=1}^{N} t_\nu,$$

$$T_1 = \sum_{\nu=1}^{N} t_\nu\,(\varepsilon_k - K + i\eta)^{-1}\,(\varepsilon_k - \varepsilon_i + U)\,(\varepsilon_k - K + i\eta)^{-1}\,t_\nu,$$

$$T_2 = \sum_{\substack{\nu,\,\nu' \\ \nu\neq\nu'}}^{N} t_\nu\,(\varepsilon_k - K + i\eta)^{-1}\,t_{\nu'}, \tag{5}$$

where

$$t_\nu = V_\nu + V_\nu\,(\varepsilon_k - K - V_\nu + i\eta)^{-1}\,V_\nu. \tag{6}$$

The impulse approximation corresponds to the replacement of T by $\sum_{\nu=1}^{N} t_\nu$; the second and the third terms in the expansion (5) characterize in the lowest order approximation respectively the effect of binding between particles of the scattering system and multiple (double) scattering of the incident particle by the particles of the system.

We substitute (5) into (3). After integration over $\mathbf{r}$ the operators in (3) acquire the meaning of quantities related to the amplitudes for the scattering of free particles and corrections to these amplitudes. Indeed, the matrix element (3), after T is replaced in it by $\sum_\nu t_\nu$ contains integrals of the form

$$\int \langle \Phi_f,\, e^{-i\mathbf{k}'\mathbf{r}}\, t_\nu e^{i\mathbf{k}\mathbf{r}}\,\Phi_i\rangle\, d\mathbf{r}$$

$$= \frac{1}{(2\pi)^{3N}} \int\!\ldots\!\int d\mathbf{p}_1', \ldots, d\mathbf{p}_N'\,\Phi_f\,(\mathbf{p}_1', \ldots, \mathbf{p}_N')\,(\chi_{\mathbf{k}'\mathbf{p}'} t_\nu \chi_{\mathbf{k}\mathbf{p}})$$

$$\times\, \Phi_i\,(\mathbf{p}_1, \ldots, \mathbf{p}_N)\, d\mathbf{p}_1, \ldots, d\mathbf{p}_N, \tag{7}$$

where $\mathbf{p}_1, \ldots, \mathbf{p}_N$ are the momenta of the bound particles, $\chi_{\mathbf{kp}} = \chi_{\mathbf{k},\mathbf{p}_1,\ldots,\mathbf{p}_N}$ are the eigenfunctions of the kinetic energy operator for all the particles; by definition

$$(2\pi)^{-3N}\,(\chi_{\mathbf{k}'\mathbf{p}'},\, t_\nu \chi_{\mathbf{k}\mathbf{p}}) = \delta\,(\mathbf{p}_1' - \mathbf{p}_1)\ldots\delta\,(\mathbf{k}' + \mathbf{p}_\nu' - \mathbf{k} - \mathbf{p}_\nu)$$

$$\times\, F\,(\mathbf{k}_\nu', \mathbf{k}_\nu)\ldots\delta\,(\mathbf{p}_N' - \mathbf{p}_N)\, 2\pi/\mu_\nu,$$

where $\mathbf{k}_\nu$ and $\mathbf{k}_\nu'$ are the relative momenta of the colliding particles before and after scattering, μ_ν is their reduced mass; $F(\mathbf{k}_\nu', \mathbf{k}_\nu)$ is the amplitude for the elastic scattering of free colliding particles in the center of mass system.

Thus, as a result of integration over $\mathbf{r}$ in (7) we have

$$t_\nu^{fi} = \int \langle \Phi_f,\, e^{-i\mathbf{k}'\mathbf{r}}\, t_\nu e^{i\mathbf{k}\mathbf{r}}\Phi_i\rangle\, d\mathbf{r} = \frac{2\pi}{\mu_\nu}\,\langle \Phi_f,\, e^{i\varkappa\mathbf{r}_\nu}\, F\,(\mathbf{k}_\nu', \mathbf{k}_\nu)\,\Phi_i\rangle, \tag{8}$$

where $\kappa = \mathbf{k} - \mathbf{k}' = \mathbf{k}_\nu - \mathbf{k}_\nu'$ is the momentum transferred to the scattering system during the collision,

$$\mathbf{k}_\nu = (m\mathbf{k} - m\mathbf{p}_\nu)/(m_\nu + m),$$

$$\mathbf{k}_\nu' = (m_\nu \mathbf{k}' - m\,(\varkappa - \mathbf{p}_\nu))/(m_\nu + m). \tag{9}$$

Taking (8) into account we now represent the expression for the probability of process (2) in the following form

$$P_{fi} = 2\pi \sum_{\nu\nu'} (\Phi_i,\, F_{\nu'}^{*} e^{-i\varkappa\mathbf{r}_{\nu'}}\Phi_f)\,(\Phi_f, e^{i\varkappa\mathbf{r}_\nu} F_\nu \Phi_i)\,\delta\,(\varepsilon + \varepsilon_i - \varepsilon_f). \tag{10}$$

Further, by utilizing the well known representation for the δ-function:

$$\delta(\gamma) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\gamma t}\, dt,$$

by taking into account the fact that $\exp(-iHt)\Phi_i = \exp(-i\epsilon_i t)\Phi_i$, and by summing over all the system states forming the complete set of wave functions Φ_f, we obtain the following expression for the differential cross section

$$d^2\sigma/d\varepsilon do = \langle \Phi_i, T^{imp} \Phi_i \rangle,$$

$$T^{imp} = \frac{k'}{k} \sum_{\nu\nu'} \frac{m^2}{\mu_\nu \mu_{\nu'}} \int_{-\infty}^{\infty} e^{-i\varepsilon t} F^*_{\nu'} e^{-i\varkappa \mathbf{r}_{\nu'}} e^{iHt} e^{i\varkappa \mathbf{r}_\nu} F_\nu e^{-iHt}\, dt. \tag{11}$$

Thus, in the impulse approximation in addition to the representation (1), in which states of the system before and after scattering are given, one can also introduce the representation (11) in which, in addition to the initial state of the system only the characteristics of pair scattering are given. Expression (11) does not require an explicit definition of the wave functions of the final state. Moreover, writing the cross section $d^2\sigma/d\epsilon\, do$ in the form of an average over the state presents a number of mathematical conveniences. Formula (11) will be utilized later (Sec. 4) for investigating the interaction of neutrons with chemically bound nuclei in the case when the pair scattering amplitudes F_ν are of a Breit-Wigner resonance character.

The conditions for the applicability of (11) can be established by substituting into (3) the correction operators T_1 and T_2 [cf., (5)] and by repeating the same arguments as were used in deriving (7) and (8). Thus, it turns out to be possible to represent the corrections to the formulas of the impulse approximation by taking binding into account in the scattering system (the operator T_1) in a simpler form than in the papers by Chew et al.[2] Specifically, they are determined directly by the pair scattering amplitudes F_ν and are of the order of $\Delta\epsilon_\nu d \ln F_\nu/dE$, where $\Delta\epsilon_\nu$ is a certain effective energy difference between the levels of the scattering system manifested in a collision with its ν-th particle (for example, the energy difference between vibrational levels of the molecule).

The condition for the applicability of the impulse approximation associated with neglecting the binding of the particles of the system can, consequently, be represented in the form

$$\Delta\varepsilon_\nu \,|\, d\ln F_\nu/dE \,| \ll 1. \tag{12}$$

Under quasiclassical conditions $F_\nu = B_\nu \times \exp iS(k_\nu, k_{\nu'})$, where $S \approx A_\nu k \gg 1$, A_ν is the effective radius of interaction between the colliding particle; therefore in this case $d \ln F_\nu/dk \approx A_\nu$. In a similar manner, in the case of scattering of slow particles (S-scattering) we obtain $d \ln F_\nu/dk \approx A_\nu$. Therefore, we can also rewrite (12) in the form

$$\Delta\varepsilon_\nu A_\nu / h v_{n\nu} \ll 1, \tag{13}$$

where $v_{n\nu}$ is the relative velocity of the colliding particles. It is essential to note that in the case when the effective speed of a bound particle exceeds significantly the speed of the incident particle v_n, the quantities $\Delta\epsilon_\nu$ turn out themselves to depend on v_n, and in such a way that condition (13) is satisfied only for sufficiently large v_n.

As an investigation shows, corrections for double scattering of the incident particle (the operator T_2) are of the order of $F_\nu/R(kR)$[2]; i.e., the condition for the applicability of the impulse approximation in which multiple scattering is not taken into account has the form

$$F_\nu / R(kR) \ll 1, \tag{14}$$

where R is the average distance between the scattering particles. This condition is always satisfied under quasiclassical conditions, i.e., for $kR \gg 1$.

3. THE IMPULSE APPROXIMATION AS A GENERALIZED PSEUDOPOTENTIAL METHOD

If the scattering amplitudes F_ν change by only a small amount within the limits of the momentum spread of the scattering particles in the initial state, then they can be taken as constant in (11) $F_\nu = a_\nu$, and then $d^2\sigma/d\epsilon\, do$ goes over into

$$\frac{d^2\sigma}{d\varepsilon do} = \frac{k'}{k} \sum_{\nu\nu'} \frac{m^2}{\mu_\nu \mu_{\nu'}} a_\nu a^*_{\nu'} \int_{-\infty}^{\infty} e^{-i\varepsilon t} \langle \Phi_i, e^{-i\varkappa \mathbf{r}_{\nu'}} e^{iHt} e^{i\varkappa \mathbf{r}_\nu} e^{-iHt} \Phi_i \rangle\, dt, \tag{15}$$

as a result of which (11) agrees exactly with the formula of Zemach-Glauber[3] for the doubly differential cross section for the scattering of neutrons by chemically bound nuclei, derived by means of the Fermi pseudopotential method (i.e., by means of writing the matrix elements T_{fi} (3) in the form of the Born approximation with an interaction potential of the delta function type).

This circumstance is not accidental. As can be easily shown, under the conditions of applicability of the impulse approximation and of the constancy of F_ν within the limits of the momentum spread of the scattering system the matrix elements for the transitions (8) can be represented in the form of a Born approximation with a certain altered potential $\hat{V}$. Indeed, in the case when the pair scattering amplitude F_ν does not depend on the momenta of the scattering system (this is equivalent to neglecting p_ν in comparison with k and κ in

(9)), the expression for the matrix element (8) has the form

$$t_\nu^{fi} = 2\pi\mu_\nu^{-1} F(\mathbf{k}'_{\nu 0}, \mathbf{k}_{\nu 0}) \langle \Phi_f e^{i\varkappa \mathbf{r}_\nu} \Phi_i \rangle, \tag{16}$$

where $\mathbf{k}_{\nu 0} = m_\nu \mathbf{k}/(m_\nu + m)$ and $\mathbf{k}'_{\nu 0} = \mathbf{k}_{\nu 0} - \boldsymbol{\kappa}$, and can be obtained by introducing an effective potential $\hat{V}_\nu$, such that

$$F_\nu(\mathbf{k}'_{\nu 0}, \mathbf{k}_{\nu 0}) = \frac{\mu_\nu}{2\pi} \int e^{i\varkappa\boldsymbol{\rho}} \hat{V}_\nu(\boldsymbol{\rho})\, d\boldsymbol{\rho}, \tag{17}$$

and by subsequently applying the Born approximation in evaluating the matrix element, i.e.,

$$t_\nu^{fi} = \int \Phi_f^* e^{i\varkappa \mathbf{r}} V_\nu \Phi_i \, d\mathbf{r}\, d\xi.$$

In the case $F_\nu = \text{const}$ (which is the case in the scattering of slow neutrons by some nuclei) it follows from (17) that $\hat{V}_\nu = (2\pi/\mu_\nu) F_\nu \delta(\mathbf{r} - \mathbf{r}_\nu)$, i.e., (16) reduces to the usual Fermi pseudopotential approximation.

The conditions for the applicability of (15) and (16) can be derived by expanding $F(\mathbf{k}'_\nu, \mathbf{k}_\nu)$ in a series in powers of $\mathbf{p}_\nu$ and by restricting ourselves to the first term of the expansion. On substituting this expansion into (11) we easily find that the corrections associated with replacing F_ν by a_ν are of order of magnitude $p_\nu\, d \ln F_\nu/dk \sim p_\nu^0 A_\nu$ for pair scattering of slow particles (S-scattering), i.e., the aforementioned condition coincides with the well known criterion for the applicability of the Fermi pseudopotential method to the scattering of neutrons by molecules $A_\nu \ll a \sim 1/p_\nu^0$ where a is the amplitude of the vibration of the atoms in the molecule.

But in the case of pair scattering of quasiclassical type $F_\nu \approx B_\nu \exp(iS_\nu)$, $S \gg 1$, when it is possible to neglect the rapidly oscillating interference terms, the condition for the applicability of (15), (16) turns out to be less restrictive, and reduces specifically to the inequality $p_\nu^0\, d \ln |F_\nu|^2/dk \ll 1$, which is always fulfilled if the classical differential cross section changes by only a small amount within the limits of the momentum spread p_ν^0, i.e., if the speed of the incident particle is large in comparison with the effective speed of the bound particle $\sqrt{p_\nu^0/m_\nu}$.

It should be noted that the quantity p_ν^0 in the inequalities quoted above has the meaning of an effective momentum spread in the system ($p_\nu^0 \sim \sqrt{m_\nu \bar{\omega}}$) only in the range of energy ϵ and of scattering angles corresponding to the maximum of the cross section determined by (15), i.e., for $|\epsilon - R| \lesssim \sqrt{R\bar{\omega}}$ ($R = \kappa^2/2m_\nu$ is the recoil energy). As can be shown, outside this region the quantity p_ν^0 is of order of magnitude $(\epsilon - R)m_\nu/\sqrt{E_a}$ ($E_a = k^2/2m$), i.e., the conditions for the applicability of the approximation (15) turn out to be more restrictive. This circumstance manifests itself, in particular, in the investigation of resonance scattering of neutrons by chemically bound nuclei (Sec. 4). Formulas (15) and (16) can be used to describe a wide range of phenomena occurring in the collisions of fast atoms with molecules (excitation, dissociation and other processes of molecular rearrangement).

4. SCATTERING OF NEUTRONS BY CHEMICALLY BOUND ATOMS IN THE PRESENCE OF BROAD NEUTRON-NUCLEAR RESONANCES

The expression (11) obtained earlier for the differential scattering cross section in the impulse approximation as applied to the scattering of neutrons by bound atoms enables us to discuss a number of peculiarities which arise in the presence of broad neutron-nuclear resonances,[2)] and, in particular, such that the width of the resonance level Γ is much greater than a certain characteristic energy of the scattering system $\bar{\omega}$: $\Gamma \gg \bar{\omega}$. In this case the amplitudes F_ν appearing in (11) have the form

$$F(\mathbf{k}'_\nu, \mathbf{k}_\nu) = \bar{A}_\nu [k_\nu^2/2\mu_\nu - E_0 + i\Gamma/2]^{-1}, \tag{18}$$

where the quantities $\bar{A}_\nu$ can be taken as constant ($\bar{A}_\nu \sim \Gamma$).

Restricting ourselves to the case $k_\nu^2/2\mu_\nu = k^2/2(m_\nu + m) - \mathbf{k}\cdot\mathbf{p}_\nu/m_\nu$ which holds for $m\bar{\omega}/m_\nu\Gamma \ll 1$, we substitute the scattering amplitudes (18) expressed in terms of the integrals

$$\left(\frac{k_\nu^2}{2\mu_\nu} - E_0 + \frac{i}{2}\Gamma\right)^{-1} = -i \int_0^\infty d\alpha \exp\left\{i\alpha\left[\frac{k_\nu^2}{2\mu_\nu} - E_0 + \frac{i\Gamma}{2}\right]\right\}$$

into (11); we obtain

$$\frac{d^2\sigma}{d\varepsilon\, do} = \frac{k'}{k} \sum_{\nu\nu'} \frac{m^2}{\mu_\nu \mu_{\nu'}} A_\nu A_{\nu'}$$
$$\times \int e^{-i\varepsilon t} \exp\left\{i\alpha\left(\frac{m_\nu}{m_\nu + m} E_a - E_0 + \frac{i}{2}\Gamma\right)\right.$$
$$\left. - i\alpha'\left(\frac{m_\nu}{m_\nu + m} E_a - E_0 - \frac{i}{2}\Gamma\right)\right\} W(\alpha, \alpha', t)\, d\alpha\, d\alpha'\, dt, \tag{19}$$

where $W(\alpha, \alpha', t)$ in the Heisenberg representation for the coordinates and the momenta has the form

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[2)] In the general case this problem has been discussed in the papers of Dzyub and Lubchenko[4] and of Kazarnovskiĭ and Stepanov[5] with the aid of quadruple time correlation functions. However, the use of this method to obtain quantitative results is in practice extremely difficult.

$$W(\alpha, \alpha', t) = \left\langle \exp\left(-i\alpha' \frac{\mathbf{k}\mathbf{p}_{\nu'}(0)}{m_{\nu'}}\right) e^{-i\varkappa\mathbf{r}_{\nu'}(0)} e^{i\varkappa\mathbf{r}_{\nu}(t)} \exp\left(i\alpha \frac{\mathbf{k}\mathbf{p}_{\nu}(t)}{m_{\nu}}\right)\right\rangle. \tag{20}$$

We now investigate on the basis of the general formula (20) the resonance scattering of neutrons by molecules and crystals. We treat the oscillations in these systems in the approximation of independent oscillators. We first of all discuss the scattering of neutrons by molecules. We shall represent the displacement of an atom from a fixed equilibrium position $\mathbf{b}_\nu$ and the corresponding momentum as usual in the form

$$\mathbf{u}_\nu = \mathbf{u}_\nu^{\mathrm{tr}} + \mathbf{u}_\nu^{\mathrm{rot}} + \sum_s \mathbf{c}_\nu^s q_s;$$

$$\mathbf{p}_\nu = m_\nu \left(\mathbf{V}_M + [\Omega \mathbf{b}_\nu] + \sum_s \mathbf{c}_\nu^s \dot{q}_s\right), \tag{21*}$$

where $\mathbf{u}_\nu^{\mathrm{tr}}$ and $\mathbf{u}_\nu^{\mathrm{rot}}$ are displacements describing the translational and the rotational parts of the motion, $\mathbf{c}_\nu^S$ is the amplitude vector associated with the nucleus ν corresponding to a vibration of frequency ω_s, q_s are normal coordinates which in the representation of the operators a^+ for the creation and of a for the annihilation of oscillations have the form $q_s = i(2\omega_s)^{-1/2}[a_s \exp(-i\omega_s t) - a_s^+ \exp(i\omega_s t)]$, $\mathbf{V}_M$, Ω are respectively the velocity of the molecule as a whole and its angular velocity.

In future we shall restrict ourselves to the case of greatest interest for applications when ϵ, R, kT $\gg \overline{\Delta E}_{\mathrm{rot}}$ ($\overline{\Delta E}_{\mathrm{rot}}$ is the average energy difference between the rotational energy levels of the molecule). We recall that while the vibrational energy is of order of tenths of eV, the value of $\overline{\Delta E}_{\mathrm{rot}}$ amounts to hundredths or even thousandths of eV. Therefore, the assumptions under consideration are satisfied over a very wide range of variables ϵ and R.

Under the condition ϵ, R, kT $\gg \overline{\Delta E}_{\mathrm{rot}}$ the interference terms are negligibly small (cf. [3,6]) and, moreover, it is possible to take the rotational transitions into account classically, which significantly simplifies the calculations. Indeed, on substituting (21) into expression (20), and utilizing the independence of the different degrees of freedom, we break up W(α, α', t) for a fixed orientation of the molecule into a product of factors describing the different transitions in the molecule:[3)]

$$W(\alpha, \alpha', t) = \langle W^{\mathrm{tr}} \; W^{\mathrm{rot}} W^{\mathrm{vib}} \rangle_{\Omega\,\mathrm{nol}},$$

$$W^{\mathrm{rot}} = \int \exp\left\{-\frac{\mathbf{l}I^{-1}\mathbf{l}}{2T}\right\} \exp\{-i(\alpha - \alpha')\,\mathbf{k}\,[\Omega\mathbf{b}_\nu]\} \times \exp\left\{it\left(\frac{1}{2}\varkappa R_\nu \varkappa + \varkappa\,[\Omega\mathbf{b}_\nu]\right)\right\} d\mathbf{l}; \tag{22}$$

where $\mathbf{l}$ is the angular momentum vector of the molecule, R_ν is a tensor related to the moment of inertia tensor of the molecule I and to the position of the scattering nucleus with respect to its center of mass [6] $\mathbf{b}_\nu$,

$$W^{\mathrm{tr}} = \int \exp\left\{-\frac{M_0 V_{\mathrm{m}}^2}{2T} - i(\alpha - \alpha')\,\mathbf{k}\mathbf{V}_{\mathrm{m}} + it\left(\frac{\varkappa^2}{2M_0} + \varkappa\mathbf{V}_{\mathrm{m}}\right)\right\} d\mathbf{V}_{\mathrm{m}}.$$

For the vibrational part of the motion the expression W^{vib} can be represented in the following manner:

$$W^{\mathrm{vib}} = \prod_s \left\langle \exp\left(-i\alpha' \frac{\mathbf{k}\mathbf{p}_\nu^s(0)}{m_\nu}\right) \exp(-i\varkappa\mathbf{u}_\nu^s(0)) \exp(i\varkappa\mathbf{u}_\nu^s(t)) \times \exp\left(i\alpha \frac{\mathbf{k}\mathbf{p}_\nu^s(t)}{m_\nu}\right)\right\rangle_T. \tag{23}$$

On taking into account the fact that $e^A e^B = \exp\{A + B + \frac{1}{2}[A, B]\}$, if (as is true in our case) [A, B] commutes with A and B (cf., for example, [3]) expression (23) can be written in the form

$$W^{\mathrm{vib}} = \prod_s \langle \exp(Q_{\nu'}^s) \rangle_T,$$

$$\begin{aligned} Q_{\nu\nu}^s = {} & i(\varkappa\mathbf{c}_\nu^s)(q_\nu^s(t) - q_\nu^s(0)) + i(\mathbf{k}\mathbf{c}_\nu^s)(\alpha\dot{q}_\nu^s(t) - \alpha'\dot{q}_\nu^s(0)) \\ & - \tfrac{1}{2}(\alpha - \alpha')(\varkappa\mathbf{c}_\nu^s)(\mathbf{k}\mathbf{c}_\nu^s)[q_\nu^s(0), \dot{q}_\nu^s(0)] \\ & + \tfrac{1}{2}(\varkappa\mathbf{c}_\nu^s)(\mathbf{k}\mathbf{c}_\nu^s)\{\alpha[\dot{q}_\nu^s(0), q_\nu^s(t)] \\ & + \alpha'[q_\nu^s(0), \dot{q}_\nu^s(t)]\} + \tfrac{1}{2}(\varkappa\mathbf{c}_\nu^s)^2[q_\nu^s(0), q_\nu^s(t)] \\ & + \tfrac{1}{2}\alpha\alpha'(\mathbf{k}\mathbf{c}_\nu^s)^2[\dot{q}_\nu^s(0), \dot{q}_\nu^s(t)]. \end{aligned}$$

We now use the well known theorem relating to the average for a system of oscillators (cf. [3])

$$\langle e^{Q_{\nu\nu}^s} \rangle_T = \exp\left\{\tfrac{1}{2}\langle (Q_{\nu\nu}^s)^2 \rangle_T\right\},$$

and then obtain

$$W^{\mathrm{vib}}(\alpha, \alpha', t) = e^{F(\alpha, \alpha', t)}, \tag{24}$$

where for the index of the exponential on the right hand side we obtain after fairly simple calculations

$$\begin{aligned} F(\alpha, \alpha', t) = \sum_s \Big\{ & (\varkappa\mathbf{c}_\nu^s)^2 [\langle q_\nu^s(0)\, q_\nu^s(t)\rangle_T - \langle q_\nu^s(0)\, q_\nu^s(0)\rangle_T] \\ & + (\alpha - \alpha')(\varkappa\mathbf{c}_\nu^s)(\mathbf{k}\mathbf{c}_\nu^s)[\langle q_\nu^s(0)\, \dot{q}_\nu^s(t)\rangle_T - \langle q_\nu^s(0)\, \dot{q}_\nu^s(0)\rangle_T] \end{aligned}$$

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*$[\Omega\mathbf{b}_\nu] = \Omega \times \mathbf{b}_\nu$.

[3)] We employ a system of units in which the Boltzmann constant k = 1. The symbol $\langle \ldots \rangle_T$ in future will denote not only quantum mechanical but also statistical averaging.

$$- \tfrac{1}{2} (\mathbf{k c}_\nu^s)^2 \left[(\alpha^2 + \alpha'^2) \langle \dot{q}_\nu^s (0)\, \dot{q}_\nu^s (0) \rangle - 2\alpha\alpha' \langle \dot{q}_\nu^s (0)\, \dot{q}_\nu^s (t) \rangle_T \right] \Big\};$$

$$\langle q_\nu^s (0)\, q_\nu^s (t) \rangle_T = \omega_s^{-2} \langle \dot{q}_\nu^s (0)\, \dot{q}_\nu^s (t) \rangle_T = \tfrac{1}{2} \omega_s^{-1} \left[(n_T + 1)\, e^{i\omega_s t} + n_T e^{-i\omega_s t} \right],$$

$$\langle q_\nu^s (0)\, \dot{q}_\nu^s (t) \rangle_T = \tfrac{1}{2} i \left[(n_T + 1)\, e^{i\omega_s t} - n_T e^{-i\omega_s t} \right], \qquad (25)$$

where $n_T = [\exp(\omega_s / T) - 1]^{-1}$ is the index of the thermal exponential.

The substitution of (24) into (22) is followed by integration over α and α'. The result depends in an essential manner on the ratio of the parameters $R_\nu = \kappa^2 / 2m_\nu$, ω and Γ. It can be seen that the terms quadratic in α and α' are of order $R\omega/\Gamma^2$ compared to unity, while the linear terms are of order R/Γ. Under the conditions $R\omega/\Gamma^2 \ll 1$ the parameter R/Γ is arbitrary and has a strong effect on the final results.

On retaining only the terms linear in α and α' we have

$$F_\nu(\alpha, \alpha', t) = \sum_s \frac{(\varkappa \mathbf{c}_\nu^s)^2}{2\omega_s} \left[(n_T + 1)\, e^{i\omega_s t} + n_T e^{-i\omega_s t} - 2n_T - 1 \right] + i (\alpha - \alpha') (\varkappa \mathbf{c}_\nu^s) (\mathbf{k c}_\nu^s) \left[(n_T + 1)\, e^{i\omega_s t} - n_T e^{-i\omega_s t} - 1 \right]. \qquad (26)$$

On substituting W^{rot}, W^{tr}, and W^{vib} into expression (22), where the symbol $\langle \ldots \rangle_{\Omega_{\text{mol}}}$ denotes averaging over the angular orientations of the molecule, we obtain after further transformations the following formula for the scattering cross section:

$$\left(\frac{d^2\sigma}{d\varepsilon\, do} \right)_\nu = \frac{k'}{k} \left(\frac{m}{\mu_\nu} \right)^2 \overline{A}_\nu^2 \int \exp \left\{ i\alpha \left(\frac{m_\nu}{m_\nu + m} E_a - E_0 + \frac{i\Gamma}{2} \right) - i\alpha' \left(\frac{m_\nu}{m_\nu + m} E_a - E_0 - \frac{i\Gamma}{2} \right) \right\} \Big\langle \frac{1}{\sqrt{\pi a^2}} \exp \left\{ - \frac{\widetilde{E}^2}{a^2} \right\}$$

$$\times \exp \left\{ - i (\alpha - \alpha') \frac{\mathbf{k} R_\nu \varkappa + \mathbf{k} \varkappa / M_0}{\varkappa R_\nu \varkappa + \varkappa^2 / M_0} \widetilde{E} \right\} \times \exp \{ F_\nu(\alpha, \alpha', t) \} \Big\rangle_{\Omega_{\text{mol}}} e^{-i(\varepsilon - \widetilde{\varepsilon})t}\, d\alpha\, d\alpha'\, dt;$$

$$a^2 = 2T (\varkappa R_\nu \varkappa + \varkappa^2 / M_0),$$

$$\widetilde{E} = \widetilde{\varepsilon} - \tfrac{1}{2} \varkappa R_\nu \varkappa - \varkappa^2 / 2M_0, \qquad \varepsilon = \widetilde{\varepsilon} + \varepsilon_{\text{vib}}, \qquad (27)$$

and for the cross section corresponding to a specified change in the vibrational state of the molecule we have ($\epsilon_{\text{vib}} = \pm n\omega_\lambda$)

$$\left(\frac{d^2\sigma}{d\varepsilon\, do} \right)_\nu^{\widetilde{\varepsilon} \pm n\omega\lambda} = \frac{k'}{k} \left(\frac{m}{\mu_\nu} \right)^2 \overline{A}_\nu^2 \Big\langle \frac{1}{\sqrt{\pi a^2}} \exp \left\{ - \frac{\widetilde{E}^2}{a^2} \right\} e^{-W_T} \times \frac{1}{n!} \left\{ \frac{(\varkappa \mathbf{c}_\nu^\lambda)^2}{2\omega_\lambda} \left[\frac{1}{e^{\omega\lambda / T} - 1} + \frac{1}{2} (1 \pm 1) \right] \right\}^n \left[1 \pm \frac{\mathbf{k c}_\nu^\lambda}{\varkappa \mathbf{c}_\nu^\lambda} \omega_\lambda \frac{d}{d\varphi} \right]^n \times \left(\varphi^2 + \frac{\Gamma^2}{4} \right)_{\varphi = \varphi_0}^{-1} \Big\rangle_{\Omega_{\text{mol}}},$$

$$W_T = \sum_s \frac{(\varkappa \mathbf{c}_\nu^s)^2}{2\omega_s} \operatorname{cth} \frac{\omega_s}{2T};$$

$$\varphi_0 = \frac{m_\nu}{m_\nu + m} E_a - E_0 + \frac{1}{2} (\varkappa \mathbf{c}_\nu^\lambda) (\mathbf{k c}_\nu^\lambda) - \frac{\mathbf{k} R_\nu \varkappa + \mathbf{k} \varkappa / M_0}{\varkappa R_\nu \varkappa + \varkappa^2 / M_0} \widetilde{E}. \qquad (28)^*$$

The calculation of the resonance scattering of neutrons by crystals is carried out in a similar manner. We expand the operator for the displacement of the nucleus from the position of equilibrium $\mathbf{r}_\nu^0$, $\mathbf{u}_\nu = \mathbf{r}_\nu - \mathbf{r}_\nu^0$, in terms of normal coordinates ($m_\nu = m_{\nu'} = M$):

$$\mathbf{u}_\nu (t) = \sum_s \mathbf{e}_s u_\nu^s (t); \qquad u_\nu^s (t) = b_\nu^s a_s e^{-i\omega_s t} - b_\nu^{s*} a_s^+ e^{i\omega_s t},$$

$$b_\nu^s = i\, (2MN\omega_s)^{-1/2} e^{i \mathbf{k}_1 \mathbf{r}_\nu^0},$$

where $\mathbf{e}_s$ is the unit polarization vector for a phonon of type s (the index s includes the propagation vector $\mathbf{k}_1$ and the nature of the phonon polarization), a_s, a_s^+ are the phonon annihilation and creation operators, N is the number of atoms in the crystal.

The derivation of $W(\alpha, \alpha', t)$ in formula (19) for crystals is fundamentally analogous to the derivation of (24), (25). We reproduce the final result which in addition also includes the coherent (interference) part of the scattering:

$$W_{\nu\nu'} (\alpha, \alpha', t) = e^{F(\alpha, \alpha', t)} e^{i\varkappa (\mathbf{r}_\nu^0 - \mathbf{r}_{\nu'}^0)},$$

$$F (\alpha, \alpha', t) = \sum_s \{ (\varkappa \mathbf{e}_s)^2 [\langle u_{\nu'}^s (0)\, u_\nu^s (t) \rangle_T - \langle u_\nu^s (0)\, u_\nu^s (0) \rangle_T] + (\alpha - \alpha') (\varkappa \mathbf{e}_s) (\mathbf{k e}_s) [\langle u_{\nu'}^s (0)\, \dot{u}_\nu^s (t) \rangle_T - \langle u_\nu^s (0)\, \dot{u}_\nu^s (0) \rangle_T] \}, \qquad (29)$$

where

$$\langle u_{\nu'}^s (0)\, u_\nu^s (t) \rangle_T = \omega_s^{-2} \langle \dot{u}_{\nu'}^s (0)\, \dot{u}_\nu^s (t) \rangle = (2MN\omega_s)^{-1} \left[(n_T + 1)\, e^{i\psi} + n_T e^{-i\psi} \right],$$

$$\langle u_{\nu'} (0)\, \dot{u}_\nu^s (t) \rangle_T = i\, (2MN)^{-1} \left[(n_T + 1)\, e^{i\psi} - n_T e^{-i\psi} \right],$$

$$\psi = k_1 (r_\nu^0 - r_{\nu'}^0) + \omega_s t.$$

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*cth = coth.

Considering for the sake of simplicity a cubic crystal we obtain from (19) and (29) for the resonance scattering of neutrons (evaluated per atom of the crystal) accompanied by the creation (upper sign) and absorption (lower sign) of n phonons of type λ in the incoherent approximation (inelastic scattering is basically incoherent; for the elastic scattering the coherent part is included in the formula given below by adding for $n = 0$ the factor

$$\left|\sum_{\nu'} \exp\{i\varkappa(r_\nu^0 - r_{\nu'}^0)\}\right|): \quad \left(\frac{d\sigma}{do}\right)^{\pm n\omega_\lambda}$$

$$= \frac{k'}{k}\left(\frac{M+m}{M}\right)^2 \overline{A}^2 e^{-W_T} \frac{1}{n!}$$

$$\times \left\{g(\omega_\lambda)\frac{\varkappa^2}{2M\omega_\lambda}\left[\frac{1}{e^{\omega_\lambda/T}-1} + \frac{1}{2}(1 \pm 1)\right]\right\}^n$$

$$\times \left\{1 \pm \frac{\mathbf{k}\boldsymbol{\varkappa}}{\varkappa^2}\omega_\lambda \frac{d}{d\varphi}\right\}^n \left(\varphi^2 + \frac{\Gamma^2}{4}\right)^{-1}_{\varphi=\varphi_0}, \tag{30}$$

where $g(\omega)$ is the phonon distribution function in the crystal,

$$W_T = \frac{\varkappa^2}{2M}\int\limits_0^{\omega_{max}} g(\omega)\frac{1}{\omega}\operatorname{cth}\frac{\omega}{2T}d\omega,$$

$$\varphi = \frac{M}{M+m}E_a - E_0 + \frac{1}{2}\frac{\varkappa\mathbf{k}}{M},$$

$\omega_{\max}$ is the maximum frequency.

For elastic scattering we have from (12) ($n = 0$, $\mathbf{k}\cdot\boldsymbol{\kappa} = \kappa^2/2$) a formula which coincides with the result of Kazarnovskiĭ and Stepanov[6] obtained for $\omega \ll \Gamma$ by a different method.

If the transferred energy ϵ is much smaller than E_0, then the quantity $\mathbf{k}\cdot\boldsymbol{\kappa}/\kappa^2$ can be replaced by $1/2$, while the quantity $\mathbf{k}\cdot\boldsymbol{\kappa}/2M$ can be replaced by $R/2$.

We now discuss the formulas (28) and (30) obtained above. As can be easily seen, for sufficiently broad resonances satisfying the condition $\epsilon, R \ll \Gamma$, we can neglect in (28) and (30) terms containing derivatives with respect to φ, and set φ_0 equal to $ME_a/(M+m) - E_0$. Then (28) and (30) coincide with the result which is obtained by the Fermi pseudopotential method if we set in it the pseudopotential $\hat{V}$ equal to

$$\hat{V} = \sum_\nu \frac{2\pi h^2}{\mu_\nu}F_\nu\delta(\mathbf{r} - \mathbf{r}_\nu),$$

where the amplitudes F_ν are not constant, but depend on the energy of the incident particle. Thus, all the results obtained by the pseudopotential method admit in the case $\epsilon, R, \omega \ll \Gamma$ a simple generalization to the case of resonance neutron-nuclear scattering by means of the replacement of the constant amplitudes a_ν by the amplitudes F_ν defined in accordance with (18).

If at least one of the quantities ϵ or R is comparable to Γ, then the situation is of a more complicated nature, and in this case it is necessary to utilize the general formulas (28) and (30) which lead, in particular, to the following conclusions. We consider the elastic scattering ($n = 0$, $\epsilon = 0$) of neutrons through a given angle (κ given). Then, for example, it follows from (30) that the dependence of the scattering cross section on the neutron energy has a Breit-Wigner character with a maximum shifted by an amount $-R/2$, i.e., at most by an amount $2mE_0/M$. For example, in the case of Cs^{55} this shift is approximately equal to 0.1 eV (for $E_0 = 5.7$ eV and $\Gamma = 0.25$ eV).

The chemical binding manifests itself in an even more significant manner when a large amount of vibrational energy is transferred. In particular, if $\epsilon \sim \Gamma$, while $R \ll \Gamma$, then we can obtain from (30) the total cross section for the excitation of n phonons in the following form:

$$\sigma^n = \sigma_\Phi^n \left\{1 + \tfrac{1}{2}\omega_\lambda\frac{d}{d\varphi}\right\}^n (\varphi^2 + \Gamma^2/4)^{-1}_{\varphi = ME_a/(M+m)-E_0}, \tag{30a}$$

where σ_Φ^n is the total cross section for the excitation of n phonons obtained by the Fermi pseudopotential method with constant scattering amplitudes.

The differential operator in (30a) yields in the case $n\omega < \Gamma$ a function with a maximum shifted by approximately $-n\omega/2$ in comparison with E_0, and, in contrast to the Breit-Wigner case, not symmetric with respect to $ME_a/(M+m) - E_0$. Analogous phenomena occur also in the case of the scattering of neutrons by molecules.

These phenomena must be taken into account in the study of the passage of neutrons through moderating substances; they must also be taken into account in the investigation of the structure and of the physico-chemical properties of different media by the methods of neutron spectroscopy which are being developed at present.

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