

*SUPPRESSION OF INELASTIC CHANNELS IN RESONANCE SCATTERING OF NEUTRONS IN  
REGULAR CRYSTALS*

Yu. KAGAN and A. M. AFANAS'EV

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A dynamical theory is developed which describes the motion of neutrons in a regular crystal when the interaction of the neutron with individual nuclei has primarily resonance character. A detailed analysis is made of the effect of suppression of inelastic channels and the distribution of the intensity of nuclear reactions over the thickness of the crystal. The problem is solved with nuclear vibration in the crystal and spin and isotopic incoherence taken into account.

## 1. INTRODUCTION

IN considering the scattering of particles by systems consisting of a large number of nuclei, we meet the problem that the interaction with individual nuclei itself begins to depend critically on the nature of the motion of the particle in the interior of such a system. Suppose that a monochromatic beam of particles is incident on a regular crystal. In moving in the interior of the crystal a particle actually loses the property of being a free particle and becomes a quasiparticle, satisfying the translational symmetry of the scattering system. The resulting state can in principle differ markedly from a plane wave, no matter how small the interaction with an individual nucleus. In fact, if the end of the wave vector of the particle is close to one of the boundaries of the Brillouin zone, the state of the particle in the crystal is a superposition of two plane waves with wave vectors differing by a vector of the reciprocal lattice, and with almost equal amplitudes. A particle in such a state will interact with the nuclei completely differently from a free particle. In particular the inelastic amplitude, (in the resonance case, the amplitude for compound state formation) may vanish or be markedly reduced, and is now simply determined by the sum of the amplitudes for each of the waves of the resulting coherent superposition.<sup>[1]</sup> This is the kind of situation that seems to occur in the scattering of slow neutrons, and consequently the neutrons in such a state will move through the crystal, being absorbed weakly even when there is a strong resonance interaction with the individual nuclei. (In the scattering of X rays by electrons one has the analogous phenomena of

“flashing”—the so-called “anomalous transmission” effect.<sup>[2]</sup>)

When the wave vector of the particles incident on the crystal is close to satisfying the Bragg condition, the initial plane wave suffers a strong deformation within a finite thickness, giving rise to the collective state described above. As a result, after almost ordinary (or even weaker) absorption in the transition layer, the particles will continue to propagate through the crystal while suffering only relatively weak absorption.

The present authors developed<sup>[1]</sup> a theory for describing the similar picture which arises in the resonance scattering of  $\gamma$  quanta. The treatment was based on solving the Maxwell equations with the actual values of the currents corresponding to individual nuclei. In the case of neutrons the theoretical analysis of the effect of suppression of inelastic channels has its own basic special features. These are connected primarily with the need to develop a dynamical theory of crystals for particles described by the Schroedinger equation.

The problem involves a general dynamical theory, taking into account the resonance character of the interaction and the presence of an intense inelastic channel as well as vibration of the nuclei in the crystal. In addition the theory must take consistent account of the spin interaction of the neutrons with the nuclei and the appearance of an additional incoherent scattering channel (the so-called “spin incoherence”). The overall problem is to decide whether the spin incoherence destroys the effect of suppression of inelastic channels. A similar problem obviously exists in connection with isotopic incoherence.

All of these questions are treated in this paper. Particular attention is devoted to analyzing how the intensity and the spatial distribution of nuclear reactions in the crystal depend on the parameters of the problem.

## 2. DYNAMICAL THEORY OF NEUTRON SCATTERING IN CRYSTALS

1. Suppose that a neutron moves through an arbitrary perfect crystal. We shall assume that the neutron energy  $E$  is sufficiently small so that  $\lambda \gg d$  ( $d$  is the nuclear size,  $\lambda$  the neutron wavelength) and that only  $s$ -scattering occurs from the individual nuclei. We also assume that the amplitude for elastic scattering by an individual nucleus  $f(\mathbf{k}, \mathbf{k}')$  is small compared to the interatomic scattering, independent of the specific character of the interaction.

The Hamiltonian for the interaction of the neutron with the crystal obviously splits into a sum of terms corresponding to interactions with individual nuclei:

$$V = \sum_m V_m.$$

We represent the  $\Psi$ -function of the neutron in the form of an expansion in plane waves:

$$\Psi(\mathbf{r}) = \sum_{\mathbf{k}} \Psi_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}.$$

Then we find from the Schroedinger equation for the coefficients  $\Psi_{\mathbf{k}}$

$$(E_{\mathbf{k}} - E)\Psi_{\mathbf{k}} + \sum_m \sum_{\mathbf{k}'} V_m(\mathbf{k}, \mathbf{k}')\Psi_{\mathbf{k}'} = 0, \quad (2.1)$$

where  $E_{\mathbf{k}} = k^2/2M$  and  $M$  is the neutron mass. (Throughout,  $\hbar = 1$ .)

The coefficients  $V_m(\mathbf{k}, \mathbf{k}')$  in (2.1) are the matrix elements of  $V_m$  between plane waves. If  $|f| \ll a$ , by a familiar technique the true interaction Hamiltonian may be replaced by an effective Hamiltonian with smeared-out interaction, for which, on the one hand, perturbation theory is valid, and on the other hand the corresponding matrix elements are uniquely related to the true amplitude for elastic scattering  $f(\mathbf{k}, \mathbf{k}')$  (cf., for example, [3]). Then

$$V_m(\mathbf{k}, \mathbf{k}') = -2\pi M^{-1} f_m(\mathbf{k}, \mathbf{k}'). \quad (2.2)$$

This treatment actually assumes that all processes leading to inelastic scattering out of the beam are incoherent and that there are no back reactions.

A consistent analysis shows that in a rigid lattice  $f_m(\mathbf{k}, \mathbf{k}')$  should be taken to mean the amplitude for elastic scattering by an individual nucleus, where its imaginary part is determined

only by the inelastic part of the cross section. Ejection from the beam associated with purely elastic scattering is already contained in Eq. (2.1) when we take (2.2) into account. Keeping in mind the treatment of resonance scattering, we shall always assume that the width  $\Gamma_2$  corresponding to inelastic channels is large compared to the elastic width  $\Gamma_1$  (in general,  $\sigma_a \gg \sigma_s$ ). We shall therefore not distinguish between the amplitude appearing in (2.2) and the true amplitude for scattering by an individual nucleus.

In the vibrating lattice the scattering of a neutron may be accompanied by the emission or absorption of phonons. These processes lead to incoherent ejection of particles from the beam, which is equivalent to an absorption. It is clear that the quantity appearing in (2.2) should be the amplitude for true elastic scattering, i.e., the amplitude diagonal in the occupation numbers. If we remember at the same time that elastic scattering corresponds to a long interaction time, it is easy to understand that this amplitude should be averaged over the equilibrium distribution of the phonons. Because of the potential character of the interaction of the neutron and the nucleus, the amplitude appearing on the right of (2.2) will depend only on the difference  $\mathbf{k} - \mathbf{k}'$ . But if the interaction has resonance character, the inclusion of nuclear vibration causes  $f_m$  to depend on  $\mathbf{k}$  and  $\mathbf{k}'$  individually (cf., below, and also [1]).

So far we have paid no attention to the neutron spin. Actually the function  $\Psi_{\mathbf{k}}$  should have a spin index, and the quantities  $V_m(\mathbf{k}, \mathbf{k}')$  and  $f_m(\mathbf{k}, \mathbf{k}')$  are actually operators in spin space. The general expression for such an operator has the form (cf., for example, [4])

$$f = \frac{1}{2I+1} [f^+(I+1) + f^-I] + \frac{2}{2I+1} [f^+ - f^-] sI. \quad (2.3)$$

Here  $f^+$  and  $f^-$  are the amplitudes for scattering of a neutron by an individual nucleus with spin  $I$ , corresponding to the two total spin values  $J = I \pm 1/2$ .

If the spin of the neutron changes during interaction with the nucleus, the resultant state is incoherent with the initial state, and such a process must be regarded as inelastic. In the absence of nuclear polarization, the true scattering amplitude corresponding to the "entrance channel" for which interference between the incident and scattered waves is typical, is just the first term in (2.3), the coherent part of the amplitude. It is this quantity that should appear on the right of (2.2).

2. In the case of a rigid lattice, near an iso-

lated resonance level the coherent scattering amplitude should have the following form:

$$f_m(\mathbf{k}, \mathbf{k}') = -a \exp [i(\mathbf{k} - \mathbf{k}') \mathbf{r}_m] - \Gamma_1' [2k(E - E_0 + i\Gamma/2)]^{-1} \exp [i(\mathbf{k} - \mathbf{k}') \mathbf{r}_m]. \quad (2.4)$$

Here  $a$  is the coherent amplitude for potential scattering,

$$\Gamma_1' = \zeta(I)\Gamma_1, \quad (2.5)$$

where  $\zeta(I)$  takes the values  $(I+1)/(2I+1)$  or  $I/(2I+1)$  depending on the total angular momentum of the resonance level.

We particularly emphasize that in the resonance term in (2.4) we have the coherent channel width  $\Gamma_1'$ , which is smaller than  $\Gamma_1$ , while the total width now contains, in addition to  $\Gamma_2$ , the width corresponding to the incoherent part of the elastic channel:

$$\Gamma_1'' = (1 - \zeta(I))\Gamma_1. \quad (2.5')$$

Now we consider the vibrating lattice and introduce explicitly the displacement vector  $\mathbf{u}_m$  of the  $m$ -th nucleus relative to its equilibrium position  $\mathbf{R}_m$ :  $\mathbf{r}_m = \mathbf{R}_m + \mathbf{u}_m$ . Keeping in mind our previous remarks and using the results of the well known paper of Lamb<sup>[5]</sup> (cf. also<sup>[4]</sup>), we find for the scattering amplitude:

$$f_m(\mathbf{k}, \mathbf{k}') = -\exp [i(\mathbf{k} - \mathbf{k}') \mathbf{R}_m] \left\{ a \langle (\exp [i(\mathbf{k} - \mathbf{k}') \mathbf{u}_m])_{\{n\}\{n'\}} \rangle + \frac{\Gamma_1'}{2k} \sum_{\{n^s\}} \langle (\exp [-i\mathbf{k}' \mathbf{u}_m])_{\{n\}\{n^s\}} (\exp [i\mathbf{k} \mathbf{u}_m])_{\{n^s\}\{n\}} \rangle \times \left[ E - E_0 - \sum_{\beta} \omega_{\beta} (n_{\beta^s} - n_{\beta}) + \frac{i}{2} \Gamma \right]^{-1} \right\}. \quad (2.6)$$

Here  $\{n\}$  is the set of occupation numbers  $n_{\beta}$  characterizing the state of the crystal;  $\omega_{\beta}$  is the frequency of the  $\beta$ 'th normal mode. The vibration problem is treated in the harmonic approximation.<sup>1)</sup> The angular brackets denote an average over the equilibrium phonon distribution.

Assuming that the crystal is perfectly regular, we introduce in place of the index  $m$  the unit cell number  $\mathbf{m}$  and the index  $j$  for atoms within one cell. Then after standard calculations we find

$$\langle (\exp [i(\mathbf{k} - \mathbf{k}') \mathbf{u}_m])_{\{n\}\{n'\}} \rangle = \exp [-Z_j(\mathbf{k} - \mathbf{k}')/2], \quad Z_j(\boldsymbol{\kappa}) = \frac{1}{2M_j} \sum_{\beta} \frac{|\boldsymbol{\kappa} \mathbf{v}_{j\beta}|^2}{\omega_{\beta}} (2\bar{n}_{\beta} + 1). \quad (2.7)$$

In the last expression  $\mathbf{v}_{j\beta}$  is the polarization vec-

tor of the  $j$ -th atom with mass  $M_j$  in the  $\beta$ 'th normal mode.

An important point is that the second term in the square brackets in (2.6) also does not depend on the number of the unit cell. Its explicit form depends to a large extent on the values of the parameters of the problem. Thus, if  $\Gamma$  or  $|E - E_0|$  are much larger than  $\omega_0$ ,  $R_j$  ( $\omega_0$  is the characteristic energy of the phonon spectrum, or the temperature,  $R_j = k^2/2M_j$ ) the phonon term in the denominator can be neglected, and the amplitude for resonance scattering by an individual nucleus has the same factor (2.7). But if these conditions are violated, the temperature dependence of the potential and resonance parts of the scattering amplitude are different. In this case it is convenient to write the resonance part as an integral over the time, as is usually done for the cross section. A direct calculation leads to the expression

$$f_m^{\text{res}}(\mathbf{k}, \mathbf{k}') = {}^{1/2} i \Gamma_1' \exp [i(\mathbf{k} - \mathbf{k}') \mathbf{R}_m - Z_j(\mathbf{k} - \mathbf{k}')/2] \times \int_0^{\infty} dt \exp \{i(E - E_0)t - {}^{1/2} \Gamma t + \varphi_j(\mathbf{k}, \mathbf{k}', t)\}, \quad (2.8)$$

$$\varphi_j(\mathbf{k}, \mathbf{k}', t) = \sum_{\beta} \frac{1}{2M_j N \omega_{\beta}} (\mathbf{k} \mathbf{v}_{j\beta}) (\mathbf{k}' \mathbf{v}_{j\beta}^*) \times [(\bar{n}_{\beta} + 1)(e^{-i\omega_{\beta} t} - 1) + \bar{n}_{\beta}(e^{i\omega_{\beta} t} - 1)]$$

( $N$  is the number of unit cells).

The relations obtained enable us to analyze the temperature dependence of the scattering amplitude in the general case. We simply note that if  $\Gamma$  or  $|E - E_0| \ll \omega_0, R_j$ , the amplitude (2.8) exhibits a markedly different temperature dependence from (2.7) (cf. <sup>[1]</sup>):

$$f_m^{\text{res}}(\mathbf{k}, \mathbf{k}') = -\frac{\Gamma_1'}{2k(E - E_0 + i\Gamma/2)} \times \exp \left[ i(\mathbf{k} - \mathbf{k}') \mathbf{R}_m - \frac{1}{2} (Z_j(\mathbf{k}) + Z_j(\mathbf{k}')) \right]. \quad (2.9)$$

If the first resonance level lies sufficiently low, the substitution  $\Gamma_1 \rightarrow \gamma \sqrt{E/E_0}$  should be made in (2.4) and (2.6). Now the dependence of the amplitude on the temperature and the phonon spectrum will depend to a large extent on the relation between  $E_0$  and  $\omega_0, R_j$ . Thus, if the inequality  $E_0 \gg \omega_0, R_j$  is not satisfied, this dependence will differ from the purely potential case (2.8) even for  $E \rightarrow 0$ , when  $f \rightarrow \text{const}$ , while for the cross section corresponding to the inelastic channels the "1/v law" is valid, i.e., the behavior of the elastic and inelastic scattering cross sec-

<sup>1)</sup>For simplicity we neglect the change in the phonon spectrum that results from the change of mass of the nucleus accompanying absorption of a neutron.

tions is the same as for the nonresonant case.

3. Keeping the above results in mind, we re-write the general expression for the scattering amplitude by an individual nucleus in the form

$$f_m(\mathbf{k}, \mathbf{k}') = \exp[i(\mathbf{k} - \mathbf{k}')(\mathbf{R}_m + \boldsymbol{\rho}_j)] f_j(\mathbf{k}, \mathbf{k}') \quad (2.10)$$

( $\boldsymbol{\rho}_j$  is the position of the  $j$ -th atom in the unit cell). In the second term of Eq. (2.2) we sum over  $m$ . Then, using (2.3), we find

$$\left(\frac{k^2}{\kappa^2} - 1\right) \Psi_{\mathbf{k}} - \sum_{\mathbf{K}} g(\mathbf{k}, \mathbf{k} + \mathbf{K}) \Psi_{\mathbf{k} + \mathbf{K}} = 0. \quad (2.11)$$

Here

$$g(\mathbf{k}, \mathbf{k}_1) = \frac{4\pi}{\kappa^2 v_0} \sum_j \exp[i(\mathbf{k} - \mathbf{k}_1) \boldsymbol{\rho}_j] f_j(\mathbf{k}, \mathbf{k}_1); \quad (2.12)$$

$\mathbf{K}$  is  $2\pi$  times a vector of the reciprocal lattice;  $v_0$  is the volume of the unit cell;  $\kappa = \sqrt{2ME}$ .

In writing (2.10) and (2.12) it was assumed that all the nuclei in the crystal are monoisotopic. If this is not the case we must again take only the coherent part of the amplitude, which in this case corresponds to simply making the substitution

$$f_j \rightarrow \bar{f}_j, \quad (2.13)$$

where the bar above denotes an isotopic average over the nuclei at the  $j$ -th site in the unit cell.

We now turn to the system of equations (2.11) and consider the case where  $\mathbf{k} = \mathbf{k}_0$ , so that for one of the diffracted waves the wave vector  $\mathbf{k}_1 = \mathbf{k}_0 + \mathbf{K}$  has a value close to that for the exact Bragg condition  $k_1^2 = k_0^2$ . Then, assuming that the interaction with an individual nucleus is sufficiently small, we can, as usual, separate out of the system (2.11) two equations, which are the same for the two values of the neutron polarization:

$$\begin{aligned} (k_0^2/\kappa^2 - 1) \Psi_{\mathbf{k}_0} &= g_{00} \Psi_{\mathbf{k}_0} + g_{01} \Psi_{\mathbf{k}_1}, \\ (k_1^2/\kappa^2 - 1) \Psi_{\mathbf{k}_1} &= g_{10} \Psi_{\mathbf{k}_0} + g_{11} \Psi_{\mathbf{k}_1}, \end{aligned} \quad (2.14)$$

where  $g_{\alpha\beta} = g(\mathbf{k}_\alpha, \mathbf{k}_\beta)$ .

The system (2.14) is similar to the system of equations considered in [1] for the case of scattering of  $\gamma$  quanta (and to the system of equations in the dynamical theory of x rays). Thus, referring the reader to [1] for details, we immediately give the final formulas.

Considering a crystal in the form of a flat plate in the Laue case (diffracted beam passes through the crystal), we have for the wave function of a neutron of arbitrary polarization in the crystal:

$$\Psi(\mathbf{r}) = \Phi_0 [\Psi_0(y) e^{i\kappa\mathbf{r}} + \Psi_1(y) e^{i\kappa_1\mathbf{r}}],$$

$$\Psi_0(y) = \frac{1}{2(\varepsilon^{(2)} - \varepsilon^{(1)})} \left\{ (2\varepsilon^{(2)} - g_{00}) \exp\left(\frac{i\kappa\varepsilon^{(1)}}{\gamma_0} y\right) \right.$$

$$\left. - (2\varepsilon^{(1)} - g_{00}) \exp\left(\frac{i\kappa\varepsilon^{(2)}}{\gamma_0} y\right) \right\},$$

$$\Psi_1(y) = -\frac{\beta g_{10}}{2(\varepsilon^{(2)} - \varepsilon^{(1)})} \left\{ \exp\left(\frac{i\kappa\varepsilon^{(1)}}{\gamma_0} y\right) - \exp\left(\frac{i\kappa\varepsilon^{(2)}}{\gamma_0} y\right) \right\}. \quad (2.15)$$

Here  $y = \mathbf{n} \cdot \mathbf{r}$ ;  $\mathbf{n}$  is the interior normal to the crystal surface;

$$\begin{aligned} \varepsilon^{(1,2)} &= 1/4(g_{00} + \beta g_{11} - \beta\alpha) \pm 1/4\{(g_{00} + \beta g_{11} - \beta\alpha)^2 \\ &+ 4\beta(g_{00}\alpha - \Delta)\}^{1/2}, \quad \Delta = g_{00}g_{11} - g_{01}g_{10}. \end{aligned} \quad (2.16)$$

The angle characterizing the deviation from the Bragg conditions is

$$\alpha = \mathbf{K}_1(\mathbf{K}_1 + 2\boldsymbol{\kappa}) / \kappa^2; \quad (2.17)$$

$\Phi_0$  is the value of the wave function at the entrance surface of the crystal;

$$\beta = \gamma_0 / \gamma_1; \quad \gamma_{0,1} = \cos \Theta_{0,1}, \quad \cos \Theta_{0,1} = \hat{\mathbf{n}} \boldsymbol{\kappa}_{0,1},$$

$$\boldsymbol{\kappa}_1 = \boldsymbol{\kappa}_0 + \mathbf{K}_1.$$

Expression (2.15) along with (2.2) and the explicit form for the scattering amplitude (2.10), (2.6)–(2.9) and (2.13) completely solves the dynamical problem for neutrons in an ideal crystal.

### 3. EFFECT OF SUPPRESSION OF INELASTIC CHANNELS. ANOMALOUS TRANSMISSION OF NEUTRONS

1. Let us examine how the yield of a nuclear reaction varies over the depth of a crystal when we have the state described in (2.15). We introduce a reaction cross section that varies over the thickness of the crystal, taking account of the true value of the neutron wave function near the nucleus and measured relative to the flux density of incident particles at the front surface of the crystal. Let us assume that the nuclear reaction has a purely resonance character. Assuming that the energy of the secondary particles is large compared to the neutron energy and the characteristic photon energy, we have

$$\begin{aligned} \tilde{d}\sigma(y_{mj}) &= \sum_{\{n^s\}} |\Psi_0(y_{mj}) f_{mj}'(\boldsymbol{\kappa}_0\{n\}; \mathbf{q}\{n^s\}) \\ &+ \Psi_1(y_{mj}) f_{mj}'(\boldsymbol{\kappa}_1\{n\}; \mathbf{q}\{n^s\})|^2 \frac{q}{\kappa} d\Omega_{\mathbf{q}}, \end{aligned} \quad (3.1)$$

where  $y_{mj} = \mathbf{n} \cdot \mathbf{R}_{mj}$ . This expression contains the reaction amplitude  $f'_{mj}$ , corresponding to the emission of a secondary particle with momentum  $\mathbf{q}$  with simultaneous transition of the phonon system from state  $\{n\}$  to state  $\{n^s\}$ .

If the formation of the compound nucleus is determined essentially by one resonance level,

$$f_{mj}'(\mathbf{x}\{n\}; \mathbf{q}\{n^s\}) = -\left(\frac{\Gamma_1 \Gamma_2}{4\kappa q}\right)^{1/2} \sum_{\{n^p\}} (\exp[-i\mathbf{q}\mathbf{u}_{mj}])_{\{n^s\}\{n^p\}} \times (\exp[i\kappa\mathbf{u}_{mj}])_{\{n^p\}\{n\}} \times \left[E - E_0 - \sum_{\beta} \omega_{\beta}(n_{\beta^p} - n_{\beta}) + \frac{i\Gamma}{2}\right]^{-1}. \quad (3.2)$$

We substitute (3.2) in (3.1) and carry out explicitly the summation over  $\{n^s\}$ , taking account of the obvious relation

$$\sum_{\{n^s\}} (\exp[i\mathbf{q}\mathbf{u}_{mj}])_{\{n^t\}\{n^s\}} (\exp[-i\mathbf{q}\mathbf{u}_{mj}])_{\{n^s\}\{n^p\}} = \delta_{\{n^t\}, \{n^p\}}.$$

Going over to an integral representation for the cross section (3.2) and performing the trivial integration over  $d\Omega_{\mathbf{q}}$ , we get

$$\tilde{\sigma}(y_{mj}) = \frac{\pi\Gamma_1 \Gamma_2}{\Gamma\kappa^2} \int_{-\infty}^{\infty} dt \exp\left[i(E - E_0)t - \frac{\Gamma}{2}|t|\right] \times F_{mj}(\mathbf{x}, \mathbf{x}_1, t), \quad (3.3)$$

$$F_{mj}(\mathbf{x}, \mathbf{x}_1, t) = \text{Sp} \{ \rho (\Psi_0^* \exp[-i\mathbf{x}\mathbf{u}_{mj}(t)] + \Psi_1^* \exp[-i\mathbf{x}_1\mathbf{u}_{mj}(t)]) \times (\Psi_0 \exp[i\mathbf{x}\mathbf{u}_{mj}] + \Psi_1 \exp[i\mathbf{x}_1\mathbf{u}_{mj}]) \} \quad (3.4)$$

( $\rho$  is the equilibrium density matrix of the crystal).

Using standard methods for calculating such correlation functions, we find for (3.4) (cf. the notation in (2.7) and (2.8)),

$$F_{mj}(\mathbf{x}, \mathbf{x}_1, t) = |\Psi_0(y_{mj})|^2 \exp[\varphi_j(\mathbf{x}, \mathbf{x}, t)] + |\Psi_1(y_{mj})|^2 \exp[\varphi_j(\mathbf{x}_1, \mathbf{x}_1, t)] + 2\text{Re}[\Psi_0(y_{mj})\Psi_1^*(y_{mj})] \times \exp[-1/2 Z_j(\mathbf{x} - \mathbf{x}_1) + \varphi_j(\mathbf{x}, \mathbf{x}_1, t)]. \quad (3.5)$$

This expression becomes considerably simpler in the limiting cases. When  $\Gamma$  or  $|E - E_0| \gg \omega_0$ ,  $R_j$ , it reduces to

$$F_{mj}' = |\Psi_0(y_{mj}) + \Psi_1(y_{mj})|^2 - 2\text{Re}[\Psi_0(y_{mj})\Psi_1^*(y_{mj})] \times \{1 - \exp[-1/2 Z(\mathbf{x} - \mathbf{x}_1)]\}. \quad (3.6)$$

In the opposite limiting case, corresponding to a narrow resonance,

$$F_{mj}'' = |\Psi_0(y_{mj}) \exp[-Z_j(\mathbf{x})/2] + \Psi_1(y_{mj}) \exp[-Z_j(\mathbf{x}_1)/2]|^2. \quad (3.7)$$

If the neutron energy lies considerably below the first resonance level, we have for the reaction cross section (3.3)

$$\tilde{\sigma}R_{(mj)} = \sigma_2 F_{mj}', \quad (3.8)$$

where  $\sigma_2$  is the reaction cross section at an isolated nucleus ( $\sigma_2 \sim \kappa^{-1}$ ).

The expressions (3.3), (3.5)–(3.8), together with (2.15) enable us to give an exhaustive analysis of the variation over the thickness of the crystal of the intensity of production of secondary particles. On the other hand, knowing (2.15), we can find the flux of primary particles at each point of the crystal.

2. Let us begin the analysis with the case of a rigid lattice. For a monatomic crystal with arbitrary symmetry, in accordance with (2.12), (2.10) and (2/4), for an arbitrary ratio of  $\text{Im } g_{\alpha\beta}$  and  $\text{Re } g_{\alpha\beta}$ , we have

$$g_{00} = g_{11} = g_{01} = g_{10}; \quad \Delta = 0. \quad (3.9)$$

If we substitute this result in (2.16) it is easy to see that when the Bragg condition is exactly satisfied, i.e., when  $\alpha = 0$ , one of the roots ( $\epsilon^{(1)}$ ) is strictly zero, while the other is equal to  $1/2 g_{00} (1 + \beta)$ . Let us consider the reaction cross section under these conditions, remembering that in a rigid lattice

$$F_{mj} = |\Psi_0(y_{mj}) + \Psi_1(y_{mj})|^2. \quad (3.10)$$

Near the entrance surface, where the condition

$$\kappa y (1 + \beta) \text{Im } g_{00} / 2\gamma_0 \ll 1,$$

is satisfied,  $\Psi_1$  is small compared to  $\Psi_0$ ; the interaction with the nuclei, and consequently the yield of secondary particles behaves as usual. But as  $\Psi_1$  increases the situation changes drastically. As  $\Psi_0$  drops a finite  $\Psi_1$  appears, and on reflection from any crystal plane  $\Psi_1(y_{mj})$  has the opposite sign from  $\Psi_0(y_{mj})$ . This leads to a much more marked decrease in the cross section for inelastic processes compared to the usual case which results from a drop in intensity of the primary beam. Finally, when

$$\kappa y (1 + \beta) \text{Im } g_{00} / 2\gamma_0 \gtrsim 1 \quad (3.11)$$

$\Psi_0$  and  $\Psi_1$  become equal in absolute value, after which (as is evident from (3.10)) compound nucleus formation ceases, and the inelastic channels are completely suppressed. Both waves retain a finite intensity and so in addition to the suppression of the inelastic channels there is an anomalous transmission of the neutrons.

Let  $\alpha \ll |g_{00}|$  but still have a finite value. We use the appropriate expansion for  $\epsilon^{(1,2)}$  (cf. Eq. (4.8) in [1]) in formula (2.15) and compute (3.10). Substituting this result in (3.3) (or (3.7)), we find for the nuclear reaction cross section, at distances where (3.11) is valid,

$$\tilde{\sigma}(y) = \sigma_2(E) \left( \frac{\beta}{1+\beta} \right)^4 \frac{\alpha^2}{|g_{00}|^2} \exp \left[ -\alpha^2 \left( \frac{y}{y_0} \right) \right],$$

$$y_0 = \frac{4\pi v_0(1+\beta)^3}{\beta^3(v_0 \kappa^3) \kappa} \frac{\sigma_1'(E)}{\sigma_t(E)}. \quad (3.12)$$

Here  $\sigma_1'(E)$ ,  $\sigma_2(E)$  and  $\sigma_t(E)$  are, respectively, the coherent scattering cross section, the reaction cross section and the total cross section for interaction with an isolated nucleus. In the case of pure resonance interaction,

$$\frac{\sigma_1'(E)}{\sigma_t(E)} = \frac{\Gamma_1'}{\Gamma} = \frac{I^* + 1/2}{2I + 1} \frac{\Gamma_1}{\Gamma}$$

(where  $I^*$  is the spin of the compound nucleus).

From (2.12) it immediately follows that

$$|g_{00}|^2 = \frac{4\pi}{v_0^2 \kappa^4} \sigma_1'(E).$$

It is interesting that for small  $\alpha$  the reaction cross section (3.11) as a function of neutron energy actually loses its resonance character. Then a yield from the nuclear reaction, though small, will be observed at thicknesses which are not usable for neutrons under ordinary conditions. We note that in the Bragg case when  $\alpha = 0$ , and (3.9) is valid, the second root  $\epsilon^{(2)} = 1/2 g_{00} (1 - |\beta|)$ . Thus, in the so-called symmetric case  $|\beta| = 1$  the root  $\epsilon^{(2)}$  also goes to zero, and in the reflection the inelastic channels are suppressed over the whole volume of the crystal.

So far we have considered crystals with one atom per unit cell. If we go over to a polyatomic lattice the picture changes. Then, as we see from (2.12), in general

$$\Delta = g_{00}g_{11} - g_{01}g_{10} \neq 0$$

and consequently neither of the roots (2.16) (or their imaginary parts) vanishes for any value of  $\alpha$ , so the effect of suppression of inelastic channels either disappears or is significantly reduced.

But in a whole variety of cases of experimental interest the effect will persist even in crystals with several atoms in the unit cell. Primarily this applies to the case where for a given neutron energy the amplitude for scattering by one of the nuclei in the unit cell,  $f_j$ , is large compared to the scattering amplitudes from the other nuclei. Then, in accordance with (2.12), under the condition  $\Delta = 0$  the effect of suppression of inelastic channels is realized fully.

It is interesting that the effect is in general destroyed in crystals with two identical atoms in the unit cell. But if the vector  $\rho_2$  can be multiplied by such an integer as to make its projection

on the basis vectors coincide with one of the nodes of the other sublattice, or if a family of crystal planes can be chosen so that  $\mathbf{K}_1 \perp \rho_2$ , then (3.9) will again be satisfied and the problem becomes equivalent to the monatomic case. This applies both to crystals with two identical atoms or with two different atoms in the unit cell.

3. Let us consider the vibrating lattice. We restrict our treatment to the case of one atom per unit cell. If there were a nucleus with such narrow resonance levels that  $\Gamma \ll \omega_0$ ,  $R_j$ , then for neutrons with energies near to resonance, according to (2.12), (2.10) and (2.9), the relation  $\Delta = 0$  would be satisfied at arbitrary values of the temperature. Then, using (3.3), (3.7) and (2.15) it is easy to see that at thicknesses satisfying the inequality (3.11), when  $\alpha = 0$  the inelastic channels are completely suppressed, although a neutron current of finite intensity proceeds through the crystal. This is connected with the vanishing in a crystal of arbitrary symmetry of the amplitude for formation of the compound nucleus, which now depends essentially on the temperature. The resulting picture is similar to that in the resonance scattering of  $\gamma$  rays by Mössbauer nuclei. We shall not discuss this case particularly, since it was treated in detail in [1].

But the existence of such narrow levels is not typical for neutrons. As a rule we have the opposite limiting case or, at least, something intermediate. Keeping this in mind, we shall give in detail the case where  $\Gamma$  or  $|E - E_0| \gg \omega_0$ ,  $R_j$  for resonance scattering, or the equivalent case of scattering in a region where the  $1/v$  law is valid.

We shall write the basic relations between the parameters characteristic for this case (cf. (3.9)):

$$g_{00} = g_{11}, \quad g_{01} = g_{10} = g_{00} e^{-Z(\mathbf{K}_1)/2};$$

$$\Delta = g_{00}^2 (1 - e^{-Z(\mathbf{K}_1)}). \quad (3.9')$$

It should be pointed out immediately that the effect of complete suppression of the inelastic channels is now absent. But for the minimal values of  $\mathbf{K}_1$  in most cases  $Z(\mathbf{K}_1) \ll 1$ ; this causes the effect of suppression to be very marked.

Let us first consider small deviations from the Bragg condition,  $\alpha \ll |g_{00}|$ . In accordance with our remarks we shall also suppose that  $\Delta \ll g_{00}^2$ . Then for  $\epsilon^{(1,2)}$  we can use formulas (4.2) from [1]. It is then not difficult to verify by direct test using (2.15) that at a thickness  $y$ , satisfying (3.11), the first term in (3.6) is quadratic in  $\Delta$

and  $\alpha$ . So, keeping only the second term, we find for the reaction cross section (3.3),

$$\tilde{\sigma}(y) = \sigma_2(E) \frac{2\beta^2}{(1+\beta)^2} \left( 1 - \exp\left[\frac{-Z(\mathbf{K}_1)}{2}\right] \right) \Phi(y), \quad (3.12')$$

$$\Phi(y) = \exp\left[-\alpha^2 \left(\frac{y}{y_0}\right) - (1 - e^{-Z(\mathbf{K}_1)}) \left(\frac{y}{y_1}\right)\right],$$

$$y_1 = \frac{(1+\beta)v_0}{\beta\gamma_0\sigma_1(E)}. \quad (3.13)$$

The reaction cross section now depends on temperature, and it is interesting that with increasing  $T$  the cross section  $\tilde{\sigma}$  always increases. Since  $Z(\mathbf{K}_1)$  tends to a finite limit (because of zero point vibrations) as  $T \rightarrow 0$ , there will be a certain detuning of the effect of suppression of inelastic channels at any temperature.

Under these same assumptions we determine from (2.15) the intensity of the primary flux of neutrons:

$$\frac{J_0(y)}{J(0)} = \left(\frac{\beta}{1+\beta}\right)^2 \left[ 1 - 4\alpha \frac{\beta}{(1+\beta)^2} \operatorname{Re} \frac{1}{g_{00}} - \frac{2(1-\beta)}{(1+\beta)^2} (1 - e^{-Z(\mathbf{K}_1)}) \right] \Phi(y).$$

Similarly for the diffracted flux,

$$\frac{J_1(y)}{J(0)} = \left(\frac{\beta}{1+\beta}\right)^2 \left[ 1 - 2\alpha \frac{\beta(1-\beta)}{(1+\beta)^2} \operatorname{Re} \frac{1}{g_{00}} + \frac{4\beta}{(1+\beta)^2} (1 - e^{-Z(\mathbf{K}_1)}) \right] \Phi(y).$$

When  $\alpha = 0$  the neutron intensity drops exponentially with effective length  $l$  at a rate  $\sim 1/Z$  times faster than when one is far from the Bragg condition. If  $T \gtrsim \omega\beta$ , then  $l \sim 1/T$ . For  $\alpha \neq 0$  there is an additional damping, independent of the temperature and the phonon spectrum. The corresponding effective length  $l_0 = y_0/\alpha^2$  (cf. (3.13)) has an extremely remarkable dependence on neutron energy. In fact, for resonance interaction  $l_0 \sim 1/E^2$ , while far from resonance, when  $\sigma_2 \gg \sigma_1$ ,  $l \sim 1/E^{3/2}$ .

It should be noted particularly that the intensity of the transmitted neutron current will show an asymmetry in  $\alpha$ , which can change sign in the vicinity of resonance as the neutron energy changes (because of the term  $\operatorname{Re} g_{00}^{-1}$ ). In the diffracted flux this asymmetry is reduced, and is altogether absent for  $\beta = 1$ .

The realization of the effects treated here requires a relatively high degree of collimation  $\Delta\Theta$  and monochromatization  $\Delta E/E$  of the neutron beam. The presence of strong interaction at resonance lowers these requirements as com-

pared with the usual potential interaction. Let us consider the example of  $\text{Gd}^{157}$ , having a resonance at  $E_0 = 0.030$  eV, with the following resonance parameters:  $\Gamma_2 = 100$  mV,  $\Gamma_1 = 0.65$  mV,  $I = 7/2$ . As we see from formulas (3.12), (3.13), on the scale determined by  $\alpha$  the characteristic angle is determined by  $\alpha_0 = \sqrt{y_0/y}$ . Then, for  $\Delta\Theta$  and  $\Delta E/E$ , from (2.17) we have

$$\Delta\Theta = \frac{\kappa}{2K \sin \Theta_B} \alpha_0, \quad \frac{\Delta E}{E} = \frac{\kappa}{K \cos \Theta_B} \alpha_0, \quad \Theta_B = \widehat{\kappa, \mathbf{K}}.$$

If we set  $v_0 = 3 \times 10^{-23}$  cm<sup>3</sup>, we will have for  $y_0$  the value  $2 \times 10^{-13}$  cm, and consequently, at a thickness  $y = 10^{-3}$  cm (very much larger than the absorption length)  $\Delta\Theta \sim 3''$  and  $\Delta E/E \sim 10^{-4}$ .

Of particular interest from the experimental point of view is the analysis of the behavior of the effect over a relatively wide range of variation of the parameter  $\alpha/|g_{00}|$ , especially the case

$$|\operatorname{Im} g_{00}| \ll |\operatorname{Re} g_{00}|. \quad (3.14)$$

We note that if we exclude the immediate neighborhood of the resonance, this inequality is usually well satisfied for neutrons.

We give the general expressions for  $\Psi_0$  and  $\Psi_1$  (2.15), corresponding to the case of (3.14):

$$\Psi_0(y) = \frac{1}{2} \left\{ \exp\left[\frac{i\kappa\varepsilon^{(1)}}{\gamma_0} y\right] + \exp\left[\frac{i\kappa\varepsilon^{(2)}}{\gamma_0} y\right] \right\} + \frac{\tilde{\alpha}}{2s} \left\{ \exp\left[\frac{i\kappa\varepsilon^{(1)}}{\gamma_0} y\right] - \exp\left[\frac{i\kappa\varepsilon^{(2)}}{\gamma_0} y\right] \right\},$$

$$\Psi_1(y) = \frac{\beta g_{10}'}{s} \left\{ \exp\left[\frac{i\kappa\varepsilon^{(1)}}{\gamma_0} y\right] - \exp\left[\frac{i\kappa\varepsilon^{(2)}}{\gamma_0} y\right] \right\},$$

$$\tilde{\alpha} = \beta\alpha + g_{00}'(1-\beta), \quad s = (\tilde{\alpha}^2 + 4\beta g_{01}' g_{10}')^{1/2},$$

$$\varepsilon^{(1,2)} = 1/4(2g_{00}' - \tilde{\alpha} \pm s) \pm 1/4 i \{ (1+\beta)g_{00}'' + s^{-1}[\tilde{\alpha}g_{00}''(1-\beta) + 2\beta(g_{01}'g_{10}'' + g_{01}''g_{10}')] \}. \quad (3.15)$$

In a lattice with one or two atoms per unit cell, in the last case, if the reflection is chosen so that  $\exp(i\mathbf{K}_1 \cdot \rho_2) = 1$ , we have

$$g_{00}' = \frac{1}{\kappa^2 v_0} \sum_j \pm [4\pi\sigma_{1j}'(E)]^{1/2}, \quad g_{00}'' = \frac{1}{4\kappa v_0} \sum_j \sigma_{1j}(E),$$

$$g_{01}' = g_{10}' = \frac{1}{\kappa^2 v_0} \sum_j \left\{ \pm [4\pi\sigma_{1j}'(E)]^{1/2} \exp\left[\frac{-Z_j(\mathbf{K}_1)}{2}\right] \right\},$$

$$g_{01}'' = g_{10}'' = \frac{1}{4\kappa v_0} \sum_j \left\{ \sigma_{1j}(E) \exp\left[\frac{-Z_j(\mathbf{K}_1)}{2}\right] \right\}. \quad (3.16)$$

From (3.15) it follows that the coefficient of the diffracted wave is symmetric around  $\alpha = 0$ , whereas in the transmitted wave the coefficient is asymmetric. But the actual asymmetry depends

rather on how strongly the two roots in (3.15) differ, and on the thickness of the crystal. We note that the minimal value again lies at  $\alpha = 0$ ; this should also result in some asymmetry in the diffracted wave. If for simplicity we take  $\beta = 1$ , then from (3.15) it follows immediately that to the left of  $\alpha = 0$  there is a range of angles where the intensity of the transmitted beam of neutrons will be lower than the intensity far from the region where the Bragg condition is satisfied, and to the right a range of angles where the intensity will be higher. Such behavior will show up the more clearly the stronger the absorption within the thickness of the crystal.

4. So far, unfortunately, there are no experiments on resonance scattering of neutrons in perfect crystals. But recently there have been interesting reports<sup>[6,7]</sup> which give results of investigations of dynamical effects appearing in the potential scattering of neutrons in such crystals as InSb, Ge, Si. Characteristic of all cases is that the inequality (3.14) is satisfied, so that for comparison we may use the results in the form of (3.15) (the intensities of the transmitted and diffracted beams of neutrons are simply proportional, respectively, to  $|\Psi_0(L)|^2$  and  $|\Psi_1(L)|^2$ ). And actually the observed appearance of angular asymmetry in the intensity of transmitted neutrons for the case of InSb (sizable absorption) and its practical absence in the case of Ge (weak absorption within the crystal for the thickness used in the experiment) agrees qualitatively with the results presented above. The observed<sup>[7]</sup> oscillation of neutron intensity with thickness in a very weakly absorbing crystal of Si directly follows from (3.15) if we take account of the difference between  $\text{Re } \epsilon^{(1)}$  and  $\text{Re } \epsilon^{(2)}$ . It is interesting that the period of oscillation must vary with the temperature (cf. (3.15)).

As for the change in intensity of inelastic processes in a crystal, the effect was first seen qualitatively by Knowles,<sup>[8]</sup> who determined the yield of the  $(n, \gamma)$  reaction from scattering of neutrons by a single crystal.

The paucity of experimental results makes comparison with theory difficult. This is true in particular for the temperature dependence, which actually first manifested itself naturally in the dynamical case. But from the point of view of the dependence on nuclear vibration, the dynamical problem for neutrons undergoing resonance scattering by nuclei with a wide level or far from resonance is similar to the dynamical theory of x rays. On the other hand, for x rays the temperature dependence of the anomalous transmission

was measured recently, and it was found that (in our notation)<sup>[9,10]</sup>

$$\text{Im } g_{01} / \text{Im } g_{00} \approx \exp(-Z(\mathbf{K}_1)/2).$$

It is easy to see that this result coincides precisely with (3.13) or (3.20), and also with the results appearing in<sup>[1]</sup>.

#### 4. THE ROLE OF SPIN AND ISOTOPIC INCOHERENCE

At first glance it might seem that the presence of the incoherent spin scattering should lead to spoiling of the effect of suppression of inelastic channels. But the results of the preceding section have shown that in any case, in a rigid lattice for  $\alpha = 0$  the effect appears at full value. It is of interest to give at least a brief analysis of the resulting situation. To be definite we restrict our discussion to the case of pure resonance interaction.

The presence of spin scattering is equivalent to the appearance of an additional inelastic channel with the width (2.5') and the corresponding "reaction" cross section:

$$\sigma_1'' = \frac{\pi}{k^2} \frac{\Gamma_1 \Gamma_1''}{(E - E_0)^2 + \Gamma^2/4}$$

Representing the scattering amplitude in the form (2.4) or (2.6), we naturally included this channel. Actually the optical theorem in this case has the form

$$\text{Im } f = \frac{k}{4\pi} (\sigma_1' + \sigma_1'' + \sigma_2)$$

(the elastic width always appears as  $\Gamma_1'$  (2.5)).

The change in the number of inelastic channels automatically changes the behavior of the  $\Psi$  function in the transition layer to some extent, but the physical picture as a whole does not change, nor does the occurrence of a paired state (cf. the Introduction). In a rigid lattice, when the Bragg condition is exactly satisfied the  $\Psi$  function has nodes at the positions of the nuclei and consequently any interaction with the nuclei, coherent or incoherent, vanishes. Thus such a state is undamped and actually insensitive to the presence of spin incoherence.

But the spin incoherence does affect the damping of the intensity when we deviate from the Bragg condition and when we include vibrations of the lattice (and also, naturally, when the collimation conditions are made poorer). (In accordance with (3.13),  $y_0 \sim \Gamma_1'$  and not  $\Gamma_1$ ).

A similar situation occurs when there is isotopic incoherence. In the preceding section some

of the results given actually were for monatomic crystals. In the general case, remembering (2.13), we must make the substitutions

$$\sigma_2 \rightarrow \bar{\sigma}_2, \quad \sigma_t \rightarrow \bar{\sigma}_t, \quad \sigma_1' \rightarrow \{(\bar{\sigma}_1)^{1/2}\}^2 \quad (4.1)$$

in the appropriate formulas.

It is easy to see that the coherent scattering amplitude, if determined in accordance with (2.13), takes into account completely the new inelastic channel coming from the isotopic incoherent scattering. Just as for the case of spin incoherence, this channel does not prevent the appearance of an undamped state, but it may make more difficult the achievement of good collimation and markedly affect the damping when there is a deviation from the Bragg condition. Thus, if the scattering of one of the isotopes predominates,  $y_0$  is proportional to the concentration of that isotope, as is easily seen from (3.13) and (4.1).

We note in conclusion that impurity atoms located at the lattice sites and not distorting the lattice, for  $\alpha = 0$  have practically no adverse ef-

fect on the suppression of the inelastic channels in the rigid lattice.

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