Fyz. čas. SAV 21 (1971), No. 2-3

ELASTIC SCATTERING OF SOUND WAVES IN NON PERIODICAL STRUCTURES

JURAJ BRACINÍK*, Žilina

This paper deals with the elastic scattering of sound waves in solids with non-periodic structure, which is the characteristic property of such systems.

I. INTRODUCTION

In an harmonic approximation the plane harmonic waves represent the exact normal modes of the system with an ideal crystalline structure. The lifetime of the corresponding phonons is therefore infinite and becomes finite only if we take into account anharmonicity, which enables the many-phonon processes. On the other hand in solids with non-periodic situated atoms as it is in amorphous solids, the plane waves are not identical with the normal modes of this system, but they can be taken as a basis for the representation. The Hamiltonian in this representation contains in general non-diagonal elements even in the quadratic approximation in potential energy. This may be interpreted as the elastic scattering of acoustic waves. In the case of a small deviation from periodicity or homogeneity the problem can be solved by adding a small perturbation term to the initial Hamiltonian [1], [2], [3].

II. ELASTIC SCATTERING

The introduction of plane-wave representation can be made by a standard procedure with respect to the fact of the non-orthogonality of the set of exponential functions (see [4]).

We express the displacement $u_\alpha(\mathbf{r}_l)$, $(\alpha = x, y, z)$ of the atom from his equilibrium position $\mathbf{r}_l$ by using the set of functions $\exp[i\mathbf{q} . \mathbf{r}_l]$ where the values of the vector $\mathbf{q}$ are given by the choice of the boundary conditions.

We shall write the displacement operator in the form

* Katedra fyziky Vysokej školy dopravnej, ŽILINA, Marxa—Engelsa 25.

$$\hat{u}_\alpha(\mathbf{r}_l) = \sum_{\mathbf{q},\lambda} \sqrt{\frac{\hbar}{2MN\omega(\mathbf{q},\lambda)}}\, e_\alpha(\mathbf{q},\lambda)\, [\hat{a}_{\mathbf{q},\lambda} e^{i\mathbf{q}.\mathbf{r}_l} + \hat{a}^+_{\mathbf{q},\lambda} e^{-i\mathbf{q}.\mathbf{r}_l}], \tag{1}$$

where M is the mass of the atom, N is the number of atoms in the whole system, e_α is the polarization vector, λ is the polarization index, $\omega(\mathbf{q}, \lambda)$ shall be determined, $\hat{a}_{\mathbf{q},\lambda}$, $\hat{a}^+_{\mathbf{q},\lambda}$ are operators satisfying the commutation relations

$$[\hat{a}_{\mathbf{q},\lambda}, \hat{a}_{\mathbf{q},\lambda'}] = [\hat{a}^+_{\mathbf{q},\lambda}, \hat{a}^+_{\mathbf{q}',\lambda'}] = 0 \qquad [\hat{a}_{\mathbf{q},\lambda}, \hat{a}^+_{\mathbf{q}',\lambda'}] = \delta_{\mathbf{q},\mathbf{q}'}\delta_{\lambda,\lambda'}. \tag{2}$$

The function $\exp[i\mathbf{q} . \mathbf{r}_l]$ do not represent the orthogonal system any longer. Therefore is is necessary in the corresponding expression for the impulse operator $\hat{\mathbf{q}}(\mathbf{r}_l)$ to use the functions $\eta(\mathbf{q}, \mathbf{r}_l)$, which form the reciprocal system to the set of the exponential functions $\exp[i\mathbf{q} . \mathbf{r}_l]$:

$$\frac{1}{N}\sum_{\mathbf{q}} e^{i\mathbf{q}.\mathbf{r}_l}\, \eta^*(\mathbf{q}, \mathbf{r}_m) = \delta_{m,l} \tag{3}$$

$$\frac{1}{N}\sum_{l} e^{i\mathbf{q}.\mathbf{r}_l}\eta^*(\mathbf{q}', \mathbf{r}_l) = \delta_{\mathbf{q},\mathbf{q}'}$$

in order that the commutation relation

$$[\hat{u}_\alpha(\mathbf{r}_l), \hat{p}_\beta(\mathbf{r}_m)] = i\hbar\delta_{\alpha,\beta}\delta_{l,m} \tag{4}$$

can be fulfilled.

Then the impulse-operator can be written as

$$\hat{p}_\alpha(\mathbf{r}_l) = i\sum_{\mathbf{q},\lambda}\sqrt{\frac{\hbar\omega(\mathbf{q},\lambda)M}{2N}}\, e_\alpha(\mathbf{q},\lambda)\, [\hat{a}^+_{\mathbf{q},\lambda}\eta^*(\mathbf{q},\mathbf{r}_l) - \hat{a}_{\mathbf{q},\lambda}\eta(\mathbf{q},\mathbf{r}_l)]. \tag{5}$$

The energy of the system in quadratic approximation is

$$E = \sum_{\alpha,l}\frac{p^2_\alpha(\mathbf{r}_l)}{2M} + \frac{1}{2}\sum_{\substack{lm\\ \alpha\beta}} \Phi_{\alpha\beta}(\mathbf{r}_l, \mathbf{r}_m)\, u_\alpha(\mathbf{r}_l)\, u_\beta(\mathbf{r}_m). \tag{6}$$

After substituting for $u_\alpha(\mathbf{r}_l)$ and $p_\alpha(\mathbf{r}_l)$ operators, the Hamiltonian of the system is

$$\hat{H} = \frac{\hbar}{4N}\sum_{\substack{\alpha,l\\ \mathbf{q},\lambda\\ \mathbf{q}',\lambda'}}\sqrt{\omega(\mathbf{q},\lambda)\,\omega(\mathbf{q}',\lambda')}\, e_\alpha(\mathbf{q},\lambda)\, e_\alpha(\mathbf{q}',\lambda')\, [\hat{a}^+_{\mathbf{q},\lambda}\eta^*(\mathbf{q},\mathbf{r}_l) -$$

$$- \hat{a}_{\mathbf{q},\lambda}\eta(\mathbf{q}, \mathbf{r}_l)]\, [\hat{a}_{\mathbf{q}',\lambda'}\eta(\mathbf{q}', \mathbf{r}_l) - \hat{a}^+_{\mathbf{q}',\lambda'}\eta^*(\mathbf{q}', \mathbf{r}_l)] +$$

$$+ \frac{\hbar}{4MN} \sum_{\substack{lm\\ \alpha\beta}} \Phi_{\alpha\beta}(\mathbf{r}_l, \mathbf{r}_m) \sum_{\substack{\mathbf{q},\lambda\\ \mathbf{q},\lambda'}} \frac{e_\alpha(\mathbf{q}, \lambda)\, e_\beta(\mathbf{q}', \lambda')}{\sqrt{\omega(\mathbf{q}, \lambda)\, \omega(\mathbf{q}', \lambda')}} [\hat{a}_{\mathbf{q},\lambda} e^{i\mathbf{q}.\mathbf{r}_l} +$$

$$+ \hat{a}^+_{\mathbf{q},\lambda} e^{-i\mathbf{q}.\mathbf{r}_l}]\, [\hat{a}_{\mathbf{q}',\lambda'} e^{i\mathbf{q}'.\mathbf{r}_m} + \hat{a}^+_{\mathbf{q}',\lambda'} e^{-i\mathbf{q}'.\mathbf{r}_m}]. \tag{7}$$

The diagonal part of the Hamiltonian (7) has the familiar form

$$\hat{H}_0 = \sum_{\mathbf{q},\lambda} \hbar\omega(\mathbf{q}, \lambda)\, [\hat{a}^+_{\mathbf{q},\lambda}\hat{a}_{\mathbf{q},\lambda} + \tfrac{1}{2}] \tag{8}$$

if $\omega(\mathbf{q}, \lambda)$ is given by

$$\omega^2(q, \lambda) = \frac{\dfrac{1}{2MN} \sum\limits_{\substack{lm\\ \alpha\beta}} \Phi_{\alpha\beta}(\mathbf{r}_l, \mathbf{r}_m)\, e_\alpha(\mathbf{q}, \lambda)\, e_\beta(\mathbf{q}, \lambda) e^{i\mathbf{q}(\mathbf{r}_m - \mathbf{r}_l)}}{1 - \dfrac{1}{2N} \sum\limits_{\mathbf{r}_l} \eta^*(\mathbf{q}, \mathbf{r}_l)\, \eta(\mathbf{q}, \mathbf{r}_l)} \tag{9}$$

The interpretation of $\omega(\mathbf{q}, \lambda)$ can be done also in the quasiclassical case, by using the state $|\mathbf{q}, \lambda>$ with quasi-determined displacements and impulses. The state vector $|\mathbf{q}, \lambda>$ satisfies the condition (see [5])

$$\hat{a}_{\mathbf{q}',\lambda'} |\mathbf{q}, \lambda> = \text{const.}\ \delta_{\mathbf{q},\mathbf{q}'} \delta_{\lambda,\lambda'} |\mathbf{q}, \lambda>. \tag{10}$$

In the absence of scattering the time dependence of $\hat{a}_{\mathbf{q},\lambda}$ would be

$$\hat{a}_{\mathbf{q},\lambda}(t) = e^{-i\omega(\mathbf{q},\lambda)t} \hat{a}_{\mathbf{q},\lambda}(0). \tag{11}$$

From (1), (10), (11) we can see that $\omega(\mathbf{q}, \lambda)$ is really the frequency of the plane harmonic wave with the wave vector $\mathbf{q}$ and the polarization λ.

If we denote

$$G\begin{pmatrix}\mathbf{q}, \mathbf{q}'\\ \lambda, \lambda'\end{pmatrix} = \frac{1}{N} \sum_l \eta^*(\mathbf{q}', \mathbf{r}_l)\, \eta(\mathbf{q}, \mathbf{r}_l) \sum_\alpha e_\alpha(\mathbf{q}, \lambda)\, e_\alpha(\mathbf{q}', \lambda'), \tag{12}$$

$$K\begin{pmatrix}\mathbf{q}, \mathbf{q}'\\ \lambda, \lambda'\end{pmatrix} = \frac{1}{MN} \sum_{\substack{lm\\ \alpha\beta}} \Phi_{\alpha\beta}(\mathbf{r}_l, \mathbf{r}_m)\, e^{i\mathbf{q}.\mathbf{r}_m} e^{-i\mathbf{q}'.\mathbf{r}_l}\, e_\alpha(\mathbf{q}', \lambda')\, e_\beta(\mathbf{q}, \lambda), \tag{13}$$

then for the case of the quasi-isotropic system the phonon lifetime can be written within the first-order approximation of the perturbation treatment as

$$\frac{1}{\tau} = \frac{V}{4\pi} \frac{1}{v^3_{\mathbf{q},\lambda}} \omega^4(\mathbf{q}, \lambda) \left\langle \left| G\begin{pmatrix}\mathbf{q}, \mathbf{q}'\\ \lambda, \lambda'\end{pmatrix} + \frac{1}{\omega^2(\mathbf{q}, \lambda)} K\begin{pmatrix}\mathbf{q}, \mathbf{q}'\\ \lambda, \lambda'\end{pmatrix} \right|^2 \right\rangle, \tag{14}$$

$$\text{where } v_{\mathbf{q},\lambda} = \frac{\omega(\mathbf{q}, \lambda)}{|\mathbf{q}|}.$$

The averaging in (14) is taken over all directions of $\mathbf{q}'$, where $|\mathbf{q}'| = |\mathbf{q}|$ and λ, λ' represent the same kind of polarization.

The evaluation of τ requests to use some model of an amorphous solid because of the statistics of the mass and force parameter distribution is needed.

The elastic scattering in non-crystalline solids is characteristic, unlike in the case of ideal crystals. In the longwavelength region, however, the long-range fluctuations of characteristic parameters are needed in order that the scattering can play an important role.

The fact of the finite lifetime of phonons due to elastic scattering may be important for the theory of many phonon processes.

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Received November 10th, 1970