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SCATTERING OF NEUTRONS BY CRYSTALS WITH IMPURITY NUCLEI AND THE PROBLEM OF RECONSTRUCTING THE VIBRATION SPECTRUM

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The scattering of neutrons by crystals of arbitrary symmetry containing isolated impurities is treated. The cross sections for coherent and incoherent scattering corresponding to one-quantum excitations of the system are found. An analysis is made of the problem of separating out the part of the incoherent cross section which is related to the scattering by the impurity atoms and by the disturbed regions near them. It is shown that this part of the cross section contains direct information about the nature of the vibration of the impurity atom, and, most important, information about the density distribution of the phonon frequency spectrum of the ideal (host) lattice.

1. INTRODUCTION

THE present paper investigates the scattering of neutrons by crystals containing arbitrary impurity nuclei. The concentration of foreign atoms in the host is assumed to be sufficiently small so that they can be considered to be isolated.

If inelastic scattering is regarded as a method for obtaining information about the excitation spectrum in a condensed medium, it makes sense to seek a solution of the inverse problem only. But it is obvious that this requires us to find a consistent solution of the direct problem which gives an explicit relation between the scattering cross section and the spectral characteristics of the medium. This in turn allows an independent solution of the dynamical problem for the macroscopic system.

The problem of the vibrations of a crystal containing an isolated impurity was investigated in its general form in a widely known series of papers by I. Lifshitz (cf., for example, [1]) and, for simple models, in papers by Montroll and coworkers.[2] This problem has also been studied in detail in connection with studies of the Mössbauer effect.[3,4] But for determining the probability of the Mössbauer effect it is necessary only to find the class of solutions to which there corresponds a nonzero vibration amplitude of the impurity atom itself. Assuming that the introduction of the impurity does not change the force constants, the problem is considerably simplified. But in the case of scattering of neutrons, the role of the impurity atom is not limited to the peculiarities of the scattering by that atom alone. In fact the neutrons suffer an additional scattering from the whole region of atoms near the impurity site, whose vibrations are perturbed. This makes it necessary to find a complete solution of the problem of the vibrations of a lattice with isolated impurity atoms. The detailed treatment of this problem is given in the second section of this paper.

Thus, for low concentrations of impurity atoms there is an additional incoherent scattering from the randomly distributed perturbed regions. This scattering gives information about both the characteristics of the impurity atom and the vibration spectrum of the initial ideal lattice. In the third section of the paper, we find the relation between the cross section for inelastic scattering of neutrons and the two types of information. We also find the conditions for separating the part of the scattering which is due to the presence of impurity atoms.

We treat monatomic lattices of arbitrary symmetry and assume that the impurity atoms are at lattice sites. The problem is solved for an arbitrary ratio of masses of impurity and host atoms on the assumption that the introduction of the impurity does not change the force constants.

Many of the points related to the scattering of neutrons by nonideal crystals have been treated earlier by Krivoglaz.[5] He studied the question of the broadening of coherent scattering peaks and the transformation of singularities in the energy spectrum of incoherent neutron scattering. These problems will not be considered here.

2. VIBRATION OF A LATTICE CONTAINING AN IMPURITY ATOM.

A. Consider a lattice with one atom per unit cell. Suppose that there is an impurity atom at one of the lattice sites (the origin). We shall assume that inserting the impurity does not change the force constants coupling the other atoms to one another and to the foreign atom. Then the equation for determining the eigenfrequencies and eigenfunctions (reduced displacements) for the vibrations of the lattice has the form

$$\omega^2\Phi^i(\mathbf{r}_n) = \sum_{n'} (m_n m_{n'})^{-1/2} A_0^{ik}(\mathbf{r}_n - \mathbf{r}_{n'})\,\Phi^k(\mathbf{r}_{n'}),$$

$$m_n = m(1 - \varepsilon\delta_{n0}) \tag{2.1}$$

with the usual periodicity conditions at the boundary. (The notation is the same as in [3,4]; we sum over repeated Latin superscripts.)

Setting $\epsilon = 0$ in (2.1), we get the equation for the vibrations of the ideal lattice. The complete system of its 3N orthonormal real solutions can be written in the form

$$\varphi^i_{\mathbf{f}\alpha 1}(\mathbf{r}_n) = \sqrt{2/N}\,e^i(\mathbf{f},\ \alpha)\cos \mathbf{f}\mathbf{r}_n; \tag{2.2'}$$

$$\varphi^i_{\mathbf{f}\alpha -1}(\mathbf{r}_n) = \sqrt{2/N}\,e^i(\mathbf{f},\ \alpha)\sin \mathbf{f}\mathbf{r}_n; \qquad 2.2'')$$

$$e^i(\mathbf{f},\ \alpha)\,e^i(\mathbf{f},\alpha') = \delta_{\alpha\alpha'}, \qquad \sum_{\alpha=1}^{3} e^i(\mathbf{f},\alpha)\,e^{i'}(\mathbf{f},\alpha) = \delta^{ii'},$$

$$\mathbf{e}(-\mathbf{f},\ \alpha) = \mathbf{e}(\mathbf{f},\ \alpha), \qquad \alpha = 1,\ 2,\ 3. \tag{2.3}$$

The wave vector **f** takes on N/2 values uniformly distributed over the region corresponding to half of the fundamental cell in the reciprocal lattice; the index $\zeta = \pm 1$ gives the parity of the solution.

From (2.1) it follows that for $\epsilon = 0$ the eigenvalues ω_0^2 are independent of ζ, so that an equal number of solutions (2.2′) and (2.2″) belong to each frequency.

Let $\{\mathbf{f}\}$ be a set of wave vectors which are connected with one another by the transformations of the point symmetry group of the crystal, the "star" of the irreducible representation. To each star of vectors **f** there correspond in general three stars of vectors $\mathbf{e}(\mathbf{f}, \alpha)$ ($\alpha = 1, 2, 3$) and three different eigenvalues. We shall number the vectors of a star by the index λ, and the different stars of vectors **e** by the index p. Then instead of the usual dependence of the squared frequency and polarization vector on wave vector and branch number

$$\omega_0^2(\mathbf{f},\ \alpha), \qquad \mathbf{e}(\mathbf{f},\ \alpha)$$

we have

$$\omega_{0p\lambda}^2, \qquad \mathbf{e}_{p\lambda},$$

where eigenvalues with the same λ coincide:

$$\omega_{0p\lambda}^2 = \omega_{0p}^2, \qquad \lambda = 1,\ 2,\ \ldots,\ \vartheta_p/2.$$

We shall assume that the frequencies are labelled by the index p in increasing order. Twice the number of vectors **e** in a star obviously gives the degree of degeneracy ϑ_p of the corresponding frequency (the factor two is due to the degeneracy in ζ).

For an overwhelmingly large number of the frequencies this multiplicity has the same value ϑ, given by the symmetry of the lattice. The exceptions occur when the wave vector **f** to which the frequency corresponds is distinguished by some symmetry element of the crystal (for example, is in a symmetry plane or along a symmetry axis), or when there is accidental degeneracy. But we shall be interested only in quantities which are obtained by summation over a macroscopic number of states. We shall therefore not use the index λ in the stars of **f** and $\mathbf{e}(\mathbf{f}, \alpha)$.

In the presence of the impurity there is a partial lifting of the degeneracy of all the levels. The frequencies which are split off fall in the interval between ω_{0p} and ω_{0p+1}. As was shown in [3], Eq. (2.1) can be transformed, for the frequencies which are split, to the following form:

$$D^{ik}(\omega^2)\, j^k = j^i, \tag{2.4}$$

where **j** is a unit vector in the direction of the displacement of the impurity atom ($\mathbf{\Phi}(0) = \Phi\mathbf{j}$), while

$$D^{ik}(\omega^2) = \frac{2\varepsilon\omega^2}{N}\sum_{\mathbf{f}\alpha}\frac{e^i(\mathbf{f},\ \alpha)\,e^k(\mathbf{f},\ \alpha)}{\omega^2 - \omega_0^2(\mathbf{f},\ \alpha)}\ . \tag{2.5}$$

Throughout the paper, summations and integrations extend over half the fundamental cell of the reciprocal lattice (this is the reason for the factor of 2 compared to [1]).

An analysis of (2.4) shows that the maximum number of frequencies split off from each level is three, the actual number depending on the symmetry of the crystal. Let us consider the various crystal systems.

1. Triclinic system. There is one non-identical symmetry transformation, the inversion. All frequencies ω_0 are degenerate with the same multiplicity $\vartheta = 2$. In the presence of the impurity atom, one frequency is split off from each degenerate level, corresponding to the value $\mathbf{j}(\omega^2)$ determined from (2.4).

2. Monoclinic system. The degree of degeneracy is $\vartheta = 4$. The symmetric tensor D^{ik} has four independent components. In the general case, two frequencies are split off—one belongs to a vibration with **j** parallel to the two-fold axis, the other is determined at the same time has its **j** in the plane perpendicular to the two-fold axis.

3. Rhombic system. The degree of degeneracy is $\vartheta = 8$. In the coordinate system with its axes along the two-fold symmetry axes, the tensor D^{ik}

is in diagonal form. Then (2.4) splits into three independent equations. We thus get three frequencies splitting off from each level, with polarization vectors j along the symmetry axes.

4. Tetragonal, trigonal, and hexagonal systems. In all these cases, the tensor D^{ik} reduces to diagonal form in a coordinate system having one of its axes along the c axis. Two of the three equations which correspond to the other two axes coincide. Thus there is a splitting off of one frequency with j parallel to the c axis, and two identical frequencies with mutually perpendicular vectors j lying in an arbitrary position in the plane perpendicular to the c axis.

5. Cubic system. From each degenerate level, three identical frequencies split off; the system of three mutually perpendicular vectors j can be chosen arbitrarily.

In accordance with the above considerations, we shall not deal in detail with cases where the directions of the vectors of the star are distinguished crystallographically, although the corresponding analysis can be done in straight-forward fashion. We mention only that for an initial frequency for which the star of vectors e lies in a symmetry plane, after introduction of the impurity atom two frequencies are split off; for frequencies to which there corresponds a star of vectors e directed along a symmetry axis, only one frequency splits off, independent of the symmetry of the crystal.

To simplify the presentation, we shall restrict ourselves in what follows to crystals with symmetry no lower than rhombic. In all these cases the number of frequencies split off is three.

B. As we have already remarked, the impurity atom participates only in vibrations whose frequencies are split off. Its displacement in all other vibrations with unchanged frequencies ω_0 is zero. As a result, for all the unsplit frequencies one can easily show that (2.1) is identical with the equation for the vibrations of the ideal lattice.

The complete system of orthonormal functions for the ideal lattice has the form (2.2). We replace f, α, ζ by the indices p, ν, where

$$\nu = \begin{cases} \lambda & \zeta = 1 \\ \lambda + \vartheta/2 & \zeta = -1. \end{cases}$$

Obviously,

$$\mathbf{f}_{\lambda+\vartheta/2} = \mathbf{f}_\lambda$$

and consequently

$$\mathbf{e}_{p\lambda+\vartheta/2} = \mathbf{e}_{p\lambda}, \qquad \omega^2_{0p\lambda+\vartheta/2} = \omega^2_{0p\lambda} = \omega^2_{0p}.$$

Then (2.2) can be rewritten as

$$\varphi^i_{p\nu}(\mathbf{r}_n) = \sqrt{2/N}\, e^i_{p\nu} \cos \mathbf{f}_{p\nu}\mathbf{r}_n, \qquad \nu = 1, 2, \ldots, \vartheta/2; \quad (2.6')$$

$$\varphi^i_{p\nu}(\mathbf{r}_n) = \sqrt{2/N}\, e^i_{p\nu} \sin \mathbf{f}_{p\nu}\mathbf{r}_n, \qquad \nu = \vartheta/2 + 1, \ldots, \vartheta. \quad (2.6'')$$

The total number of independent functions in (2.2) and (2.6) is, of course, the same and equal to 3N.

We make an orthogonal transformation and replace (2.6) by a new system of functions:

$$\psi^i_{p\nu}(\mathbf{r}_n) = \sum_{\delta=1}^{\vartheta/2} S_{\nu\delta}(p)\, \varphi^i_{p\delta}(\mathbf{r}_n), \qquad \nu = 1, 2 \ldots, \vartheta/2;$$
$$\varphi^i_{p\nu}(\mathbf{r}_n), \qquad \nu = \vartheta/2 + 1, \ldots, \vartheta \qquad (2.7)$$

and require that for $\nu = 4, \ldots, \vartheta/2$

$$\psi^i_{p\nu}(0) = 0$$

or

$$\sum_{\delta=1}^{\vartheta/2} S_{\nu\delta}(p)\, e^i_{p\delta} = 0. \qquad (2.8)$$

It is easy to show that an orthogonal matrix satisfying the $3(\vartheta/2 - 3)$ $(i = 1, 2, 3)$ conditions (2.8) can be constructed for any crystal with symmetry equal to rhombic or higher; this matrix is determined to within an orthogonal transformation which leaves invariant the subspaces of functions (2.7) with $\nu = 1, 2, 3$ [cf. (2.15)] and with $\nu = 4, \ldots, \vartheta/2$ [and consequently also the conditions (2.8)]. For crystals of the triclinic and monoclinic systems $(\vartheta/2 < 3)$, all the possible solutions of equation (2.1) are exhausted by the functions (2.6″) and the functions corresponding to the split-off frequencies [cf. later in (2.17)], so that there is no need for the construction given here.

Thus for each p we have determined $\vartheta - 3$ functions $\psi_{p\nu}(\mathbf{r}_n)$ $(\nu = 4, \ldots, \vartheta/2)$ and $\varphi_{p\nu}(\mathbf{r}_n)$ $(\nu = \vartheta/2 + 1, \ldots, \vartheta)$, which are eigenfunctions of the vibration problem for the ideal lattice, correspond to ω^2_{0p}, and vanish for $\mathbf{r}_n = 0$.

We now find the explicit form of the functions $\psi^i_{p\nu'}(\mathbf{r}_n)$ for $\nu' = 1, 2, 3$. The condition that they be orthogonal to the functions (2.7) with $\nu = 4, \ldots, \vartheta/2$ gives the relation

$$\sum_n \psi^i_{p\nu'}(\mathbf{r}_n)\, \psi^i_{p\nu}(\mathbf{r}_n) = \sum_{\delta=1}^{\vartheta/2} S_{\nu'\delta}(p)\, S_{\nu\delta}(p) = 0. \qquad (2.9)$$

We choose $S_{\nu'\delta}(p)$ in the form

$$S_{\nu'\delta}(p) = C_{\nu'}(p)\, e^i_{p\delta} j^i_{p\nu'}, \qquad (2.10)$$

where $\mathbf{j}_{p\nu'}$ is an arbitrary unit vector. Then, if we use (2.8) we see that condition (2.9) is satisfied identically.

Let $\nu'' = 1, 2, 3$. Then

$$\sum_n \psi^i_{p\nu'}(\mathbf{r}_n)\, \psi^i_{p\nu''}(\mathbf{r}_n) = C_{\nu'}(p)\, C_{\nu''}(p) \sum_{\delta=1}^{\vartheta/2} e^i_{p\delta} e^k_{p\delta} j^i_{p\nu'} j^k_{p\nu''}. \qquad (2.11)$$

We introduce the tensor

$$L^{ik}(p) = \sum_{\delta=1}^{\vartheta/2} e^i_{p\delta} e^k_{p\delta}. \qquad (2.12)$$

We choose the vectors $\mathbf{j}_{p\nu'}$ so that they are eigenvectors of the tensor $L^{ik}(p)$, i.e.,

$$L^{ik}(p)\, j^k_{p\nu'} = \eta_{\nu'}(p)\, j^i_{p\nu'}, \qquad \nu' = 1, 2, 3. \qquad (2.13)$$

Because they are mutually orthogonal, (2.11) vanishes for $\nu' \neq \nu''$, while the condition for normalization of the functions (2.7) to unity gives the relation

$$C_{\nu'}(p) = 1/\sqrt{\eta_{\nu'}(p)}. \qquad (2.14)$$

Thus

$$\psi^i_{p\nu}(\mathbf{r}_n) = [\eta_{\nu'}(p)]^{-1/2} \sum_{\delta=1}^{\vartheta/2} (\mathbf{j}_\nu \mathbf{e}_{p\delta})\, \varphi^i_{p\delta}(\mathbf{r}_n), \qquad \nu = 1, 2, 3. \qquad (2.15)$$

Starting with the rhombic system, the vectors $\mathbf{j}_{p\nu} = \mathbf{j}_\nu$ are along the fixed principal axes of the crystal. Then

$$\sum_{\nu=1}^{3} \eta_\nu(p) = L^{ii}(p) = \vartheta/2.$$

In particular, in a cubic crystal

$$L^{ik}(p) = {}^1\!/_6\, \vartheta \delta^{ik}, \qquad \eta_\nu(p) = \vartheta/6. \qquad (2.16)$$

The functions (2.7) and (2.6″) form a complete system of eigenfunctions for the problem of vibration of an ideal lattice. In the presence of the impurity atom, the system of eigenfunctions changes. It is now formed by the functions (2.6″) and the functions (2.7) for $y = 4, \ldots, \vartheta/2$ (taking (2.8) into account), while new functions corresponding to the split-off frequencies appear in place of (2.15). These functions, which are actually superpositions of the functions (2.15) with different p and ν, were found in [3] and can be written, taking account of normalization, in the following form:

$$\Phi^i_{p\nu}(\mathbf{r}_n) = \left(\frac{d \ln \omega^2_{p\nu}}{d\varepsilon}\right)^{1/2} j^k_\nu \frac{2}{N} \sum_{\mathbf{f}\alpha} \left[\varepsilon \omega^2_{p\nu} \frac{e^i(\mathbf{f}, \alpha)\, e^k(\mathbf{f}, \alpha)}{\omega^2_{p\nu} - \omega^2_0(\mathbf{f}, \alpha)} + \frac{1}{3}\left(\sqrt{1-\varepsilon} - 1\right)\delta^{ik}\right] \cos \mathbf{f}\mathbf{r}_n, \qquad \nu = 1, 2, 3; \qquad (2.17)$$

$$\frac{d \ln \omega^2_{p\nu}}{d\varepsilon} = \left\{\frac{2\varepsilon^2 \omega^4_{p\nu}}{N} \sum_{\mathbf{f}\alpha} \frac{(\mathbf{j}_\nu \mathbf{e}(\mathbf{f}, \alpha))^2}{[\omega^2_{p\nu} - \omega^2_0(\mathbf{f}, \alpha)]^2} - \varepsilon\right\}^{-1}. \qquad (2.18)$$

Thus if we use $\Phi^i_{p\nu}(\mathbf{r}_n)$ to denote the complete system of orthonormal functions for the problem of the vibration of the lattice in the presence of the impurity atom, then for $\nu = 1, 2, 3$, these functions coincide with (2.17) (the corresponding eigenvalues are $\omega^2_{p\nu}$), for $\nu = 4, \ldots, \vartheta/2$ they coincide with (2.7)—(2.8), and for $\nu = \vartheta/2 + 1, \ldots, \vartheta$, with (2.6″) ($\omega^2_{p\nu} = \omega^2_{0p}$ for $4 \leq \nu \leq \vartheta$).

C. We shall again limit ourselves to crystals with symmetry no lower than rhombic. Then, from (2.4) and (2.5), in a coordinate system whose axes are along the principal symmetry axes of the crystal, we have three independent equations for determining the shifted frequencies:

$$\frac{2\varepsilon\omega^2_{p\nu}}{N} \sum_{\mathbf{f}\alpha} \frac{[e^\nu(\mathbf{f}, \alpha)]^2}{\omega^2_{p\nu} - \omega^2_0(\mathbf{f}, \alpha)} = 1, \qquad \nu = 1, 2, 3. \qquad (2.19)$$

These equations, in addition to the quasicontinuous spectrum $0 < \omega^2_{p\nu} < \omega^2_{0\,\max}$ ($\omega_{0\,\max}$ is the limiting frequency of the quasicontinuous spectrum of the regular lattice), can have solutions in the form of discrete frequencies $\omega^2_{p\nu} > \omega^2_{0\,\max}$.

For $\omega^2 > \omega^2_{0\,\max}$ the denominator in (2.19) does not vanish, and we can change from summation over f to integration. As a result, to determine the discrete frequencies, if they exist, we have an equation analogous to the one found by I. Lifshitz [1]:

$$\varepsilon\omega^2 \int_0^{\omega^2_{0\,max}} \frac{g^{(\nu)}(\omega^2_0)\, d\omega^2_0}{\omega^2 - \omega^2_0} = 1, \qquad \nu = 1, 2, 3, \qquad (2.20)$$

where

$$g^{(\nu)}(\omega^2_0) = \frac{2v_0}{(2\pi)^2} \sum_\alpha \int_{\omega^2_0(\mathbf{f}, \alpha) = \omega^2_0} \frac{[e^\nu(\mathbf{f}, \alpha)]^2}{|\nabla\omega^2_0(\mathbf{f}, \alpha)|}\, d\Omega_{\mathbf{f}} \qquad (2.21)$$

(v_0 is the volume of the unit cell). The integration in (2.21) extends over those portions of the surface $\omega^2_0(\mathbf{f}, \alpha) = \omega^2_0$ which are located within the region chosen initially—half the fundamental cell of the reciprocal lattice.

The quantity

$$g(\omega^2_0) = \frac{1}{3} \sum_{\nu=1}^{3} g^{(\nu)}(\omega^2_0) = \frac{2v_0}{3(2\pi)^3} \sum_\alpha \int_{\omega^2_0(\mathbf{f}, \alpha) = \omega^2_0} \frac{d\Omega_{\mathbf{f}}}{|\nabla\omega^2_0(\mathbf{f}, \alpha)|} \qquad (2.22)$$

is a function of the density of the squared frequencies for the initial ideal lattice. From the very definitions (2.21) and (2.22) it follows that the functions $g^{(\nu)}(\omega^2_0)$ and $g(\omega^2_0)$ satisfy the normalization

$$\int_0^{\omega^2_{0\,max}} g^{(\nu)}(\omega^2_0)\, d\omega^2_0 = 1, \qquad \int_0^{\omega^2_{0\,max}} g(\omega^2_0)\, d\omega^2_0 = 1. \qquad (2.23)$$

All the considerations about the degeneracy of the split-off frequencies obviously remain valid for the discrete frequencies. Thus in a cubic crystal $g^{(\nu)}(\omega^2_0) = g(\omega^2_0)$, and we arrive at the single equation (2.20) for determining the threefold degenerate frequency.

It is easy to show that each of the equations (2.20) has a unique solution if and only if

$$\varepsilon > \left[\int_0^{\omega^2_{0max}} \frac{g^{(\nu)}(\omega^2_0)\, d\omega^2_0}{1 - \omega^2_0/\omega^2_{0max}}\right]^{-1}. \qquad (2.24)$$

This inequality is the condition which the spectrum of the system must satisfy in order to have discrete frequencies. Their number can vary up to three, depending on the values of ν for which (2.24) is valid.

Because the right side of (2.24) is positive, discrete frequencies appear only when the impurity atoms are lighter than the host atoms, and for the usual vibration spectra m_0/m must be considerably less than unity. (For example, in a simple cubic lattice, with nearest neighbor interactions, and with equal central and noncentral force constants, the discrete frequency appears only when $m_0/m < 0.670$.)

D. In the quasicontinuous spectrum, as in [1,3], we represent $\omega_{p\nu}^2$ in the form

$$\omega_{p\nu}^2=\omega_{0p}^2+\Delta\omega_{p\nu}^2, \qquad \Delta\omega_{p\nu}^2=z_{p\nu}\delta\omega_{0p}^2,$$
$$\delta\omega_{0p}^2=\omega_{0p+1}^2-\omega_{0p}^2, \qquad 0\leqslant z_{p\nu}\leqslant 1. \tag{2.25}$$

Taking a quasiequidistant distribution of the squared frequencies ω_{0p}^2, we find the value of $z_{p\nu}$ from Eq. (2.19) by the usual method (cf. [1,3]). Going to the limit $\delta\omega_{0p}^2 \to 0$, $N \to \infty$, so that $\omega_{0p}^2 = \omega^2$ is unshifted, we finally get

$$z_\nu(\omega^2)=\frac{1}{\pi}\operatorname{arc\,tg}\left\{\left|\left[1-\varepsilon\omega^2\fint_0^{\omega_{0\,max}^2}\frac{g^{(\nu)}(\omega_0^2)\,d\omega_0^2}{\omega^2-\omega_0^2}\right]\right|\frac{1}{\pi\varepsilon\omega^2 g^{(\nu)}(\omega^2)}\right\}. \tag{2.26*}$$

This result can be used immediately for computing quantities having the form of sums over the shifted frequencies of the quasicontinuous spectrum with weights $d\ln\omega_{p\nu}^2/d\epsilon$. Using the relation

$$\frac{d\ln\omega_{p\nu}^2}{d\varepsilon}=\frac{\delta\omega_{0p}^2}{\omega_{0p}^2}\frac{\partial z_{p\nu}}{\partial\varepsilon},$$

which follows from (2.25), we quickly get

$$\lim_{N\to\infty}\sum_{\substack{p\\(\omega^2=0)}}^{(\omega_{0\,max}^2)}\frac{d\ln\omega_{p\nu}^2}{d\varepsilon}(\ldots)=\int_0^{\omega_{0\,max}^2}d\omega^2 f_\nu(\omega^2)(\ldots), \tag{2.27}$$

where

$$f_\nu(\omega^2)\equiv\frac{1}{\omega^2}\frac{\partial z_\nu(\omega^2)}{\partial\varepsilon}$$
$$=g^{(\nu)}(\omega^2)\left\{\left|\left[1-\varepsilon\omega^2\fint_0^{\omega_{0\,max}^2}\frac{g^{(\nu)}(\omega_0^2)\,d\omega_0^2}{\omega^2-\omega_0^2}\right]\right|^2+[\pi\varepsilon\omega^2g^{(\nu)}(\omega^2)]^2\right\}^{-1} \tag{2.28}$$

(assuming, of course, that the integral in (2.27) exists).

One can get an important normalization relation for the quantity $f_\nu(\omega^2)$. To derive it, we set $\mathbf{r}_n = \mathbf{r}_{n'}$, $i = i'$ (no summation!) in the relation

$$\sum_{p\nu}\Phi_{p\nu}^i(\mathbf{r}_n)\,\Phi_{p\nu}^{i'}(\mathbf{r}_n')=\delta^{ii'}\delta_{\mathbf{r}_n\mathbf{r}_{n'}}, \tag{2.29}$$

which follows from the completeness of the orthonormal function system $\Phi_{p\nu}^i(\mathbf{r}_n)$. Remembering that

$$\mathbf{\Phi}_{p\nu}(0)=\begin{cases}\sqrt{1-\varepsilon}\,(d\ln\omega_{p\nu}^2/d\varepsilon)^{1/2}\,\mathbf{j}_\nu, & \nu=1,2,3\\ 0 & \nu=4,\ldots,\vartheta\end{cases} \tag{2.30}$$

[cf. (2.17) and (2.4)], and also that $j_\nu^i = \delta^{i\nu}$, we get

$$(1-\varepsilon)\sum_p d\ln\omega_{p\nu}^2/d\varepsilon=1. \tag{2.31}$$

Changing from summation to integration over the quasicontinuous spectrum, we get the required relation

$$(1-\varepsilon)\int_0^{\omega_{0\,max}^2}f_\nu(\omega^2)\,d\omega^2+(1-\varepsilon)\,d\ln\omega_{D\nu}^2/d\varepsilon=1. \tag{2.32}$$

The second term comes from the discrete frequency. As expected, for $\epsilon = 0$ (2.32) goes over into the first of the conditions (2.23).

If we know the partial density function for the squared frequencies $g^{(\nu)}(\omega_0^2)$, the quantity $d\ln\omega_{D\nu}^2/d\epsilon$ as a function of $\omega_{D\nu}^2$ is given by

$$\frac{d\ln\omega_{D\nu}^2}{d\varepsilon}=\left\{\varepsilon^2\omega_{D\nu}^2\int_0^{\omega_{0\,max}^2}\frac{g^{(\nu)}(\omega_0^2)\,d\omega_0^2}{(\omega_{D\nu}^2-\omega_0^2)^2}-\varepsilon\right\}^{-1}, \tag{2.33}$$

which follows immediately from (2.18) when we change to integration.

The numerical value of $d\ln\omega_{D\nu}^2/d\epsilon$ as a function of ϵ alone can be found in principle from (2.32) as an integral of $f_\nu(\omega^2)$, or by determining $\omega_{D\nu}^2 = \omega_{D\nu}^2(\epsilon)$ from Eq. (2.20).

E. Let us write the displacement of an arbitrary atom as an expansion in normal vibrations:

$$u^i(\mathbf{r}_n)=\sum_{p\nu}u_{p\nu}^i(\mathbf{r}_n). \tag{2.34}$$

It is not difficult to show that

$$u_{p\nu}^i(\mathbf{r}_n)=\sqrt{\hbar/m_n\omega_{p\nu}}\,\Phi_{p\nu}^i(\mathbf{r}_n)\,q_{p\nu}, \tag{2.35}$$

where $q_{p\nu}$ is a dimensionless real normal coordinate, corresponding to the vibration with frequency $\omega_{p\nu}$.

3. SCATTERING OF SLOW NEUTRONS; DISCRETE FREQUENCIES ABSENT

Let us consider the scattering of neutrons by crystals with impurity atoms. We assume that the concentration of impurities is so low that the scattering occurs independently from the isolated regions of disturbance around the impurity atoms. We can then restrict the treatment to neutron scattering by a crystal with a single impurity nucleus, and make use of the results obtained above.

The general expression for the interaction of a neutron with an arbitrary crystal lattice can be written as follows (cf. [6]):

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*tg = tan.

$$V(\mathbf{r}) = \sum_n [A_n \hat{I} + B_n (\hat{\mathbf{S}}\hat{\mathbf{K}}_n)]\, \delta(\mathbf{r} - \mathbf{R}_n). \qquad (3.1)$$

Here $\hat{\mathbf{S}}$ is the neutron spin operator; $\hat{\mathbf{K}}_n$ is the spin operator for the nucleus at the n-th lattice site; A_n and B_n are nuclear parameters; $\mathbf{R}_n = \mathbf{r}_n + \mathbf{u}(\mathbf{r}_n)$.

Let us consider the matrix element of (3.1) corresponding to a transfer of momentum $\hbar\mathbf{k} = \hbar(\mathbf{k}_1 - \mathbf{k}_2)$ to the lattice with a simultaneous change in occupation numbers of $r_{p\nu} = n'_{p\nu} - n_{p\nu}$. Remembering (2.35), after averaging over the initial equilibrium state of the crystal and averaging over the initial and summing over the final states for the projection of the neutron and nuclear spins, we find for the square modulus of the matrix element

$$\begin{aligned} M(\{r_{p\nu}\}, \mathbf{k}) &= \sum_n \sum_{n'} A_n A_{n'} \exp[i\mathbf{k}(\mathbf{r}_n - \mathbf{r}_{n'})] \exp\left(-\frac{w_n + w_{n'}}{2}\right) \\ &\times \prod_{p\nu} \exp\left(\frac{r_{p\nu}\hbar\omega_{p\nu}}{T}\right) I_{r_{p\nu}}\left[\frac{\hbar(\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))(\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_{n'}))}{2\sqrt{m_n m_{n'}}\,\omega_{p\nu}} \operatorname{sh}^{-1}\frac{\hbar\omega_{p\nu}}{2T}\right] \\ &+ \frac{1}{4}\sum_n B_n^2 K_n(K_n+1) e^{-w_n} \prod_{p\nu} \exp\left(\frac{r_{p\nu}\hbar\omega_{p\nu}}{2T}\right) I_{r_{p\nu}} \\ &\times \left[\frac{\hbar(\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))^2}{2m_n\omega_{p\nu}} \operatorname{sh}^{-1}\frac{\hbar\omega_{p\nu}}{2T}\right], \end{aligned} \qquad (3.2)^*$$

$$w_n = \frac{\hbar}{2m_n}\sum_{p\nu}\frac{(\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))^2}{\hbar\omega_{p\nu}}(2\bar{n}_{p\nu} + 1). \qquad (3.3)$$

We have used the relation[4]

$$\langle n + r | \exp[i\sqrt{2x}q] | n\rangle = \begin{cases} e^{-x/2}(i\sqrt{x})^r \sqrt{n!/(n+r)!}\, L_n^r(x), & r > 0 \\ e^{-x/2}(i\sqrt{x})^{|r|} \sqrt{(n+r)!/n!}\, L_{n+r}^{|r|}(x), & r \leqslant 0 \end{cases}$$

and the summation formula[7]

$$\begin{aligned} (1 - z)\sum_{n=0}^{\infty}\frac{n!}{(n+r)!} L_n^r(x) L_n^r(y)\, z^n \\ = \exp\left\{-(x+y)\frac{z}{1-z}\right\}(xyz)^{-r/2} I_r\left\{\frac{2(xyz)^{1/2}}{1-z}\right\}. \end{aligned}$$

Here L_n^r is a generalized Laguerre polynomial, I_r is the Bessel function of r-th order and pure imaginary argument, T is the crystal temperature in energy units.

We note that the expressions (3.2)—(3.3) are valid for the scattering of a neutron by an arbitrary system of harmonically interacting particles. The particular properties of the system find their expression in the explicit form of the functions $\Phi_\beta^i(\mathbf{r}_n)$ and the spectrum of frequencies ω_β^2.

In this section we assume that there are no localized vibrations with discrete frequencies, i.e., there is only a quasicontinuous spectrum. Remembering that the amplitudes of the atomic displacements in each normal vibration belonging to the quasicontinuous spectrum $\sim N^{-1/2}$, we should restrict ourselves to cases where all the $|r_{p\nu}| \leq 1$. Then

$$\exp\left\{\pm\frac{\hbar\omega}{2T}\right\} I_{\pm 1}\left[(xy)^{1/2}\frac{1}{\operatorname{sh}(\hbar\omega/2T)}\right] = (xy)^{1/2}\left(\bar{n} + \frac{1}{2} \pm \frac{1}{2}\right). \qquad (3.4)$$

In addition suppose that the regular lattice consists of quite heavy nuclei. Then at not too high temperatures we can neglect the contribution of multiquantum transitions and treat only scattering processes which are accompanied by the creation or absorption of one quantum of the vibration p, ν. For such a process, using (3.4), Eq. (3.2) takes the form

$$\begin{aligned} M_{p\nu} &= \left\{\left|\sum_n \frac{A_n}{\sqrt{m_n}} e^{-w_n/2} e^{i\mathbf{k}\mathbf{r}_n}(\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))\right|^2 \right. \\ &\left. + \frac{1}{4}\sum_n \frac{B_n^2}{m_n} K_n(K_n+1) e^{-w_n}(\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))^2\right\} \\ &\times \frac{\hbar}{2\omega_{p\nu}}\left(\bar{n}_{p\nu} + \frac{1}{2} \pm \frac{1}{2}\right). \end{aligned} \qquad (3.5)$$

(From here on the upper sign refers to creation, the lower to absorption by the neutron of a vibration quantum.)

Let us make some remarks about the quantity e^{-w_n} in (3.3), the Debye-Waller factor. At sufficiently high temperatures, when

$$T \gtrsim \hbar\omega_{0\,max} \sim \Theta \qquad (3.6)$$

(Θ is the Debye temperature), the relation

$$2\bar{n}_{p\nu} + 1 \approx \frac{2T}{\hbar\omega_{p\nu}}\left[1 + \frac{1}{12}\left(\frac{\hbar\omega_{p\nu}}{T}\right)^2\right]. \qquad (3.7)$$

holds. We then have for w_n,

$$w_n = 2TR_n\frac{1}{\hbar^2}\sum_{p\nu}\frac{1}{\omega_{p\nu}^2}(\boldsymbol{\varkappa}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))^2 + \frac{R_n}{6T}\sum_{p\nu}(\boldsymbol{\varkappa}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))^2. \qquad (3.8)$$

Here R_n is the recoil energy of atom n:

$$R_n = \frac{\hbar^2 k^2}{2m_n} = R\frac{1}{(1 - \varepsilon\delta_{n0})}, \qquad R = \frac{\hbar^2 k^2}{2m}, \qquad \boldsymbol{\varkappa} = \frac{\mathbf{k}}{k}. \qquad (3.9)$$

Because of (2.29), the last term in (3.8) is simply equal to $R_n/6T$. To calculate the first term in (3.8), in complete analogy with the procedure in [4], we multiply both sides of (2.1) (for the p, ν vibration) by

$$\omega_{p\nu}^{-2}\Phi_{p\nu}^k(\mathbf{r}_l)(m_l m_n)^{1/2}[A_0^{-1}(\mathbf{r}_l - \mathbf{r}_n)]^{ji}$$

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*sh = sinh.

($[A_0^{-1}(\mathbf{r}_l - \mathbf{r}_n)]^{ik}$ is the matrix inverse to $A_0^{ik}(\mathbf{r}_l - \mathbf{r}_n)$) and sum over $\mathbf{r}_n$, i, p, ν. Using (2.29), we get

$$\sum_{p\nu} \omega_{p\nu}^{-2} \Phi_{p\nu}^{i}(\mathbf{r}_l)\, \Phi_{p\nu}^{k}(\mathbf{r}_l) = m_l\, [A_0^{-1}(0)]^{ik}. \qquad (3.10)$$

A similar relation holds for the original ideal lattice:

$$\sum_{\mathbf{f}\alpha\zeta} \omega_0^{-2}(\mathbf{f}, \alpha)\, \varphi_{\mathbf{f}\alpha\zeta}^{i}(\mathbf{r}_l)\, \varphi_{\mathbf{f}\alpha\zeta}^{k}(\mathbf{r}_l)$$
$$= \frac{2}{N} \sum_{\mathbf{f}\alpha} \omega_0^{-2}(\mathbf{f}, \alpha)\, e^{i}(\mathbf{f}, \alpha)\, e^{k}(\mathbf{f}, \alpha) = m\, [A_0^{-1}(0)]^{ik} \qquad (3.11)$$

Comparing (3.8), (3.10), and (3.11) we finally get

$$w_n = 4RT \frac{1}{\hbar^2} \frac{1}{N} \sum_{\mathbf{f}\alpha} \omega_0^{-2}(\mathbf{f}, \alpha)\, (\varkappa \mathbf{e}(\mathbf{f}, \alpha))^2 + \frac{R_n}{6T}. \qquad (3.12)$$

In the case of a cubic crystal, the quantity w_n becomes isotropic and takes the form

$$w_n = \frac{2RT}{\hbar^2} \langle \omega_0^{-2} \rangle + \frac{R_n}{6T}, \qquad \langle \omega_0^{-2} \rangle = \frac{2}{3N} \sum_{\mathbf{f}\alpha} \omega_0^{-2}(\mathbf{f}, \alpha). \qquad (3.12')$$

Thus, neglecting the second term in (3.12) (which is already small for $T \sim \hbar\omega_{0\,\max}$), we see that the Debye-Waller factor is independent of n when (3.6) is satisfied.

On the other hand, when $T < \hbar\omega_{0\,\max}$, for a lattice consisting of sufficiently heavy atoms, such as we are considering, w_n is itself small, and in this case there is a small error if we neglect its dependence on n. In accordance with this, we assume throughout the constancy of w_n for all n.

We average (3.5) over the isotopic composition of the host lattice, using the standard method (cf., for example,[6]). Denoting quantities referring to the impurity nucleus by the subscript 0, we get

$$\overline{M}_{p\nu} = e^{-w} \Big\{ \frac{1}{m} \overline{A}^2 \Big| \sum_{n \neq 0} (\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))\, e^{i\mathbf{k}\mathbf{r}_n} \Big|^2 + \frac{1}{m} C \sum_{n} (\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))^2$$
$$+ \frac{2}{(mm_0)^{1/2}} A_0 \overline{A}\, (\mathbf{k}\boldsymbol{\Phi}_{p\nu}(0)) \sum_{n \neq 0} (\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n)) \cos \mathbf{k}\mathbf{r}_n$$
$$+ \Big[\frac{1}{m_0} \big(A_0^2 + \tfrac{1}{4} B_0^2 K_0 (K_0 + 1)\big)$$
$$- \frac{1}{m} C \Big] (\mathbf{k}\boldsymbol{\Phi}_{p\nu}(0))^2 \Big\} \frac{\hbar(\overline{n}_{p\nu} + 1/2 \pm 1/2)}{2\omega_{p\nu}}, \qquad (3.13)$$

$$C = \overline{A^2} - \overline{A}^2 + {}^1/_4\, \overline{B^2 K (K+1)}. \qquad (3.14)$$

First let us consider the third and fourth terms in (3.13). They differ from zero only for $\nu = 1, 2, 3$, since only for these values is $\boldsymbol{\Phi}_{p\nu}(0) \neq 0$. Substituting (2.17) and (2.30) in the third and fourth terms in (3.13), after simple transformations we arrive at the expression

$$\frac{1}{m} \frac{d \ln \omega_{p\nu}^2}{d\varepsilon} \Big\{ 2\overline{A} A_0 (\mathbf{j}_\nu \mathbf{k}) \Big[\varepsilon \omega_{p\nu}^2 \sum_{\alpha} \frac{(\mathbf{k}\mathbf{e}(\mathbf{k}, \alpha))(\mathbf{j}_\nu \mathbf{e}(\mathbf{k}, \alpha))}{\omega_{p\nu}^2 - \omega_0^2(\mathbf{k}, \alpha)} - \mathbf{j}_\nu \mathbf{k} \Big] + (\mathbf{j}_\nu \mathbf{k})^2 [A_0^2 + {}^1/_4\, B_0^2 K_0 (K_0 + 1) - (1 - \varepsilon) C] \Big\},$$
$$\nu = 1, 2, 3. \qquad (3.15)$$

For the first and second terms in (3.13), using (2.6)—(2.8) and (2.17), we find respectively

$$\Big| \sum_{n \neq 0} (\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))\, e^{i\mathbf{k}\mathbf{r}_n} \Big|^2 = \begin{cases} \dfrac{d \ln \omega^2}{d\varepsilon} \Big[\varepsilon \omega^2 \sum\limits_{\alpha} \dfrac{(\mathbf{k}\mathbf{e}(\mathbf{k}, \alpha))(\mathbf{j}_\nu \mathbf{e}(\mathbf{k}, \alpha))}{\omega^2 - \omega_0^2(\mathbf{f}, \alpha)} - \mathbf{j}_\nu \mathbf{k} \Big]^2, \quad \nu = 1, 2, 3, & (3.16a) \\ \dfrac{N}{2} \sum\limits_{\delta=1}^{\vartheta/2} [S_{\nu\delta}(p)]^2 (\mathbf{k}\mathbf{e}_{p\delta})^2 (\delta_{\mathbf{f}_{p\delta}, \mathbf{k}} + \delta_{\mathbf{f}_{p\delta}, -\mathbf{k}}), \quad \nu = 4, \ldots, \vartheta/2, & (3.16b) \\ \dfrac{N}{2} (\mathbf{k}\mathbf{e}_{p\nu})^2 (\delta_{\mathbf{f}_{p\nu}, \mathbf{k}} + \delta_{\mathbf{f}_{p\nu}, -\mathbf{k}}), \quad \nu = \vartheta/2 + 1, \ldots, \vartheta; & (3.16c) \end{cases}$$

$$\sum_{n} (\mathbf{k}\boldsymbol{\Phi}_{p\nu}(\mathbf{r}_n))^2 = \begin{cases} \dfrac{d \ln \omega^2}{d\varepsilon} \Big[\dfrac{2\varepsilon^2\omega^4}{N} \sum\limits_{\mathbf{f}\alpha\alpha'} \dfrac{(\mathbf{k}\mathbf{e})(\mathbf{j}_\nu \mathbf{e})(\mathbf{k}\mathbf{e}')(\mathbf{j}_\nu \mathbf{e}')}{(\omega^2 - \omega_0^2)(\omega^2 - \omega_0'^2)} - \varepsilon (\mathbf{j}_\nu \mathbf{k})^2 \Big], \quad \nu = 1, 2, 3, & (3.17a) \\ \sum\limits_{\delta=1}^{\vartheta/2} [S_{\nu\delta}(p)]^2 (\mathbf{k}\mathbf{e}_{p\delta})^2, \quad \nu = 4, \ldots, \vartheta/2, & (3.17b) \\ (\mathbf{k}\mathbf{e}_{p\nu})^2, \quad \nu = \vartheta/2 + 1, \ldots, \vartheta. & (3.17c) \end{cases}$$

We have used the abbreviated notation

$$\omega^2 = \omega_{p\nu}^2, \qquad \mathbf{e} = \mathbf{e}(\mathbf{f}, \alpha), \quad \mathbf{e}' = \mathbf{e}(\mathbf{f}, \alpha'), \qquad \omega_0^2 = \omega_0^2(\mathbf{f}, \alpha),$$
$$\omega_0'^2 = \omega_0^2(\mathbf{f}, \alpha').$$

We go from (3.13) to the differential scattering cross section:

$$\frac{d^2\sigma(\mathbf{k}, \Delta E)}{dE\, d\Omega} = \frac{\mu^2 k_2}{4\pi^2 \hbar^4 k_1} \sum_{p} \sum_{\nu=1}^{\vartheta_p} \overline{M}_{p\nu} \delta(\Delta E \mp \hbar\omega_{p\nu}). \qquad (3.18)$$

Here μ is the mass of the neutron, $\mathbf{k}_1$ and $\mathbf{k}_2$ are the wave vectors of the neutron before and after scattering,

$$\Delta E = E_1 - E = \hbar^2 (k_1^2 - k_2^2) / 2\mu. \qquad (3.19)$$

In measuring the differential cross section (3.18) there is an unavoidable averaging over a small energy interval which nevertheless contains a macroscopic number of frequencies; the weighting function $\gamma(\Delta E - \Delta E')$ is determined by the experimental resolution ($\int \gamma(\Delta E - \Delta E')\, d\Delta E' = 1$). We see that in this case $\gamma(\Delta E \mp \hbar\omega_{p\nu})$ appears in the expression (3.18) for the cross section in place of the δ function. In particular the transition from summation over the quasicontinuous spectrum to integration is done immediately.

In order to solve the inverse problem, it is necessary to separate out the part of the scattering cross section which is related to the scattering by the impurity nucleus and by the disturbed region in its vicinity. We look at the sum over ν from 4 to $\vartheta/2$ in (3.18). Only the terms (3.16b) and (3.17b) contribute to it. Remembering that for an orthogonal matrix

$$\sum_{\nu=1}^{\vartheta/2} [S_{\nu\delta}(p)]^2 = 1, \tag{3.20}$$

and also relations (2.10) and (2.14), we have

$$\begin{aligned}\frac{N}{2}\sum_{\nu=4}^{\vartheta/2}\sum_{\delta=1}^{\vartheta/2} [S_{\nu\delta}(p)]^2 (\mathbf{k}\mathbf{e}_{p\delta})^2 (\delta_{\mathbf{f}_{p\delta},\mathbf{k}} + \delta_{\mathbf{f}_{p\delta},-\mathbf{k}}) \\ = \frac{N}{2}\sum_{\delta=1}^{\vartheta/2} (\mathbf{k}\mathbf{e}_{p\delta})^2 (\delta_{\mathbf{f}_{p\delta},\mathbf{k}} + \delta_{\mathbf{f}_{p\delta},-\mathbf{k}}) \\ - \frac{N}{2}\sum_{\delta=1}^{\vartheta/2} (\mathbf{k}\mathbf{e}_{p\delta})^2 \sum_{\nu=1}^{3} \eta_\nu^{-1}(p)\, (\mathbf{j}_\nu \mathbf{e}_{p\delta})^2 (\delta_{\mathbf{f}_{p\delta},\mathbf{k}} + \delta_{\mathbf{f}_{p\delta},-\mathbf{k}});\end{aligned} \tag{3.21}$$

$$\begin{aligned}\sum_{\nu=4}^{\vartheta/2}\sum_{\delta=1}^{\vartheta/2} [S_{\nu\delta}(p)]^2 (\mathbf{k}\mathbf{e}_{p\delta})^2 = \sum_{\delta=1}^{\vartheta/2} (\mathbf{k}\mathbf{e}_{p\delta})^2 \\ - \sum_{\delta=1}^{\vartheta/2} (\mathbf{k}\mathbf{e}_{p\delta})^2 \sum_{\nu=1}^{3} \eta_\nu^{-1}(p) (\mathbf{j}_\nu \mathbf{e}_{p\delta})^2.\end{aligned} \tag{3.22}$$

The first term in (3.21) and (3.16c) leads to the usual expression for the coherent scattering cross section

$$\frac{d^2\sigma_{\text{coh}}^{(0)}(\mathbf{k}, \Delta E)}{dE\, d\Omega} = \frac{\mu^2 \bar{A}^2 R k_2 e^{-w}}{4\pi^2\hbar^4 k_1} N \sum_{\alpha} (\varkappa \mathbf{e}(\mathbf{k}, \alpha))^2 \times \frac{1}{\hbar\omega_0(\mathbf{k}, \alpha)} \delta(\Delta E \mp \hbar\omega_0(\mathbf{k}, \alpha)), \tag{3.23}$$

while the first term in (3.22) and (3.17c) gives the usual expression for the incoherent scattering cross section

$$\frac{d^2\sigma_{\text{inc}}^{(0)}(\mathbf{k}, \Delta E)}{dE\, d\Omega} = \frac{\mu^2 C R k_2 e^{-w}}{2\pi^2\hbar^4 k_1} \sum_{\mathbf{f}\alpha} (\varkappa \mathbf{e}(\mathbf{f}, \alpha))^2 \times \frac{1}{\hbar\omega_0(\mathbf{f}, \alpha)} \delta(\Delta E \mp \hbar\omega_0(\mathbf{f}, \alpha)) \tag{3.24}$$

of the original ideal lattice. (In deriving (3.23) one must consider that of the two vectors $\mathbf{k}$ and $-\mathbf{k}$ only one can belong to the region of summation over $\mathbf{f}$, corresponding to half the fundamental cell of the reciprocal lattice.)

Now we separate the coherent and incoherent scattering. To do this we use the idea developed in [8]: we assume that the differential cross section (3.21) is measured as a function of ΔE for fixed momentum transfer $\mathbf{k} = 2\pi\mathbf{b}$ (where $\mathbf{b}$ is a vector of the reciprocal lattice). Then for $\Delta E \neq 0$ the quantity $d^2\sigma_{\text{coh}}^{(0)}(\mathbf{k} = 2\pi\mathbf{b}, \Delta E)/dE\, d\Omega$ is zero since $\omega_0(2\pi\mathbf{b}, \alpha) = 0$. At the same time the contribution to the cross section of the second term in (3.21) vanishes.

After substituting $\mathbf{k} = 2\pi\mathbf{b}$, the expressions (3.15) and (3.16a) give

$$(D/m)\, (\mathbf{j}_\nu \mathbf{k})^2 d \ln \omega_{p\nu}^2 / d\varepsilon, \tag{3.25}$$

$$D = [\bar{A}(1-\varepsilon) - A_0]^2 + {}^1/_4\, B_0^2 K_0 (K_0 + 1) - (1-\varepsilon)\, C. \tag{3.26}$$

It is easy to see that if we neglect the anisotropy of the Debye-Waller factor, the cross section (3.18) for $\mathbf{k} = 2\pi\mathbf{b}$ can be represented in the following form ($\Delta E \neq 0$):

$$d^2\sigma(\mathbf{k} = 2\pi\mathbf{b}, \Delta E)/dE\, d\Omega = R\varkappa^i \varkappa^k T^{ik}(\Delta E), \tag{3.27}$$

where $T^{ik}(\Delta E)$ is a tensor with the symmetry of the crystal. By measuring the cross section in the general case for three values $\mathbf{k} = 2\pi\mathbf{b}$ (cf. [8]) which are not coplanar, we can find the principal values of the tensor $T^{ik}(\Delta E)$ and consequently $\operatorname{Sp} T(\Delta E)$.

For the case of uniaxial crystals it is sufficient to measure the cross section for just two different values $\mathbf{k} = 2\pi\mathbf{b}$, while for the cubic crystal only one value is needed.

If the coherent scattering is small ($\bar{A} \approx 0$), the need for fixing $\mathbf{k} = 2\pi\mathbf{b}$ disappears. Measurement of the total cross section for three orientations of the single crystal which differ by cyclic permutation of the axes (cf. [8,9]) or for a polycrystal, again gives the value of $\operatorname{Sp} T(\Delta E)$.

Thus we shall assume that the value of $\operatorname{Sp} T(\Delta E)$ is known and, on this basis we shall treat the contribution to the cross section of the remaining terms (3.17a) and the second term in (3.22). Considering (2.12), (2.13), and (2.18), to within a multiplicative factor the contribution of these terms to the cross section (3.18) is given by the expression (including the average over a small energy interval)

$$\sum_p \sum_{\nu=1}^{3} \frac{\bar{n}(\omega_{p\nu}) + {}^1\!/_2 \pm {}^1\!/_2}{\omega_{p\nu}} \gamma(\Delta E \mp \hbar\omega_{p\nu})$$

$$- 3 \sum_p \frac{\bar{n}(\omega_{0p}) + {}^1\!/_2 \pm {}^1\!/_2}{\omega_{0p}} \gamma(\Delta E \mp \hbar\omega_{0p}). \quad (3.28)$$

We note that for the special case of a cubic crystal the three frequencies $\omega_{p\nu}$, $\nu = 1, 2, 3$, coincide. Keeping this in mind and also the relation (2.16), we immediately arrive at an expression of the type (3.28) after summation of (3.17a) over ν.

Using (2.25), the transformation (3.28) gives

$$\sum_p \sum_{\nu=1}^{3} \delta\omega_{0p}^2 z_{p\nu} \frac{\partial}{\partial\omega_{0p}^2} \left\{ \frac{n(\omega_{0p}) + {}^1\!/_2 \pm {}^1\!/_2}{\omega_{0p}} \gamma(\Delta E \mp \hbar\omega_{0p}) \right\}.$$

Changing from summation over p to an integration, and then integrating by parts, we finally get the expression

$$- \sum_{\nu=1}^{3} \int d\omega^2 \frac{\partial z_\nu(\omega^2)}{\partial\omega^2} \frac{\bar{n}(\omega) + {}^1\!/_2 \pm {}^1\!/_2}{\omega} \gamma(\Delta E \mp \hbar\omega). \quad (3.29)$$

Suppose that the relative concentration of impurity atoms is η. Then going to the cross section and taking it as usual per atom of the crystal, if we assume good resolution we get an expression of the form (3.27) with the following value of Sp T(ΔE) [cf. (3.25) and (3.29)]:

$$\mathrm{Sp}T(\Delta E) = \mathrm{Sp}T_0(\Delta E) + \eta\, \mathrm{Sp}T_1(\Delta E), \quad (3.30)$$

where Sp T_0(ΔE) is determined in an obvious way from (3.24), while

$$\mathrm{Sp}T_1(\Delta E) = \frac{\mu^2 k_2 e^{-w}}{2\pi^2\hbar^6 k_1} \sum_{\nu=1}^{3} \left[D f_\nu(\omega^2) - C \frac{\partial z_\nu(\omega^2)}{\partial\omega^2} \right]$$

$$\times \left[\bar{n}(\omega) + \frac{1}{2} \pm \frac{1}{2} \right] \Bigg|_{\omega = |\Delta E|/\hbar} \quad (3.31)$$

The last expression is obviously entirely due to the scattering from impurity atoms. [In deriving (3.31) we have used the relation (2.27).]

In the case of a cubic crystal there is no need for three independent measurements, and we get directly

$$\frac{d^2\sigma^{(1)}(\mathbf{k} = 2\pi\mathbf{b}, \Delta E)}{dE\, d\Omega} = \frac{R}{3} \eta\, \mathrm{Sp}T_1(\Delta E)$$

$$= \frac{R\mu^2 k_2 e^{-w}}{2\pi^2\hbar^6 k_1} \eta \left[D f(\omega^2) - C \frac{\partial z(\omega^2)}{\partial\omega^2} \right] \left[\bar{n}(\omega) + \frac{1}{2} \pm \frac{1}{2} \right] \Bigg|_{\omega = |\Delta E|/\hbar}. \quad (3.31')$$

As already mentioned, if the coherent scattering is small (3.31) and (3.31′) hold for arbitrary **k**. Let $\epsilon = 0$. Then

$$D = (\bar{A} - A_0)^2 + {}^1\!/_4 B_0^2 K_0 (K_0 + 1) - C;$$
$$\partial z_\nu(\omega^2) / \partial\omega^2 = 0, \qquad f_\nu(\omega^2) = g^{(\nu)}(\omega^2). \quad (3.32)$$

If the selected atom belongs to the isotopic mixture of the regular lattice, we find, by averaging (3.32), that D = 0 and expression (3.31) vanishes.

If C ≪ D, the need for calculating the contribution to (3.18) from (3.17a) and the second term in (3.22) disappears; the same remark applies to the averaging of the polarization vectors which is done only to simplify the final formulas. In this case we find from (3.25) and (3.26) that the cross section due to the impurity atoms is

$$\frac{d\sigma^{(1)}(\mathbf{k} = 2\pi\mathbf{b}, \Delta E)}{dE\, d\Omega} = R\eta\varkappa^i\varkappa^k T_1^{ik}(\Delta E), \quad (3.33)$$

$$T_1^{ik}(\Delta E) = \frac{\mu^2 k_2 e^{-w} D}{2\pi^2\hbar^6 k_1} \left[\sum_{\nu=1}^{3} j_\nu^i j_\nu^k f_\nu(\omega^2) \right] \left[\bar{n}(\omega) + \frac{1}{2} \pm \frac{1}{2} \right] \Bigg|_{\omega = |\Delta E|/\hbar}, \quad (3.34)$$

$$D = [\bar{A}(1 - \varepsilon) - A_0]^2 + {}^1\!/_4 B_0^2 K_0 (K_0 + 1). \quad (3.35)$$

We see that the tensor T^{ik}(ΔE) has a very simple form, directly accessible to analysis, while its principal values, which are again found by making the required number of independent measurements (three, two, or one, depending on the symmetry of the crystal), are equal to

$$T_1^{\nu\nu}(\Delta E) = \frac{\mu^2 k_2 e^{-w} D}{2\pi^2\hbar^6 k_1} f_\nu(\omega^2) \left[\bar{n}(\omega) + \frac{1}{2} \pm \frac{1}{2} \right] \Bigg|_{\omega = |\Delta E|/\hbar}. \quad (3.36)$$

This case is of the greatest interest for the analysis of the vibration spectrum of the crystal.

4. SCATTERING OF SLOW NEUTRONS WHEN DISCRETE FREQUENCIES ARE PRESENT

When condition (2.24) is satisfied, there are discrete frequencies in addition to the quasicontinuous spectrum. Although the number of such frequencies is small, their relative importance for the scattering cross section corresponding to the impurity atoms is considerable, while in some cases they may play a decisive role. This is related to the fact that, because of their spatial localization, the discrete frequencies correspond to larger displacement amplitudes of the impurity atom, comparable with or exceeding the total amplitude of its vibration in all the frequencies of the quasicontinuous spectrum.

Formula (3.12), which was derived using only Eq. (2.1) and the orthogonality and completeness of its solutions, and all the remarks concerning the Debye-Waller factor which were made in the preceding section, are also valid here. The change is the appearance of a factor in the form of a Bessel function, since the displacement amplitude in a localized vibration does not have the factor $\sim N^{-1/2}$.

It should be mentioned that when there are localized normal modes the question of strict degeneracy of such discrete frequencies plays a special role (cf. [4]). In calculating the differential cross section we are faced with the necessity of summing over all final states with a fixed energy, corresponding to different occupation numbers of the localized normal oscillators, i.e., we must consider multiquantum processes for such oscillators.

In the case of scattering with $|\Delta E| \leq \hbar\omega_{0\,\max}$, i.e., when only phonons of the quasicontinuous spectrum are excited, we arrive at an expression for the square modulus of the matrix element which differs from (3.5) by the substitution

$$A_n A_{n'} \to A_n A_{n'} \prod_{\lambda=1}^{3}{}' I_0(X_{nn'}^{(\lambda)}), \qquad B_n^2 \to B_n^2 \prod_{\lambda=1}^{3}{}' I_0(X_{nn}^{(\lambda)}), \tag{4.1}$$

where for brevity we have introduced the notation

$$X_{nn'}^{(\lambda)} = \sum_{(\lambda)} \frac{\hbar\,(\mathbf{k}\boldsymbol{\Phi}_{D\lambda}(\mathbf{r}_n))\,(\mathbf{k}\boldsymbol{\Phi}_{D\lambda}(\mathbf{r}_{n'}))}{2\omega_{D\lambda}\sqrt{m_n m_{n'}}}\,\mathrm{sh}^{-1}\frac{\hbar\omega_{D\lambda}}{2T}. \tag{4.2}$$

The symbol $\prod_{\lambda}'$ denotes a product over the various discrete frequencies, $\sum_{(\lambda)}$ is a summation over all the normal vibrations corresponding to a given discrete frequency $\omega_{D\lambda}$. In deriving (4.1)—(4.2), we have used the following summation formula for Bessel functions:

$$\sum_{n_1=-\infty}^{\infty} \cdots \sum_{n_s=-\infty}^{\infty} \prod_{i=1}^{s} I_{n_i}(x_i) = I_m\Big(\sum_{i=1}^{s} x_i\Big),$$
$$\sum_{i=1}^{s} n_i = m$$

Similarly by using (3.2) we can write an expression corresponding to creation or absorption of a quantum of the discrete frequency $\omega_{D\nu}(|\Delta E|) = \hbar\omega_{D\nu}$:

$$\begin{aligned} M_{D(\nu)} = {} & \sum_{n}\sum_{n'} A_n A_{n'} \exp\{i\mathbf{k}(\mathbf{r}_n - \mathbf{r}_{n'})\} \\ & \times \exp\Big(-\frac{w_n + w_{n'}}{2}\Big)\exp\Big(\pm\frac{\hbar\omega_{D\nu}}{2T}\Big) I_1(X_{nn'}^{(\nu)}) \prod_{\lambda\neq\nu}{}' I_0(X_{nn'}^{(\lambda)}) \\ & + \frac{1}{4}\sum_{n} B_n^2 K_n(K_n+1)e^{-w_n}\exp\Big(\pm\frac{\hbar\omega_{D\nu}}{2T}\Big) \\ & \times I_1(X_{nn}^{(\nu)}) \prod_{\lambda\neq\nu}{}' I_0(X_{nn}^{(\lambda)}). \end{aligned} \tag{4.3}$$

But it is easy to see that for $T \ll \hbar\omega_{0\,\max}$ the arguments of the Bessel functions in (4.2) are much less than unity, and consequently it is again meaningful to expand as in (3.4); also

$$I_0 \approx 1.$$

On the other hand assuming that $R'/\hbar\omega_{0\,\max} < 1$, these expansions can be used over the whole temperature range in which the one-quantum approximation is valid. Considering this region, we find that all the results of the preceding section for the case of excitation of quanta of the quasicontinuous spectrum ($|\Delta E|) \leq \hbar\omega_{0\,\max}$) also remain valid in the presence of discrete frequencies.

We note that in the limiting case of $m_0/m \ll 1$, which corresponds to a marked localization of the normal vibrations for the discrete frequencies, it is useful to keep the true value for w_0. In other words, in this case when using the formulas of the preceding section it is sensible to make the replacement

$$A_0^2 e^{-w} \to A_0^2 e^{-w_0} \prod_{\nu=1}^{3} I_0(X_{00}^{(\nu)}), \qquad B_0^2 e^{-w} \to B_0^2 e^{-w_0} \prod_{\nu=1}^{3} I_0(X_{00}^{(\nu)}), \tag{4.4}$$

leaving the other terms unchanged [including those linear in A —cf. (4.1)—(4.2)]. Obviously because of (2.30) and (4.2),

$$X_{00}^{(\nu)} = \sum_{(\nu)} \frac{R\,(\varkappa\mathbf{j}_\nu)^2}{\hbar\omega_{D\nu}}\,\frac{d\ln\omega_{D\nu}^2}{d\varepsilon}\,\mathrm{sh}^{-1}\frac{\hbar\omega_{D\nu}}{2T}. \tag{4.5}$$

Now we determine the cross section for scattering with excitation of a discrete frequency. In view of the above remarks, the derivation is analogous to that in the previous section for the quasicontinuous spectrum. The difference is that the only contributions to the cross section (3.18) in this case come from (3.15), (3.16), and (3.17a), where $\omega^2 = \omega_{D\nu}^2$. The result is

$$\begin{aligned} \frac{d^2\sigma(\mathbf{k},\Delta E)}{dE\,d\Omega} = {} & \frac{\mu^2 k_2 R e^{-w}}{4\pi^2\hbar^4 k_1}\,\eta \sum_{\nu=1}^{3} \frac{1}{\hbar\omega_{D\nu}}\,\frac{d\ln\omega_{D\nu}^2}{d\varepsilon}\Big\{\Big[\overline{A}\Big(\mathbf{j}_\nu\boldsymbol{\varkappa} - \varepsilon\omega_{D\nu}^2 \\ & \times \sum_{\alpha}\frac{(\boldsymbol{\varkappa}\mathbf{e}(\mathbf{k},\alpha))\,(\mathbf{j}_\nu\mathbf{e}(\mathbf{k},\alpha))}{\omega_{D\nu}^2 - \omega_0^2(\mathbf{k},\alpha)}\Big) - A_0(\mathbf{j}_\nu\boldsymbol{\varkappa})\Big]^2 + \Big[\frac{1}{4}B_0^2 K_0(K_0+1) \\ & - (1-\varepsilon)C\Big](\mathbf{j}_\nu\boldsymbol{\varkappa})^2 + C\Big[\frac{2\varepsilon^2\omega_{D\nu}^4}{N}\sum_{\mathbf{f}\alpha\alpha'}\frac{(\boldsymbol{\varkappa}\mathbf{e})\,(\mathbf{j}_\nu\mathbf{e})\,(\boldsymbol{\varkappa}\mathbf{e}')\,(\mathbf{j}_\nu\mathbf{e}')}{(\omega^2-\omega_0^2)\,(\omega^2-\omega_0'^2)} \\ & - \varepsilon(\mathbf{j}_\nu\boldsymbol{\varkappa})^2\Big]\Big\}\Big(\overline{n}_{D\nu} + \frac{1}{2} \pm \frac{1}{2}\Big)\delta(\Delta E \mp \hbar\omega_{D\nu}). \end{aligned} \tag{4.6}$$

Expression (4.6) actually determines the total cross section for scattering of neutrons by the lattice ($|\Delta E| > \hbar\omega_{0\,\max}$), excluding the multiquantum background, which we are neglecting (cf. below). There is therefore no need for additional conditions ($\mathbf{k} = 2\pi\mathbf{b}$) for eliminating the coherent scattering. Nevertheless, to simplify (4.2) we shall fix $\mathbf{k} = 2\pi\mathbf{b}$, or assume that $\mathbf{k}$ is arbitrary, but sufficiently small so that

$$\omega_0^2(\mathbf{k},\alpha) \ll \omega_{D\nu}^2. \tag{4.7}$$

As a result we get

$$\begin{aligned} \mathrm{Sp}\,T(\Delta E) = {} & \frac{\mu^2 k_2 e^{-w}}{4\pi^2\hbar^5 k_1}\sum_{\nu=1}^{3}\frac{1}{\omega_{D\nu}}\Big(D\frac{d\ln\omega_{D\nu}^2}{d\varepsilon} + C\Big) \\ & \times \Big(\overline{n}_{D\nu} + \frac{1}{2} \pm \frac{1}{2}\Big)\delta(\Delta E \mp \hbar\omega_{D\nu}) \end{aligned} \tag{4.8}$$

for the case of a crystal of arbitrary symmetry, and

$$\frac{d^2\sigma(\mathbf{k},\,\Delta E)}{dE\,d\Omega} = \eta\,\frac{\mu^2 R k_2 e^{-w}}{4\pi^2\hbar^5 k_1 \omega_D}\left(D\,\frac{d\ln\omega_D^2}{d\varepsilon} + C\right)$$

$$\times\ \left(\bar{n}_D + \frac{1}{2} \pm \frac{1}{2}\right)\delta(\Delta E \mp \hbar\omega_D) \tag{4.9}$$

for the case of cubic symmetry. The value of the quantity $d \ln \omega_{D\nu}^2/d\epsilon$ is determined by (2.32) or by the expression (2.33), using (2.20).

The procedure for obtaining (4.8) is the same as in the preceding section—one uses a polycrystal [with $\bar{A} \approx 0$ and arbitrary $\mathbf{k}$, or with arbitrary $\bar{A}$ and $\mathbf{k}$ satisfying (4.7)], or measures the cross section for the appropriate number of independent values of $\mathbf{k}$ (equal to $2\pi\mathbf{b}$ or satisfying (4.7)) using a single crystal.

The excited states of the discrete normal oscillator exist for a finite time even when $T = 0$. Introducing a width for the excited state $\Gamma_{D\nu}$, and approximating the instrument resolution curve $\gamma(\Delta E - \Delta E')$ (cf. the preceding section) by a function of Lorentz type with characteristic parameter Γ, we get expressions which differ from (4.6), (4.8)—(4.9) by the replacement

$$\delta(\Delta E \mp \hbar\omega_{D\nu}) \to \frac{1}{\pi}\,\frac{(\Gamma_{D\nu} + \Gamma)/2}{(\Delta E \mp \hbar\omega_{D\nu})^2 + (\Gamma_{D\nu} + \Gamma)^2/4}\,. \tag{4.10}$$

As direct calculations show, the ratio $\Gamma_D/\hbar\omega_D$ for $T \ll \Theta$ is of order 10^{-2}, while it is even much less for $\omega_0 > 2\omega_{0\,\max}$. Thus for sufficiently good resolution, when $\Delta E = \hbar\omega_{D\nu}$ one should see sharp peaks. Obviously from the area under the peaks one can determine the corresponding values of $d \ln \omega_{D\nu}^2/d\epsilon$.

When $\Delta E > \hbar\omega_{0\,\max}$, in addition to one-phonon scattering corresponding to the discrete levels, one will also see two-phonon scattering. The possibility of observing neutron scattering with excitation of discrete levels is obviously essentially connected with the assumption that the two-phonon scattering is small. Let us estimate the cross section for such a process.

Let the one-phonon scattering from the ideal host be primarily coherent. Then, computing the cross section for the two-phonon process for $\mathbf{k} = 2\pi\mathbf{b}$, we find

$$\frac{d^2\sigma_2(\mathbf{k} = 2\pi\mathbf{b},\,\Delta E)}{dE\,d\Omega} \sim \frac{\mu^2 A_{\varsigma}^2 k_2}{\pi^2\hbar^5 k_1}\,e^{-w}\left(\frac{R}{\Delta E}\right)^2\psi\left(\frac{\Delta E}{\hbar}\right)\left[\bar{n}\left(\frac{\Delta E}{\hbar}\right) + 1\right],$$

$$\Delta E > 0, \tag{4.11}$$

where $\psi(\omega)$ is the normalized distribution function for the frequencies in the phonon spectrum.

Analysis of (4.11) shows that the cross section for two-phonon scattering, compared to R times (4.8), (4.10) [or (4.9), (4.10)] contains the small parameter $R/\Delta E$, while for sufficiently good resolution it contains another small parameter $\Gamma_{D\nu}/\hbar\omega_{0\,\max}$. Thus by suitably choosing the parameters of the impurity nucleus and limiting the temperature one can comparatively easily guarantee conditions in which one will observe sharp peaks in the cross section corresponding to discrete levels, with a low concentration of impurity atoms.

We note that for a large mass difference $(m_0/m \ll 1)$ the values of the cross section for two-quantum excitations of localized oscillators also become significant. Thus in addition to the maxima in the scattering cross section for $\Delta E = \hbar\omega_{D\nu}$, satellites should appear at $\Delta E = 2\hbar\omega_{D\nu}$, etc. $(\Delta E > 0)$.

5. DISCUSSION OF RESULTS

The results obtained in the preceding sections allow us to analyze what information concerning the vibration spectrum can be gotten from measurements of the cross section for scattering of slow neutrons by crystals containing isolated impurity atoms.

The decisive point for the inverse problem is the possibility of separating out the actual cross section for scattering by the impurity atom and the disturbed region which is produced around it. The problem is solved most simply if one can use impurity nuclei whose scattering is anomalously large in the energy region of interest. Several isotopes with low-lying resonance levels are known at present. But the energies of all these levels are of the order of one eV, so that the use of these isotopes requires the development of a special experimental technique.

If, however, the total scattering from the impurity nuclei does not predominate, the problem of separating out $d^2\sigma^{(1)}/dE\,d\Omega$ is more complicated. To isolate the coherent scattering one must measure the scattering cross section of single crystals as a function of ΔE for fixed momentum transfer $\mathbf{k} = 2\pi\mathbf{b}$. If the coherent scattering is negligibly small, the measurement can be made on a polycrystal, where a complete averaging of the polarization occurs (cf. [8] and also Sec. 3). Thus in both cases we at least get the quantity (3.30), and if $d^2\sigma^{(1)}/dE\,d\Omega$ is comparable to $d^2\sigma^{(0)}_{inc}/dE\,d\Omega$, the quantity η Sp $T_1(\Delta E)$, which is what we want, can be separated out.

But the most interesting question is whether, from experiments on scattering of neutrons by crystals with low impurity concentrations, one can establish the distribution function for the squared frequencies of the initial ideal lattice, (2.22).

The possibility of separating $d^2\sigma^{(1)}/dE\,d\Omega$ when $\eta \ll 1$ definitely assumes that

$$D \gg C. \tag{5.1}$$

In this case, as shown in Sec. 3, measuring the cross section for three noncoplanar values of $\mathbf{k} = 2\pi\mathbf{b}$ (for uniaxial crystals two independent measurements are sufficient, for a cubic crystal, one) for a fixed value $\Delta E \neq 0$, one can find the principal values of the tensor $T^{ik}(\Delta E)$ of (3.36) and consequently the quantities $f_\nu(\omega^2)$. The existence of the functional relation (2.28) between $f_\nu(\omega^2)$ and $g^{(\nu)}(\omega^2)$ then allows us to get $g^{(\nu)}(\omega^2)$, and thus we can affirm that it is possible to determine $g(\omega^2)$. (To calculate the integral appearing in (3.28) in first approximation one can use some simple model, and then use the method of successive approximations.)

One should remember that the whole theory is based on the assumption that the force constants are unchanged by the introduction of the foreign atom. But when the masses m_0 and m are markedly different, one can apparently neglect changes in the force constants (cf, also[4]), so that this assumption becomes completely reasonable.

A very important point is the possibility of detecting from experiments on scattering the presence of discrete frequencies and to determine their magnitude as well as the quantity $d \ln \omega^2_{D\nu}/d\epsilon$. Agreement between the experimental values of $\omega_{D\nu}$ and those which are computed from the solution of (2.20), or, for a cubic crystal, are given by the equation

$$\varepsilon\omega_D^2 \int\limits_0^{\omega^2_{0max}} \frac{g(\omega^2)\,d\omega^2}{\omega_D^2 - \omega^2} = 1, \tag{5.2}$$

would serve as a good confirmation of the correctness of the initial assumption of unchanged values of the force constants. In solving (2.20) we can again choose $g^{(\nu)}(\omega^2)$ from some crude model. If $\omega_{D\nu}$ is sufficiently high, to find it (as shown in [3,4]) it is sufficient to know only the first moments of the function $g^{(\nu)}(\omega^2)$, which can be determined to good accuracy by an independent method. In particular, in the case of a cubic crystal the first moment $\langle\omega^2\rangle$ can be found from the deviation of the specific heat from its classical limit at high temperatures.

We remark that there is particular interest in determining $g(\omega^2)$ for a host with very weak one-phonon incoherent scattering.

If Eq. (5.1) is not satisfied, we must use for D the general expression in the form (3.26). From the form of this expression it follows that one can get a marked increase in $d^2\sigma^{(1)}/dE\,d\Omega$ by using heavy impurity atoms ($m_0/m \gg 1$), or by using atoms for which A_0 has the opposite sign from A.

As shown in earlier papers of the authors,[3,4] when $m_0/m \gg 1$ the quantity f_ν (2.28) has a strong resonant character:

$$f_\nu(x) = \frac{1}{\pi|\varepsilon|}\sqrt{\frac{x}{x_\nu}}\,\frac{\lambda_\nu}{(x - x_\nu)^2 + \lambda_\nu^2}, \tag{5.3}$$

where

$$x = \frac{\omega^2}{\omega^2_{0\,max}}, \qquad x_\nu = \frac{1}{|\varepsilon|\,\langle x^{-1}\rangle_\nu}, \qquad \lambda_\nu = \frac{\pi d_\nu}{|\varepsilon|^{3/2}\,\langle x^{-1}\rangle_\nu^{5/2}}. \tag{5.4}$$

The symbol $\langle\ldots\rangle_\nu$ denotes an average with weight $g^{(\nu)}$ (2.21), so that

$$\langle x^{-1}\rangle_\nu \equiv \int\limits_0^1 \frac{g^{(\nu)}(x)\,dx}{x};$$

d_ν is a constant determined from the low frequency limit ($x \ll 1$) of the function $g^{(\nu)}(x)$, which has the form

$$g^{(\nu)}(x) = d_\nu\sqrt{x}.$$

Because of this, the cross section for one-quantum excitations (3.33)—(3.34) will be localized in a narrow energy interval around

$$\Delta E = \frac{\hbar\omega_{0max}}{|\varepsilon|^{1/2}\,\langle x^{-1}\rangle_\nu^{1/2}}, \tag{5.5}$$

while the intensity at the maximum will be $\sim 1/\lambda_\nu$ times the usual scattering cross section from the impurity centers. Apparently this case is very favorable for detecting the one-quantum scattering of neutrons from impurity atoms when their concentration is low.

We remark that in the case considered the two-quantum (multiquantum) excitations may become important, which will correspond to peaks in the neutron scattering cross section for

$$\Delta E = \frac{2\hbar\omega_{0max}}{|\varepsilon|^{1/2}\,\langle x^{-1}\rangle_\nu^{1/2}} \qquad \left(\Delta E = \frac{n\hbar\omega_{0max}}{|\varepsilon|^{1/2}\,\langle x^{-1}\rangle_\nu^{1/2}}\right).$$

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