# Neutron scattering by a crystal in an external alternating field

A. Ya. Dzyublik

*Nuclear Research Institute, Ukrainian Academy of Sciences*
(Submitted 1 March 1983; resubmitted 13 June 1983)
Zh. Eksp. Teor. Fiz. **85**, 1658–1665 (November 1983)

A dynamic theory is developed for neutron scattering by a crystal that executes forced vibrations under the influence of an external alternating field. The interference of coherent neutron waves having different frequencies leads to the appearance of a pendellosung effect in such crystals, to suppression of reactions, and to temporal intensity beats. The possibility is also demonstrated of resonant suppression of the anomalous passage of neutrons by ultrasound, of enhancement of the temporal beats, and of a change of the character of the pendellosung oscillations (neutron-acoustic resonance).

PACS numbers: 61.80.Hg, 63.20. – e

## 1. INTRODUCTION

The influence of forced crystal-atom oscillations excited by external alternating fields (laser, ultrasound, etc.) on neutron scattering and on nuclear reactions in which neutrons participate has been investigated in many studies.[1–6] Inelastic scattering of neutrons by polaritons produced by laser-wave mixing with phonons were considered.[1] A kinematic theory was constructed[2] for potential scattering of neutrons by crystals with account taken of the anharmonicity of the oscillations. The possibility was discussed[3] of neutron acceleration in a medium in which a laser excites intramolecular oscillations. Also considered[4] was the effect of laser radiation on magnetic scattering of neutrons. The cross section for nuclear reactions in the small-oscillation approximation was calculated in Refs. 1 and 5. The cross section for oscillations of arbitrary amplitude was calculated in Ref. 6. Many earlier studies (see, e.g., Refs. 7 and 8) were devoted to the effect of low-frequency crystal vibrations on neutron diffraction. In this article is developed a theory of multiple neutron scattering by a crystal that executes coherent forced vibrations of arbitrary amplitude under the influence of alternating fields.

## 2. BASIC EQUATIONS

It is known that an oscillator executes in an alternating field quantum oscillations about an instantaneous equilibrium position that vibrates classically in turn. The forced vibration of the equilibrium position have the frequency $\Omega$ of the external force. Therefore the radius vector of the $\varkappa$-th atom of the l–th unit cell of a crystal in an alternating field is

$$\mathbf{R}_{l\varkappa}(t)=\mathbf{R}_{l\varkappa}^{(0)}+\mathbf{X}_{l\varkappa}(t)+\mathbf{u}_{l\varkappa}', \quad \mathbf{R}_{l\varkappa}^{(0)}=\mathbf{l}+\boldsymbol{\rho}_{\varkappa}, \tag{1}$$

where the vector $\boldsymbol{\rho}_\varkappa$ determines the equilibrium position of the $\varkappa$-th atom in the cell, $\mathbf{X}_{l\varkappa}(t)$ is the displacement, due to the classical vibrations, from the instantaneous equilibrium position of this atom, and $\mathbf{u}'_{l\varkappa}$ is the displacement, due to the quantum motion, from the instantaneous equilibrium position. Assume that a traveling displacement wave having a wave vector $\mathbf{q}$ and an amplitude $\mathbf{A}_\varkappa$ is excited in the crystal:

$$\mathbf{X}_{l\varkappa}(t)=\mathbf{A}_\varkappa\cos(\mathbf{ql}-\Omega t). \tag{2}$$

The operator of the interaction of the neutron with the $i$-th ($i=\mathbf{l},\varkappa$) atom of the crystal, $\hat{v}_i^{(\mathrm{neut})}(t)=\hat{v}_H(\mathbf{r}-\mathbf{R}_i(t))$, where $\mathbf{r}$ is the neutron radius vector, is then a periodic function of the time with a period $T=2\pi/\Omega$.

We represent the Hamiltonian of the neutron + crystal system in an alternating field in the form

$$\hat{\mathscr{H}}(t)=\hat{\mathscr{H}}_0+\hat{V}(t). \tag{3}$$

The operator $\hat{\mathscr{H}}_0$ is equal to the sum of the neutron kinetic-energy operator $\hat{\mathscr{K}}$, of the Hamiltonian $\hat{H}_c$ of the quantum oscillations of the crystal, and of the Hamiltonian $\hat{H}\gamma$ of that part of the electromagnetic field which corresponds to the $\gamma$ quanta. The perturbation operator is

$$\hat{V}=\sum_i\hat{v}_i(t), \quad \hat{v}_i(t)=\hat{v}_i^{(\mathrm{neut})}(t)+\hat{v}_i^{(\gamma)}, \tag{4}$$

where $v_i^\gamma$ is the interaction of the nucleus with the field. We denote the eigenfunctions of the operator $\hat{\mathscr{H}}_0$ by $|a\rangle$, $|b\rangle$, $|c\rangle$ or $X_{a,b,c}$, and the corresponding eigenvalues by $E_{a,b,c}$. Let the initial state of the system as $t\to-\infty$ be described by the function $\chi_a=|\alpha\rangle\exp(i\mathbf{k}_0\mathbf{r})$, where $|\alpha\rangle$ is the initial quantum state of the scatterer and $\mathbf{k}_0$ is the wave vector of the incident neutron having an energy $E=\hbar^2k_0^2/2m$. The initial energy $E_a$ of the quantum motions of the system is equal to the sum of $E$ and of the energy $\mathscr{E}_a$ of the quantum oscillations of the crystal.

The system wave function $\Psi(t)$ satisfies the Schrödinger equation

$$i\hbar\partial\Psi(t)/\partial t=\hat{\mathscr{H}}(t)\Psi(t). \tag{5}$$

Its solution that satisfies the chosen initial condition can be reduced to a simple form by changing to a new Hilbert space of functions that are periodic in time with a period $T$. Whereas usually the time enters as a parameter and the scalar product of the functions is defined as an integral only over the spatial variables $x$ of the system, here we regard the time as a variable on a par with $x$. We define the scalar product of the functions $\varphi(x,t)$ and $\psi(x,t)$ as

$$\{\psi(x,t)|\varphi(x,t)\}=\int_0^T dt\int dx\,\psi^*(x,t)\varphi(x,t). \tag{6}$$

The orthonormalized basis vectors take in the new space the form $|a;n\}=\chi_aT^{-1/2}\exp(in\Omega t)$. Any function of the new space can be expanded in a series in the vectors $|a;n\}$ with constant coefficients. We introduce in the new space the operator $\tilde{\mathscr{H}}_0 = \hat{\mathscr{H}}_0 - i\hbar\partial/\partial t$ in place of $\hat{\mathscr{H}}_0$. The vectors $|a, n\}$ are the eigenvectors of the operator $\tilde{\mathscr{H}}_0$ with corresponding eigenvalues $E_a + n\hbar\Omega$. In the new space, the interaction operator $\tilde{V} = \hat{V}(t)$ has the matrix

$$\{a'; n'|\tilde{V}|a; n\} = \frac{1}{T}\int_0^T dt e^{-i(n'-n)t} V_{a'a}(t) = V_{a'a}(n'-n), \quad (7)$$

where $V_{a'a}(n)$. The total Hamiltonian is $\tilde{\mathscr{H}} = \tilde{\mathscr{H}}_0 + V$. The wave function of the system then takes the form

$$\Psi(t) = \psi_a^+(x, t)\exp(-iE_a t/\hbar),$$
$$\psi_a^+ = \chi_a + (E_a + i\eta - \tilde{\mathscr{H}}_0)^{-1}\tilde{\mathscr{T}}\chi_a, \quad \eta \to +0. \quad (8)$$

The scattering operator is defined by the expression

$$\tilde{\mathscr{T}} = \tilde{V} + \tilde{V}(E_a + i\eta - \tilde{\mathscr{H}})^{-1}\tilde{V}. \quad (9)$$

We consider now neutron scattering by the $i$-th atom of the crystal. If a neutron wave $\exp(i\mathbf{k}_0 \cdot \mathbf{r})$ is incident, the scattered wave $\psi_a^+ - \chi_a$ is a coherent sum of waves $\sim\exp(in\Omega t)$. These waves can be further rescattered in the crystal. Using the proposed formalism, we calculate the matrix of neutron scattering by the $i$-th nucleus:

$$\{b'; n'|\tilde{t}_i|b; n\} = v_{b'b}^{(\mathrm{neut})}(n'-n)_i + \sum_c \sum_{n''} \frac{v_{b'c}^{(\mathrm{neut})}(n'-n'')_i v_{cb}^{(\mathrm{neut})}(n''-n)_i}{E_a - E_c - n''\hbar\Omega + i\Gamma/2}, \quad (10)$$

where $|c\rangle$ are all the intermediate system states produced when a neutron is captured by the nucleus on a resonant level of width $\Gamma$ and energy $E_0$. The amplitude for scattering by the $i$-th nucleus as the scatterer goes from the state $|\alpha\rangle$ into $|\alpha'\rangle$, when $n'$-$n$ of the $\hbar\Omega$ quanta are given up by the neutron to the external field, is connected with the $t$-matrix by the relation

$$f_{\alpha\alpha'}^{(n'-n)}(\mathbf{k}, \mathbf{k}')_i = -\frac{m}{2\pi\hbar^2}\{\alpha', \mathbf{k}'; n'|\tilde{t}_i|\alpha, \mathbf{k}; n\}\exp\{-i(\mathbf{k} - \mathbf{k}' - (n'-n)\mathbf{q})\mathbf{R}_i^{(0)}\}. \quad (11)$$

Averaging the amplitude $f_{\alpha\alpha}^{(n'-n)}$ over the states of the scatterer and over the isotopes we obtain the amplitude for coherent neutron scattering by the $\varkappa$-th nucleus:

$$f_{\mathrm{coh}}^{(n'-n)}(\mathbf{k}, \mathbf{k}')_\varkappa = i^{n'-n}\Big[-\bar{b}_\varkappa \exp(-W_\varkappa(\mathbf{Q}))J_{n'-n}(\mathbf{QA}_\varkappa) + \sum_{l=-\infty}^{\infty} J_{l-n'}(\mathbf{k}'\mathbf{A}_\varkappa)J_{l-n}(\mathbf{kA}_\varkappa)f_{\mathrm{res}}(E - l\hbar\Omega)\Big], \quad (12)$$

whee $\bar{b}$ is the coherent-scattering length, $\mathbf{Q} = \mathbf{k} - \mathbf{k}'$, $J_n(z)$ is a Bessel function of order $n$, $f_{\mathrm{res}}(E)$ the amplitude of resonant scattering of neutrons by the nucleus in the absence of forced vibrations:

$$f_{\mathrm{res}}(E) = -p_\varkappa \frac{2I+1}{2(2I_0+1)}\frac{\Gamma_{\mathrm{neut}}}{2k_0} \times \sum_{n_s', n_s^0} w(n_s^0)\frac{\langle n_s^0|e^{-i\mathbf{k}'\mathbf{u}_i'}|n_s'\rangle\langle n_s'|e^{i\mathbf{k}_0\mathbf{u}_i'}|n_s^0\rangle}{E - E_0 - \sum_s \hbar\omega_s(n_s' - n_s^0) + i\Gamma/2}, \quad (13)$$

$p_\varkappa$ is the relative number of resonant nuclei in the $\varkappa$-th site, $I_0$ and $I$ are the spins of the initial and compound nuclei, $\Gamma_{\mathrm{neut}}$ is the partial neutron width, $n_s^0$ and $n_s'$ are the numbers of phonons having a frequency $\omega_s$ in the initial and intermediate states, and $\omega(n_s^0)$ is the Gibbs distribution over the phonons.

In the kinematic approximation we obtain for the cross section for coherent neutron scattering by the crystal the expression

$$\left(\frac{d^2\sigma}{d\Omega\, dE'}\right)_{\mathrm{coh}} = \sum_{n=-\infty}^{\infty}\frac{k'}{k_0}|F^{(n)}(\mathbf{k}_0, \mathbf{k}')|^2 \times \frac{(2\pi)^3}{v_0}N'\sum_\tau \delta(\mathbf{Q} - n\mathbf{q} + \boldsymbol{\tau})\delta(E' - E + n\hbar\Omega), \quad (14)$$

where $N'$ is the number of unit cells with volume $v_0$, $\boldsymbol{\tau}/2\pi$ is the reciprocal-lattice vector, and $F^{(n)}$ is the amplitude for coherent scattering by one cell of the crystal:

$$F^{(n)}(\mathbf{k}, \mathbf{k}') = \sum_\varkappa \exp(i\mathbf{Q}\boldsymbol{\rho}_\varkappa)f_{\mathrm{coh}}^{(n)}(\mathbf{k}, \mathbf{k}')_\varkappa. \quad (15)$$

It can be seen from (14) that within the framework of the kinematic theory one obtains coherent peaks on rigorous satisfaction of the generalized Bragg conditions

$$E' = E - n\hbar\Omega, \quad \mathbf{k}' = \mathbf{k}_0 - n\mathbf{q} + \boldsymbol{\tau}. \quad (16)$$

## 3. DYNAMIC THEORY

We consider a crystal in the form of a plane-parallel plate with lattice vector $\mathbf{l} = l_1\mathbf{a}_1 + l_2\mathbf{a}_2 + l_3\mathbf{a}_3$, where $\mathbf{a}_i$ are the basis vectors $l_1, l_2 = 0, \mp 1, \mp 2, ..., \mp\infty$; $l_3 = 0, 1, 2, ..., N_3 - 1$. Let the origin of the $(x,y,z)$ coordinate system be at the point $\mathbf{l} = 0$, the axes $x$ and $y$ lie in the $(\mathbf{a}_1, \mathbf{a}_2)$ plane, the $z$ axis be directed towards the interior of the plate, and $k_{0z} > 0$. The thickness; of one layer of the unit cells is $d = \mathbf{a}_3 \cdot \mathbf{e}_z$ where $\mathbf{e}_z$ is a unit vector along the $z$ axis. From (8) and (9) follows a system of exact equations that determine the multiple scattering of the neutrons by the crystal:

$$\psi_a^+ = \chi_a + \sum_{i=1}^{N}(E_a + i\eta - \tilde{\mathscr{H}}_0)^{-1}\tilde{t}_i\psi_i,$$
$$\psi_i = \chi_a + \sum_{j(\neq i)=1}^{N}(E_a + i\eta - \tilde{\mathscr{H}}_0)^{-1}\tilde{t}_j\psi_j, \quad (17)$$

where $N$ is the number of atoms and $\psi_i$ is the effective wave incident on the $i$-th atom. Since $f \ll d$, the system (17) can be replaced by an approximate equation for the coherent neutron function $\psi(\mathbf{r}, t)$ in the medium:

$$\psi(\mathbf{r}, t) = e^{i\mathbf{k}_0\mathbf{r}} + \sum_{i=1}^{N}(E + i\eta - \tilde{\mathscr{H}})^{-1}\langle\tilde{t}_i\psi(\mathbf{r}, t)\rangle,$$
$$\tilde{\mathscr{H}} = \hat{\mathscr{H}} - i\hbar\partial/\partial t, \quad (18)$$

where the angle brackets $\langle\ \rangle$ denote averaging over the states of the crystal and over the isotopes. It can be verified by direct substitution that the solution of (18) is of the form

$$\psi(\mathbf{r},t)=\sum_{n=-\infty}^{\infty}\sum_{\nu}C(n,\nu)\exp\{i\mathbf{K}(n,\nu)\mathbf{r}+in\Omega t\},\qquad(19)$$

where the wave vectors in the crystal take on the values

$$\mathbf{K}(n,\nu)=\mathbf{K}_0+\boldsymbol{\tau}_\nu-n\mathbf{q}\quad(\boldsymbol{\tau}_0=0).\qquad(20)$$

From the boundary conditions at $z=0$ it follows that

$$\mathbf{K}_0=\mathbf{k}_0+\delta\mathbf{e}_z.\qquad(21)$$

Substitution of (19) in (18) yields the system of algebraic equations

$$[K^2(n,\nu)+n(2m\Omega/\hbar)-k_0^2]C(n,\nu)$$
$$=\sum_{n'=-\infty}^{\infty}\sum_{\nu'}\frac{4\pi}{v_0}F^{(n-n')}(\mathbf{K}(n',\nu'),\ \mathbf{K}(n,\nu))C(n',\nu').\qquad(22)$$

Let the Bragg conditions (16) be satisfied approximately only for the wave with $\mathbf{K}_1=\mathbf{K}_0+\boldsymbol{\tau}_1-n_1\mathbf{q}$. In this case the deviation from the exact Bragg condition is determined by the parameter

$$\varepsilon=\frac{1}{4k_{1z}}\left[-2\mathbf{k}_0\mathbf{Q}_1+Q_1^2+n_1\left(\frac{2m\Omega}{\hbar}\right)\right],\qquad(23)$$

where $\mathbf{Q}_1=n_1\mathbf{q}-\boldsymbol{\tau}_1$, $\mathbf{k}_1=\mathbf{k}_0-\mathbf{Q}_1$. The two-wave approximation is satisfied if

$$|\hbar\Omega/E-\mathbf{k}_{0,1}\mathbf{q}/k_0^2|\gg2\pi|F|/k_0^2v_0.\qquad(24)$$

Following Ref. 10, we distinguish between two cases. If the neutron wavelength is constant and the direction of incident is varied then

$$\varepsilon=\frac{1}{2\gamma_1}|\mathbf{Q}_1|\cos\theta_B(\theta_B-\theta),\qquad(25a)$$

where $\gamma_1=k_{1z}/k_1$, $\theta$ is the angle between $\mathbf{k}_0$ and the plate surface, and $\theta_B$ is the Bragg angle. If, however $\theta=\theta_B$ and $\lambda$ is varied, then

$$\varepsilon=\frac{1}{2\gamma_1}|\mathbf{Q}_1|\sin\theta_B\left(\frac{\lambda-\lambda_B}{\lambda}\right).\qquad(25b)$$

The vectors $\mathbf{K}_0$, $\mathbf{K}_1$ and the corresponding wave amplitudes $C_0$, $C_1$ are defined by the equations

$$(a_{00}-\delta)C_0+a_{01}C_1=0,\quad a_{10}C_0+(a_{11}-2\varepsilon-\delta)C_1=0,\qquad(26)$$

where

$$a_{\mu\nu}=\frac{2\pi}{k_{\mu z}v_0}F^{((\mu-\nu)n_1)}(\mathbf{K}_\nu,\mathbf{K}_\mu).\qquad(27)$$

The roots of Eqs. (26) are

$$\delta_{1,2}=\frac{a_{00}+a_{11}}{2}-\varepsilon\mp\left[\left(\frac{a_{00}+a_{11}}{2}-\varepsilon\right)^2+2a_{00}\varepsilon-\Delta\right]^{1/2},$$
$$\Delta=a_{00}a_{11}-a_{01}a_{10}.\qquad(28)$$

Furthermore, the plus and minus signs correspond to $\delta_1$ and $\delta_2$, respectively. At $n_1=0$ the equations obtained agree with the results of the theory of elastic deformation of neutrons.[11] For Laue diffraction the wave amplitudes are

$$C_0^{(1)}=\frac{\delta_2-a_{00}}{\delta_2-\delta_1},\quad C_0^{(2)}=-\frac{\delta_1-a_{00}}{\delta_2-\delta_1},$$
$$C_1^{(2)}=-C_1^{(1)}=a_{10}/(\delta_2-\delta_1).\qquad(29)$$

Near the Bragg conditions, the two pairs of waves corresponding to the values of $\delta_1$ and $\delta_2$ have amplitudes $\sim1$. One of these pairs, $\psi_1(\mathbf{r},t)$ is more damped, and the other $\psi_2(\mathbf{r},t)$, is less damped. To suppress the inelastic scattering and the $(n,\gamma)$ reaction completely we must have $\Delta=0$.[11] By way of example we consider the case of an isolated resonance, when $\Gamma\gg\hbar\omega$, $\mathscr{R}$, where $\mathscr{R}$ is the recoil energy of the nucleus. The resonant scattering amplitude is then $f_{\rm res}(E)\sim(E-E_0+i\Gamma/2)^{-1}$.[11] If in addition $E\approx E_0$, $\hbar\Omega\gg\Gamma$, as well as $k_{1z}=k_{0z}$ (the analog of symmetric Laue diffraction), we have

$$\Delta\sim(J_0(z)J_{n_1}(z')-e^{-2W(\mathbf{Q}_1)}J_0(z')J_{n_1}(z)),\qquad(30)$$

where $z\equiv\mathbf{k}\cdot\mathbf{A}$ and $z'\equiv\mathbf{k}'\cdot\mathbf{A}$. By changing the orientations of $\mathbf{k}$ and $\mathbf{k}'$ relative to $\mathbf{A}$ we can attain total suppression of the reaction ($\Delta=0$). The coherent wave

$$\psi_2(\mathbf{r},t)=e^{i\delta_2z}(C_0^{(2)}e^{i\mathbf{k}_0\mathbf{r}}+C_1^{(2)}e^{i\mathbf{k}_1\mathbf{r}+in_1\Omega t})\qquad(31)$$

moves then without the damping due to the reaction (anomalous passage). The reason is that the amplitude for the capture of such a neutron by a nucleus is $\sim\Delta=0$, i.e., no compound nucleus is produced under these conditions.

In Laue diffraction, energy is also pumped from the refracted wave into the diffracted one and back upon penetration into the interior of the crystal (pendellosung effect). Beats are consequently produced between the transmitted and diffracted neutron beams when the wavelength or the plate thickness is changed. In the case of potential scattering, when $\mathrm{Im}\,\bar{b}\ll\mathrm{Re}\,\bar{b}$ and the crystal can be regarded as nonabsorbing, total energy transfer from one wave to the other takes place at $k_{1z}=k_{0z}$. One period of these oscillations takes place over the extinction length $d_e$:

$$d_e=k_{0z}v_0\left[2\left|\sum_\varkappa\bar{b}_\varkappa\exp(i\mathbf{Q}_1\boldsymbol{\rho}_\varkappa)\exp(-W_\varkappa(\mathbf{Q}_1))J_{n_1}(\mathbf{Q}_1\mathbf{A}_\varkappa)\right|\right]^{-1}.\qquad(32)$$

We consider now Bragg diffraction by a semi-infinite crystal. The reflection coefficient, which determines the relative number of reflected neutrons, takes then the form

$$R=\frac{|k_{1z}|}{k_0}\left|\frac{\delta_1-a_{00}}{a_{01}}\right|,\quad\mathrm{Im}\,\delta_1\geq0.\qquad(33)$$

If the crystal is non-absorbing we have total reflection of the neutrons ($R=1$) when $\varepsilon$ varies in an interval of $|\varepsilon-(a_{11}-a_{00})/2|\leqslant(-a_{01}a_{10})^{1/2}$ having a width

$$2(-a_{01}a_{10})^{1/2}=\left(\frac{k_{0z}}{|k_{1z}|}\right)^{1/2}\frac{2\pi}{d_e}.\qquad(34)$$

Thus, the intensity of the reflected neutrons is $\sim |J_{n_1}(\mathbf{Q}_1\mathbf{A})|$. The solution obtained above for the pair of waves $|\mathbf{K}_0\rangle$, and $|\mathbf{K}_1\rangle$ can be regarded as the zeroth approximation, and the small amplitudes of the remaining waves can be obtained from (22) by iteration. Their superposition leads to small temporal beats of the neutron fluxes. The resultant equations contain Bessel functions, so that the physical results should oscillate when the argument of the functions $\mathbf{k}_{0,1}\cdot\mathbf{A}$ or $\mathbf{Q}\cdot\mathbf{A}$ changes.

#### 4. NEUTRON-ACOUSTIC RESONANCE

We solve now Eqs. (22) in the $kA \ll 1$ approximation. Let a sound wave $\mathbf{q} = q\mathbf{e}_z$ propagate in the crystal along the $z$ axis, and let condition (24) not be satisfied. The essential role in the expansion (19) is played then by neutron waves with $n = 0, \mp 1$. Their amplitudes $C(n, \nu)$ can be formally regarded as components of the vector $\mathbf{C}$ in a six-dimensional Euclidean space with basis unit vectors $|n, \nu\rangle$, i.e.,

$$\mathbf{C}=\sum_{n=-1}^{1}\sum_{\nu=0,1} C(n,\nu)\,|n,\nu\rangle. \tag{35}$$

We then rewrite the algebraic equations (22) in the form

$$(\hat{\mathscr{A}}-\delta\hat{I})\mathbf{C}=0,\quad \hat{\mathscr{A}}=\hat{\mathscr{A}}_0+\hat{\mathscr{A}}',\quad \hat{\mathscr{A}}_0=\sum_{n=-1}^{1}\hat{\mathscr{A}}_0(n). \tag{36}$$

The $n$-th zeroth-approximation operator $\hat{\mathscr{A}}_0(n)$ acts here only in the $n$-th subspace with unit vectors $|n, 0\rangle$ and $|n, 1\rangle$, where it has the matrix

$$\begin{gathered}\mathscr{A}_0(n)_{00}=a_{00}+ns,\quad \mathscr{A}_0(n)_{01}=a_{01},\\ \mathscr{A}_0(n)_{10}=a_{10},\quad \mathscr{A}_0(n)_{11}=a_{11}+2\varepsilon+ns,\quad s\equiv q-m\Omega/\hbar k_{0z},\end{gathered} \tag{37}$$

and the detuning parameter of the elastic diffraction is defined by Eq. (24) with $n_1 = 0$. At $\Omega \sim 10^8\ \mathrm{sec}^{-1}$ both terms in $s$ are of the same order of magnitude. We confine ourselves to consideration of symmetric Laue diffraction ($\boldsymbol{\tau}_1\cdot\mathbf{e}_z = 0$) in a crystal with one atom per unit cell. The nonzero matrix elements of the operator $\hat{\mathscr{A}}'$ are then

$$\begin{gathered}\langle\mp1,0|\hat{\mathscr{A}}'|0,1\rangle=\langle0,0|\hat{\mathscr{A}}'|\mp1,1\rangle=-\langle\mp1,1|\hat{\mathscr{A}}'|0,0\rangle\\ =-\langle0,1|\hat{\mathscr{A}}'|\mp1,0\rangle=-ia,\\ a=\frac{\pi(\boldsymbol{\tau}_1\mathbf{A})}{k_{0z}v_0}\bar{b}e^{-W(\boldsymbol{\tau}_1)}.\end{gathered} \tag{38}$$

The eigenvalues of the operator $\hat{\mathscr{A}}_0(n)$ are

$$\delta_i^{(0)}(n)=\delta_i^{(0)}+ns\quad (i=1,2), \tag{39}$$

where $\delta_i^{(0)}$ is given in (28). The corresponding eigenvectors $\mathbf{e}_i(n)$ are obtained by rotation of the basis vectors $|n, 0\rangle$ and $|n, 1\rangle$. By varying the ultrasound frequency $\Omega$ one can make the branches of the dispersion surface $\delta_i^{(0)}(n)$ intersect, so that at a certain value of $\varepsilon$

$$\begin{gathered}\mathrm{Re}\,\delta_2^{(0)}(1)=\mathrm{Re}\,\delta_2^{(0)}+s=\mathrm{Re}\,\delta_1^{(0)},\\ \mathrm{Re}\,\delta_1^{(0)}(-1)=\mathrm{Re}\,\delta_1^{(0)}-s=\mathrm{Re}\,\delta_2^{(0)}.\end{gathered} \tag{40}$$

We call such an intersection of the branches neutron-acoustic resonance, by analogy with the x-ray acoustic resonance.[12-14] Even a small perturbation of $\hat{\mathscr{A}}'$ in the vicinity of the intersection of the dispersion branches mixes substantially the vectors $\mathbf{e}_i^{(0)}(n)$ and distorts $\delta_i^{(0)}(n)$. When the unit vectors $\mathbf{e}_1^{(0)}(0)$ and $\mathbf{e}_2^{(0)}(1)$ are mixed we obtain the following eigenvectors of the operator $\hat{\mathscr{A}}$:

$$\begin{gathered}\mathbf{e}_+=\mathbf{e}_1^{(0)}(0)\cos(\varphi/2)+\mathbf{e}_2^{(0)}(1)\sin(\varphi/2),\\ \mathbf{e}_-=-\mathbf{e}_1^{(0)}(0)\sin(\varphi/2)+\mathbf{e}_2^{(0)}(1)\cos(\varphi/2),\end{gathered} \tag{41}$$

where the angle $\varphi$ is defined as[1]

$$\mathrm{tg}\,\varphi=-2a/(\delta_1^{(0)}-\delta_2^{(0)}-s). \tag{42}$$

Corresponding to these vectors are the eigenvalues

$$\delta_\pm=\frac{\delta_1^{(0)}+\delta_2^{(0)}+s}{2}\pm\frac{1}{2}[(\delta_2^{(0)}+s-\delta_1)^2+4a^2]^{1/2}. \tag{43}$$

In addition, we have also a pair of vectors $\mathbf{e}'_\pm$, which are obtained from (41) by replacing $\mathbf{e}_1^{(0)}(0)$ by $\mathbf{e}_2^{(0)}(0)$ and $\mathbf{e}_2^{(0)}(1)$ by $\mathbf{e}_1^{(0)}(-1)$. They correspond to values $\delta'_\pm = \delta_\pm - s$. Thus, in the absence of ultrasound, waves with eigenvalues $\delta_1^{(0)}$ and $\delta_2^{(0)}$ propagated in the crystal and anomalous passage of the wave with $\delta_2^{(0)}$ took place, since $\mathrm{Im}\delta_2^{(0)} < \mathrm{Im}\delta_1^{(0)}$. Resonant mixing of these waves by ultrasound leads to the appearance of new waves with $\delta_\pm$ and $\delta'_\pm$, for which $\mathrm{Im}\delta_\pm > \mathrm{Im}\delta_2^{(0)}$ (at $s = \mathrm{Re}\Delta K$ and $2a = \mathrm{Im}\Delta K$, where $\Delta K = \delta_1^{(0)} - \delta_2^{(0)}$, we have $\mathrm{Im}\delta_\pm = \mathrm{Im}(\delta_1^{(0)} + \delta_2^{(0)})/2$). As a result of which, in neutron-acoustic resonance, when $\mathbf{q}\|\mathbf{e}_z$, the anomalous passage of the neutrons through the crystal is suppressed.

Using the conditions for the continuity of the wave function on the boundary $z = 0$, we obtain at $\varepsilon = 0$ the following expression for the coherent wave function of the neutron inside the crystal:

$$\begin{gathered}\psi(\mathbf{r},t)=e^{-i\zeta}[(\cos^2(\varphi/2)e^{i\delta_+z}\\ +\sin^2(\varphi/2)e^{i\delta_-z})(\cos\zeta e^{i\mathbf{k}_0\mathbf{r}}+i\sin\zeta e^{i\mathbf{k}_1\mathbf{r}})\\ -{}^1/_2\sin\varphi(e^{i\delta_+z}-e^{i\delta_-z})(\cos(3\zeta+\Omega t)e^{i\mathbf{k}_0\mathbf{r}}\\ -i\sin(3\zeta+\Omega t)e^{i\mathbf{k}_1\mathbf{r}})],\end{gathered} \tag{44}$$

where $\mathbf{k}_1 = \mathbf{k}_0 + \boldsymbol{\tau}_1$ and $\zeta = qz/2$. It can be seen from (44) that in the case of neutron-acoustic resonance the intensity of the transmitted and diffracted neutron beams is subject to strong temporal beats. In addition, the pendellosung intensity beats take place at several frequencies, i.e., are described by a sum of several sinusoids. In contrast to Ref. 13, we did not use a quasistatic approximation, so that the results need not be time-averaged.

1) If $s < 0$, $s$ is replaced in (42)–(44) by $|s|$.


[1]V. M. Agranovich and I. I. Lalov, Zh. Eksp. Teor. Fiz. **69**, 647 (1975) [Sov. Phys. JETP **42**, 328 (1975)].
[2]A. F. Lubchenko and A. M. Korostil', Teor. Mat Fiz. **32**, 416 (1977).
[3]D. F. Zaretskiĭ and V. V. Lomonosov, Yad. Fiz. **26**, 443 (1977) [Sov. J. Nucl. Phys. **26**, 227 (1977)].
[4]D. F. Zaretskiĭ and V. V. Lomonosov, *ibid.* **27**, 1268 (1978) [**27**, 671 (1978)].
[5]V. G. Baryshevskiĭ, Pis'ma Zh. Tekh. Fiz. **8**, 136 (1982 [Sov. J. Tech. Phys. Lett. **8**, 58 (1982)].
[6]A. Ya. Dzublik, Zh. Eksp. Teor. Fiz. **82**, 977 (1982) [Sov. Phys. JETP **55**, 573 (1982)].

[7]R. Michalec, L. Sedlakova, B. Chalupa, D. Galociova, and V. Petrzilka, Acta Cryst. **A27**, 410 (1971).
[8]T. F. Parkinson, E. Gürmen, S. K. Lyalka, and L. D. Muhlestein, J. App. Phys. **45**, 2021 (1974).
[9]A. I. Baz', Ya. B. Zel'dovich, and A. M. Perelomov, Scattering, Reactions, and Decay in Nonrelativistic Quantum Mechanics, Wiley, 1969.
[10]W. H. Zachariasen, theory of x-ray Diffraction in Crystals, Wiley, 1946, p. 118.
[11]Yu. Kagan and A. M. Afanas'ev, Zh. Eksp. Teor. Fiz. **49**, 1505 (1965) [*sic*].
[12]I. R. Éntin, Pis'ma Zh. Eksp. Teor. Fiz. **26**, 392 (1977) [JETP Lett. **26**, 269 (1977).
[13]I. R. Éntin, Zh. Eksp. Teor. Fiz. **77**, 214 (1979) [Sov. Phys. **50**, 110 (1979)].
[14]K. P. Assur and I. R. Éntin, Fiz. Tverd. Tela (Leningrad) **24**, 2122 (1982) [Sov. Phys. Solid State **24**, 1209 (1982)].

Translated by J. G. Adashko