LOCALIZED VIBRATIONS OF LINE DEFECTS IN A DIATOMIC CUBIC LATTICE

IVA KARASOVÁ, Bratislava

INTRODUCTION

Recently a number of authors turned from the investigation of point defects to the problems of localized vibrations caused by extended defects. On the model of a simple monoatomic lattice there were studied localized vibrations of planes and lines of impurity atoms [1—4], localized vibrations of dislocations [5] and dislocation dipoles [6]. It was found that in contrast to the point defects whole frequency bands arise, and those are ascribed to localized vibrations. The bands have their own disperse relations of an optical or an acoustic character and can be partially overlapped by the frequency band of an ideal lattice.

In this paper the investigation of models is further extended to the investigation of a diatomic lattice. The main points of interest are here localized vibrations caused by a line defect.

EQUATIONS FOR LOCALIZED MODES

Let us consider a perfect simple cubic lattice with N^3 atoms (N even). Every cell contains two atoms with the masses m_1 and m_2. Interaction is considered only between the nearest neighbours and is characterized by the central force constant α_1 and the noncentral force constants α_2, α_3. If the interaction between the various components of the atom displacement vector is neglected, then using the relation

$$\mathbf{X} = \mathrm{e}^{\mathrm{i}\omega t}\boldsymbol{u}$$

for vibrations in the direction of the axis Ox (and similarly for the directions Oz, Oy) we can write:
for an odd lattice point

$$[m_1\omega^2 - 2\sum_{i=1}^{3}\alpha_i]u_{i,j,k} = -\alpha_1[u_{i,j,k+1} + u_{i,j,k-1}] - \qquad (1)$$

$$- \alpha_2[u_{i,j+1,k} + u_{i,j-1,k}] -$$

$$(i + j + k = \text{odd}) \qquad - \alpha_3[u_{i+1,j,k} + u_{i-1,j,k}]$$

and for an even lattice point

$$[m_2\omega^2 - 2\sum_{i=1}^{3}\alpha_i]u_{i,j,k} = - \alpha_1[u_{i,j,k+1} + u_{i,j,k-1}] - \qquad (2)$$

$$- \alpha_2[u_{i,j+1,k} + u_{i,j-1,k}] -$$

$$(i + j + k = \text{even}) \qquad - \alpha_3[u_{i+1,j,k} + u_{i-1,j,k}].$$

The choice of the displacement subscripts is evident from Fig. 1. Assuming the Born—Kárman periodic conditions in all three directions and using the properties of the cyclic matrices [8] we can rewrite the equations (1) and (2) as follows

$$\mathscr{M}\omega^2\mathbf{u}_{N^3} = \{[\mathbf{I}_N \times \mathbf{\Phi}^2_{N^2}] - [\mathbf{\Omega}_N \times \mathbf{P}_{N^2} + \mathbf{\Omega}_N^{-1} \times \mathbf{P}_{N^2} - 2\mathbf{I}_N \times \mathbf{P}_{N^2}]\} \times \mathbf{u}_{N^3} \qquad (3)$$

where

$$\mathbf{P}_{N^2} = \alpha_3\mathbf{I}_{N^2} \qquad \mathscr{M} = \mathbf{I}_{N/2} \times \begin{pmatrix} \mathbf{M}^1_{N^2} & 0 \\ 0 & \mathbf{M}^2_{N^2} \end{pmatrix}$$

$$[\mathbf{\Omega}_N]_{ij} = \delta_{i,j-1} \quad \text{mod } N$$

and $\times$ means the direct product of matrices.

Matrix $\mathbf{M}^1_{N^2}$ (and similarly matrix $\mathbf{M}^2_{N^2}$) is a diagonal matrix of the order N^2, whose elements are masses of the atoms of the particular lattice points

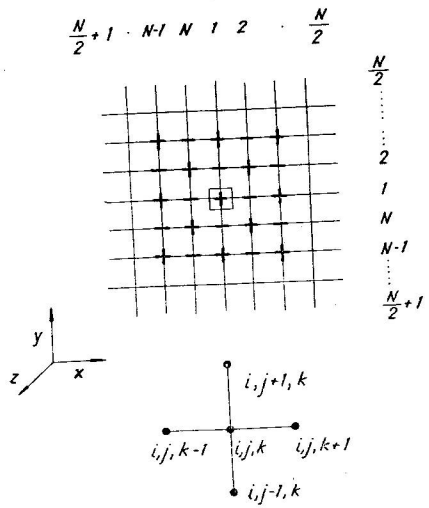

Fig. 1.

at odd walls (or even walls, respectively) and the matrix $\mathbf{\Phi}^2_{N^2}$ is a matrix of force constants of the two-dimensional lattice and has the structure

$$\mathbf{\Phi}^2_{N^2} = \begin{pmatrix} \mathbf{A} & \mathbf{B} & & \mathbf{B} \\ \mathbf{B} & \ddots & 0 & \\ & 0 & \ddots & \mathbf{B} \\ \mathbf{B} & & \mathbf{B} & \mathbf{A} \end{pmatrix} = - \alpha_1[\mathbf{I}_N \times \mathbf{\Omega}_N + \mathbf{I}_N \times \mathbf{\Omega}_N^{-1} - 2\mathbf{I}_{N^2}] - \qquad (4)$$

$$- \alpha_2[\mathbf{\Omega}_N \times \mathbf{I}_N + \mathbf{\Omega}_N^{-1} \times \mathbf{I}_N - 2\mathbf{I}_{N^2}]$$

$$A_{ii} = 2(\alpha_1 + \alpha_2) \qquad A_{i,i+1} = A_{i,i-1} = -\alpha_1$$

$$B_{ii} = -\alpha_2$$

Let us now assume that a lattice is disturbed by the introducing of the line of defect atoms oriented in the direction of the axis z in such a way that it goes through a lattice point with the coordinates (1.1). The masses of the defect atoms are $m_1' = m_1(1 - \varepsilon_1)$, $m_2' = m_2(1 - \varepsilon_2)$ and the force constants between defect atoms are $\alpha_3' = \alpha_3(1 - \gamma)$. The displacements of the particular atoms are again described by equation (3), if in the matrices $\mathscr{M}$ and $\mathbf{P}_{N^2}$ appropriate changes in the force constants and the masses are made. After solving this equation we could obtain frequencies of localized vibrations. In this direct treatment difficulties connected with the evaluation of the Green's functions arise and therefore we shall use the approximation on a monoatomic lattice to solve this problem.

In order to do this let us return to the illustrative equations (1) and (2) and enlarge them by the equations valid for the lattice points containing a defect atom. If we define a mass M^* [7] as

$$[M^*\omega^2 - 2\sum_{i=1}^{3}\alpha_i] = [m_1\omega^2 - 2\sum_{i=1}^{3}\alpha_i]^{1/2}[m_2\omega^2 - 2\sum_{i=1}^{3}\alpha_i]^{1/2} \qquad (5)$$

and displacements as

$$u_{i,j,k} = \begin{cases} \left[m_2\omega^2 - 2\sum_{i=1}^{3}\alpha_i\right]^{1/2} w_{i,j,k} \text{ for an odd lattice point} \\ \left[m_1\omega^2 - 2\sum_{i=1}^{3}\alpha_i\right]^{1/2} w_{i,j,k} \text{ for en even lattice point} \end{cases}$$

then with respect to the designation

$$\Delta^{1,2}(\omega^2) = \frac{\left[m_{1,2}\omega^2 - 2\sum_{i=1}^{3}\alpha_i\right]^{1/2}}{\left[m_{2,1}\omega^2 - 2\sum_{i=1}^{3}\alpha_i\right]^{1/2}} \quad \text{and} \quad \mathbf{F}_{N^2} = \left.\begin{pmatrix} 1 & & \\ & 0 & \\ & & \ddots \\ & & & 0 \end{pmatrix}\right\} N^2$$

the equation (3) will be in the form

$$\left\{M^*\omega^2\mathbf{I}_{N^3} - \omega^2\mathbf{I}_{N/2} \times \begin{pmatrix} m_1\varepsilon_1\Delta^2 & 0 \\ 0 & m_2\varepsilon_2\Delta^1 \end{pmatrix} \times \mathbf{F}_{N^2}\right\}\mathbf{w}_{N^3} = \tag{6a}$$

$$= \left\{[\mathbf{I}_N \times \mathbf{\Phi}^2_{N^2}] - \alpha_3[\mathbf{\Omega}_N + \mathbf{\Omega}_N^{-1} - 2\mathbf{I}_N] \times \mathbf{I}_{N^2} + \right.$$

$$\left. + \alpha_3\gamma\left[\mathbf{\Omega}_N + \mathbf{\Omega}_N^{-1} - 2\mathbf{I}_{N/2} \times \begin{pmatrix} \Delta^2 & 0 \\ 0 & \Delta^1 \end{pmatrix}\right] \times \mathbf{F}_{N^2}\right\}\mathbf{w}_{N^3}.$$

To be able to use translation symmetry in the direction of the axis z let us arrange the right side of the equation (6a) as follows

$$\left\{\left[\mathbf{I}_{N/2} \times \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \times \mathbf{\Phi}^2_{N^2}\right] - \alpha_3\left[\mathbf{I}_{N/2} \times \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \mathbf{\Omega}_{N/2} \times \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \right.\right.$$

$$+ \mathbf{\Omega}^{-1}_{N/2} \times \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - 2\mathbf{I}_N\Big] \times \mathbf{I}_{N^2} + \alpha_3\gamma\left[\mathbf{I}_{N/2} \times \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \mathbf{\Omega}_{N/2} \times \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \right.$$

$$\left.\left. + \mathbf{\Omega}^{-1}_{N/2} \times \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - 2\mathbf{I}_{N/2} \times \begin{pmatrix} \Delta^2 & 0 \\ 0 & \Delta^1 \end{pmatrix}\right] \times \mathbf{F}_{N^2}\right\}. \tag{6b}$$

As the eigen-values and the eigen-vectors of the cyclic matrices are known [8]

$$\mathbf{\Omega}_N\mathbf{w}_N(\varphi) = e^{i\varphi}\mathbf{w}_N(\varphi),\ [\mathbf{w}_N(\varphi)]_n = N^{-1/2}e^{i\varphi n},\ \varphi = \frac{2\pi}{N}k;\ k, n = 1, 2, \ldots N$$

the solution of equation (6) can be found in the form of the direct product

$$\mathbf{w}_{N^3} = \mathbf{v}_{N/2}(\varphi_3) \times \mathbf{q}_{2N^2}(\varphi_3). \tag{7}$$

Putting (7) into (6) we obtain

$$\{\mathbf{D}_{2N^2}(\varphi_3) - M^*\omega^2\mathbf{I}_{2N^2}\}\mathbf{q}_{2N^2}(\varphi_3) = 0 \tag{8}$$

where

$$\mathbf{D}_{2N^2}(\varphi_3) = \mathbf{D}^0_{2N^2}(\varphi_3) + \mathbf{R}(\omega^2; \varphi_3)$$

$$\mathbf{D}^0_{2N^2}(\varphi_3) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \times \mathbf{\Phi}^2_{N^2} - \alpha_3 \begin{pmatrix} -2 & 1 + e^{-i\varphi_3} \\ 1 + e^{i\varphi_3} & -2 \end{pmatrix} \times \mathbf{I}_{N^2}$$

$$\mathbf{R}(\omega^2; \varphi_3) = \left\{\alpha_3\gamma \begin{pmatrix} -2\Delta^2(\omega^2) & 1 + e^{-i\varphi_3} \\ 1 + e^{i\varphi_3} & -2\Delta^1(\omega^2) \end{pmatrix} + \omega^2 \begin{pmatrix} m_1\varepsilon_1\Delta^2(\omega^2) & 0 \\ 0 & m_2\varepsilon_2\Delta^1(\omega^2) \end{pmatrix}\right\} \times \mathbf{F}_{N^2}$$

and φ_3 is a parameter acquiring $N/2$ values from 0 to 2π. As the matrix $\mathbf{R}$ has only a few non-zero elements, let us introduce Green's functions and instead of the equation (8) let us solve the following equation

$$\{\mathbf{I}_{2N^2} + (\mathbf{D}^0_{2N^2} - M^*\omega^2\mathbf{I}_{2N^2})^{-1}\mathbf{R}(\omega^2; \varphi_3)\}\mathbf{q}_{2N^2}(\varphi_3) = 0. \tag{9}$$

Further, it is advantageous to arrange the displacements in such a way that the non-zero elements of the matrix $\mathbf{R}$ may form only one submatrix different from zero

$$\mathbf{R} = \left(\begin{array}{c:c} \bullet & \bullet \\ \hdashline \bullet & \bullet \end{array}\right)\begin{matrix}\}N^2 \\ \}N^2\end{matrix} \rightarrow \left(\begin{array}{c:c} \bullet\bullet & \\ \bullet\bullet & \\ \hdashline & \end{array}\right).$$

Similarly we must arrange the matrix of Green's functions, which is then divided in the following way

$$(\mathbf{D}^0_{2N^2} - M^*\omega^2\mathbf{I}_{2N^2})^{-1} = \begin{pmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{pmatrix}$$

where $\mathbf{K}_{11}(M^*\omega^2)$ is the square matrix corresponding to the non-zero elements of the matrix $\mathbf{R}$ (for simplicity we keep to original notation).

Eq. (9) can then be rewritten as

$$\left(\begin{array}{c:c} \mathbf{I} + \mathbf{K}_{11}\mathbf{R} & 0 \\ \hdashline \mathbf{K}_{21}\mathbf{R} & \mathrm{I} \end{array}\right)\begin{pmatrix} \mathbf{q}_1 \\ \mathbf{q}_2 \end{pmatrix} = 0.$$

Hence it can be seen that the frequencies of the searched localized vibrations and of the corresponding components $\mathbf{q}_1$ (which characterize the disturbed region) of the vector $\mathbf{q}_{2N^2}$ are the solution of the equation

$$\{\mathbf{I} + \mathbf{K}_{11}(M^*\omega^2; \varphi_3)\mathbf{R}(\omega^2; \varphi_3)\}\mathbf{q}_1(\varphi_3) = 0. \tag{10}$$

Equation (8) describes the vibrations of a $2N^2$-dimensional lattice, whose matrix of force constants, for $\mathbf{R} = 0$, is the matrix $\mathbf{D}^0_{2N^2}$. The matrix $\mathbf{D}_{2N^2}$ is of a Hermite type and its eigen-values are therefore real. In our case, however, due to the frequency-dependent defect, the $M^*\omega^2$-local, which satisfies the equation (8), is generally not an eigen-value of the matrix $\mathbf{D}_{2N^2}$. We must thus assume that the values $M^*\omega^2$ are not only real, but also complex. From definition (5)[1]), it can be seen that the complex values $M^*\omega^2$ correspond to the frequencies in the forbidden space between the optical and acoustical band of a three-dimensional diatomic lattice. These frequencies satisfy the relation $\omega_1^2 < \omega^2 < \omega_2^2$. Real $M^*\omega^2$ — local correspond then to the region $\omega^2 > \omega_2^2$ or $\omega^2 < \omega_1^2$ (see Fig. 2b). In order to determine, where the local frequencies, e. g. frequencies complying with (10), are situated, we must know the eigen-frequencies of a lattice, which are described by the matrix of the force constants $\mathbf{D}^0_{2N^2}$. Therefore we shall return to the problem of the

[1]) We consider only the positive root of the square roots $(m_1\omega^2 - 2\sum_{i=1}^{3}\alpha_i)^{1/2}$ and $(m_2\omega^2 - 2\sum_{i=1}^{3}\alpha_i)^{1/2}$.

possition of the local frequencies later and now turn our attention to the matrix of Greene's functions.

THE INVERSE MATRIX $(\mathbf{D}^0_{2N^2} - M^*\omega^2\mathbf{I}_{2N^2})^{-1}$

In order to carry out the required inversion, we concern ourselves with eigen-values of the matrix $\mathbf{D}^0_{2N^2}(\varphi_3)$, which are designated by λ^0, and therefore we determine the solution of the equation

$$\{\mathbf{D}^0_{2N^2}(\varphi_3) - \lambda^0\mathbf{I}_{2N^2}\}\mathbf{q}_{2N^2}(\varphi_3) = 0. \tag{11}$$

Substituting the relation (4) in place of $\mathbf{\Phi}^2_{N^2}$ we can see that the solution of equation (11) can be found in the form of the direct product

$$\mathbf{q}_{2N^2} = \mathbf{v}_2 \times \mathbf{v}_N(\varphi_1) \times \mathbf{v}_N(\varphi_2) \tag{12}$$

where

$$\varphi_i = \frac{2\pi}{N}k \qquad \begin{matrix} i = 1, 2 \\ k = 1, 2, \ldots N \end{matrix}$$

Substituting (12) into (11) we obtain for the vectors $\mathbf{v}_2$ and the eigen values λ^0

$$\mathbf{v}^j_2 = \begin{pmatrix} \dfrac{(-1)^{j+1}}{\sqrt{2}} \dfrac{(1+e^{-i\varphi_3})}{2\cos\varphi_2/2} \\ 1/\sqrt{2} \end{pmatrix} \tag{13}$$

$$\lambda^0_j = 4\sum_{i=1}^{2}\alpha_i \sin\varphi_i/2 + \begin{cases} 4\alpha_3 \sin^2\varphi_3/4 & j = 1 \\ 4\alpha_3\cos^2\varphi_3/4 & j = 2 \end{cases}$$

We point out again that the dependence of the eigen-values λ^0_j on the masses m_1 and m_2 is defined by the relation (5) as we in fact put $M^*\omega^2 = \lambda$. Now we can easily accomplish the required inversion of the expression $(\mathbf{D}^0_{2N^2} - M^*\omega^2\mathbf{I}_{2N^2})$.

For $N \to \infty$

$$(\mathbf{D}^0_{2N^2} - M^*\omega^2\mathbf{I}_{2N^2})^{-1} = \underset{\substack{slm \\ s'l'm'}}{}$$

$$= \frac{1}{(2\pi)^2}\sum_{j=1}^{2}\int_0^{2\pi}\int \frac{v^*_{js}(\varphi_3)v_{js'}(\varphi_3)}{-M^*\omega^2 + \lambda^0_j}\exp i[(m-m')\varphi_1 + (l-l')\varphi_2]d\varphi_1 d\varphi_2 \tag{14}$$

$$= \frac{1}{(2\pi)^2}\sum_{j=1}^{2} v^*_{js}(\varphi_3)v_{js'}(\varphi_3)\int_0^{2\pi}\int \frac{\exp i[(m-m')\varphi_1 + (l-l')\varphi_2]}{-\eta_j + 4\alpha_1\sin^2\varphi_1/2 + 4\alpha_2\sin^2\varphi_2/2}\,d\varphi_1 d\varphi_2$$

where

$$\eta_j = M^*\omega^2 - 2\alpha_3\left[1 + (-1)^j\cos\frac{\varphi_3}{2}\right].$$

As we are interested in local vibrations, e. g. we require $M^*\omega^2 \neq \lambda^0_j$ hence also $\eta_j \neq 4\sum_{i=1}^{2}\alpha_i\sin^2\dfrac{\varphi_i}{2}$.

The integral (14) is, however, with the exception of the constants, Greene's function of an ideal two-dimensional monoatomic lattice and has been relatively well analysed already [4], [9]. It is convergent for $\eta_j < 0, \eta_j > 4(\alpha_1 + \alpha_2)$ and divergent only on the boundaries. This difficulty can be avoided. As demonstrated in [9], Greene's function can be divided into two parts, where one is then divergent for $\eta_j \to 0$, $\eta_j \to 4(\alpha_1 + \alpha_2)$ and the other gets a finite value. The integral (14) is convergent also for a complex η.

ANALYSIS OF THE LOCATION OF LOCAL FREQUENCIES

In order to analyse local vibrations let us return again to the right-hand side of equation (5). It can be expressed also as

$$[m_1\omega^2 - 2\sum_{i=1}^{3}\alpha_i]^{1/2}[m_2\omega^2 - 2\sum_{i=1}^{3}\alpha_i]^{1/2} = \pm K(\varphi_1, \varphi_2, \varphi_3). \tag{15}$$

A simple substitution makes it clear that for $K > 0$ a plus sign corresponds to the frequencies ω^2 from the optical branch and a minus sign to the frequen-

Table 1

The boundaries of the frequency bands (Fig. 2a).

Upper bound	$(4\sum_{i=1}^{2}\alpha_i, 4\sum_{i=1}^{2}\alpha_i + 2\alpha_3)$	$(4\sum_{i=1}^{2}\alpha_i + 2\alpha_3, 4\sum_{i=1}^{3}\alpha_i)$
Lower bound	$(0, 2\alpha_3)$	$(2\alpha_3, 4\alpha_3)$
(—) lattice	$0 < \varphi_3 < \pi \quad j = 1$	$\pi < \varphi_3 < 2\pi \quad j = 1$
	$2\pi < \varphi_3 < \pi \quad j = 2$	$\pi < \varphi_3 < 0 \quad j = 2$
(+) lattice	$2\pi < \varphi_3 < \pi \quad j = 1$	$\pi < \varphi_3 < 0 \quad j = 1$
	$0 < \varphi_3 < \pi \quad j = 2$	$\pi < \varphi_3 < 2\pi \quad j = 2$

cies from the acoustic branch. We shall therefore, in accordance with (5), define the mass M^* in two ways so that the following defining equations may hold

$$[M^*\omega^2]_- - 2\sum_{i=1}^{3}\alpha_i = -K(\varphi_1, \varphi_2, \varphi_3) \quad (-) \text{ lattice} \tag{16}$$

$$[M^*\omega^2]_+ - 2\sum_{i=1}^{3}\alpha_i = +K(\varphi_1, \varphi_2, \varphi_3) \quad (+) \text{ lattice}$$

For $K > 0$ the acoustic branch of the diatomic lattice spectrum is transformed into the monoatomic lattice characterized by $[M^*\omega^2]_-$ ((−) lattice) and similarly the optical branch of a diatomic lattice is transformed into $[M^*\omega^2]_+$, i. e. the vibration problem of a diatomic lattice becomes the vibration problem of two monoatomic lattices (for $K < 0$ the mutual assignment of the mono- and diatomic spectrum is just a reverse one).

In deriving equations (6)—(14) we have used a formal expression $M^*\omega^2 - 2\sum_{i=1}^{3}\alpha_i$, i. e. we have not specified, if the (+) or the (−) lattice is chosen. If we compare now equation (13) with (16) we may find that equation (13) can be assigned to the (−) lattice. From (13) we can see further that by the simple transformation

$$\varphi_j^* = \varphi_j \pm \pi \quad j = 1, 2$$
$$\varphi_3^* = \varphi_3 \pm 2\pi$$

the (+) lattice characterized by the quantities φ_i^* ($i = 1, 2, 3$) has formally the same dispersion law as the (−) lattice. Then $+K(\varphi_1, \varphi_2, \varphi_3) = -K(\varphi_1^*,$

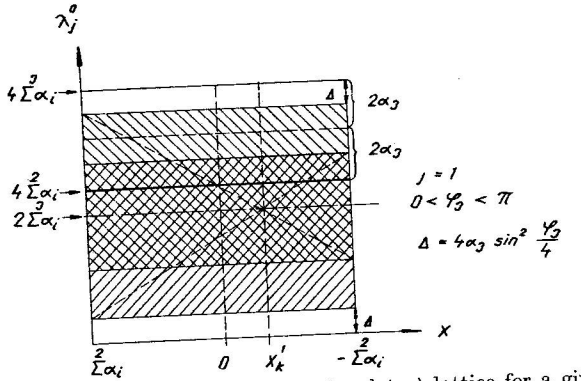

Fig. 2a. ▨ — the frequency band of a $2N^2$-dimensional (—) lattice for a given value of the parameter φ_3. ▥ — the frequency band of a $2N^2$-dimensional (+) lattice for a given value of the parameter φ_3. The band boundaries are in the intervals given by Table 1.

φ_2^*, φ_3^*) and therefore also equations (6)—(14) will be valid for the (+) lattice (instead of φ_i we write φ_i^*). When determining the local frequencies of the lattice, described by equation (3), (e. g. $[M^*\omega^2]_\pm \neq \lambda_{j\pm}^0$) these must be simultaneously the local frequencies of the (+) lattices and the (−) lattices. The same results would have been obtained by using one of the lattices only and applying then the translation symmetry. In our case this procedure would be less clear than that shown above.

Fig. 2a presents the frequency analysis of the (+) and (−) lattices described

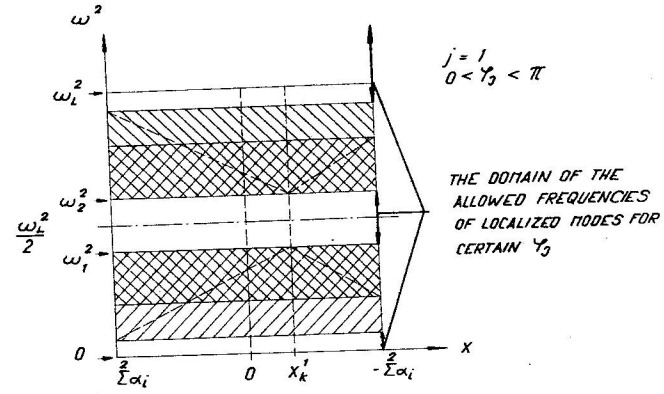

Fig. 2b. The frequency bands of a $2N^2$-dimensional diatomic lattice approximated by the (+) lattice and the (—) lattice for a given value of the parameter φ_3. They are determined by the frequencies of the optical (plus sign) and the acoustic (minus sign) branch.

$$\omega_j^2 = \frac{1}{2}\omega_L^2 \pm \left[\left(\frac{\omega_2^2 - \omega_1^2}{2}\right)^2 + \frac{4}{m_1 m_2}(\alpha_1 \cos\varphi_1 + \alpha_2 \cos\varphi_2 + (-1)^{j+1}\alpha_3 \cos\varphi_3/2)^2\right]^{1/2}$$

where

$$\omega_L^2 = \omega_1^2 + \omega_2^2 = 2(\alpha_1 + \alpha_2 + \alpha_3)\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \text{ for } m_1 > m_2.$$

Introducing the notation $X = \sum \alpha_i \cos\varphi_i$ (it is summed over i which has the value 1, 2) we can see that X can get values from the interval $(\sum\alpha_i, -\sum\alpha_i)$. By a similar method as in [10], the expressions (15) and (16) can be analysed and we arrive at the conclusion that to the (—) lattice there correspond acoustic frequencies from the interval $(\sum\alpha_i, X_k^j)$ and optical frequencies from the interval $(X_k^j, -\sum\alpha_i)$. To the (+) lattice there correspond optical frequencies from the interval $(\sum\alpha_i, X_k^j)$ and acoustic frequencies from the interval $(X_k^j, -\sum\alpha_i)$. The quantity X_k^j depends on φ_3, j and is defined as $X_k^j = \sum \alpha_i \cos\varphi_i^k = -(-1)^{j+1}\alpha_3 \cos\varphi_3/2$.

by equation (13) for a given value of the parameter φ_3, from the interval $(0, \pi)$. The frequencies of the corresponding diatomic lattice are then obtained by inserting (5) into (13) as can be seen on Fig. 2b. After a similar analysis for φ_3 from the interval $(\pi, 2\pi)$ we arrive at the conclusion that for the calculation of the local frequencies above and in the optical band of an ideal three-dimensional lattice the (+) lattice is used, for the local frequencies in the acoustic band, however, the (−) lattice, provided φ_3 is in the interval $(0, \pi)$. For φ_3 from the interval $(\pi, 2\pi)$ the situation is just an opposite one. Fig. 3 elucidates the case — the white areas correspond to the possible local frequencies for a given φ_3.

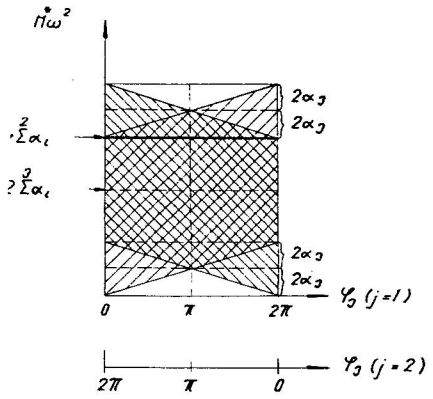

Fig. 3. The dependence $[M^*\omega^2]_\pm$ on the parameter φ_3. For orientation a rough dependence is sufficient and therefore the curves can be approximated by straight lines.

Similarly as in the case of a linear defect in the monoatomic lattice, bands of local frequencies can be expected. These may be located above and in the band of the optical vibrations, in the band of the acoustic vibrations and in the forbidden frequency band of a three-dimensional ideal diatomic lattice (see Fig. 3). In the last case it is interesting that a possible band of local frequencies in the forbidden space between the optical and acoustical band does not exceed the boundary frequencies of an ideal lattice. The matrix $\mathbf{D}_{2N^2}$ being a Hermite symmetric one, and the matrix $\mathbf{R}$ being frequency-dependent, we cannot perform a general consideration about the dependence of the local frequencies on the parameter φ_3, which characterizes a band, without a concrete calculation. All that can be said is that, if for a certain $\omega^2(\varphi_3)$ equation (10) is satisfied, then we can get the whole band of local frequencies

for all φ_3 only under the condition stated in Fig. 3. Otherwise only incomplete or disrupted bands result.

Numerical calculation of the local frequencies will be dealt with later.[2])

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Fyzikálny ústav SAV, Bratislava

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