PHYSICS

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1958

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Abstract

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PHYSICS

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NORMAL COORDINATES OF A CRYSTAL LATTICE WITH RETARDATION OF THE INTERACTION TAKEN INTO ACCOUNT

(Presented by Academician N. N. Bogolyubov, 8 IV 1958)

1. The consideration of a number of properties of a crystal is based on the introduction of normal coordinates. This problem is solved elementarily for purely mechanical vibrations, when the retarded electromagnetic interaction between the particles of the crystal is not taken into account ([1]). However, for a consistent consideration of the optical properties of a crystal it is necessary to take the indicated retardation into account, and therefore the problem of introducing normal coordinates must be solved in this general case. We shall consider a crystal lattice in the dipole approximation, when the variables are taken to be the displacements of the atoms $\mathbf{u}_s^l$ and the dipole moments $\mathbf{p}_s^l$ caused by deformation of the electron shells (l is the number of the unit cell, s the number of the atom in it) ([2]).

Neglecting the inertia of the dipole moments, the equations of motion are

$$m_s \ddot{\mathbf{u}}_s^l = -\frac{\partial U}{\partial \mathbf{u}_s^l} + e_s \vec{\mathcal{E}}_s^l, \qquad 0 = -\frac{\partial U}{\partial \mathbf{p}_s^l} + \vec{\mathcal{E}}_s^l, \tag{1}$$

where m_s, e_s are the mass and charge of the s-th ion; U is the potential energy, a homogeneous quadratic form in $\mathbf{u}_s^l, \mathbf{p}_s^l$; $\vec{\mathcal{E}}_s^l$ is the electric-field strength at the lattice point with coordinates $\mathbf{r}_s^l$.

We seek the solution of (1) in the form of plane monochromatic waves

$$\mathbf{u}_s^l = \mathbf{u}_s \exp(-i\omega t + i\mathbf{k}\mathbf{r}_s^l), \qquad \mathbf{p}_s^l = \mathbf{p}_s \exp(-i\omega t + i\mathbf{k}\mathbf{r}_s^l),$$

$$\vec{\mathcal{E}}_s^l = \vec{\mathcal{E}}_s \exp(-i\omega t + i\mathbf{k}\mathbf{r}_s^l), \tag{2}$$

where ([3])

$$\vec{\mathcal{E}}_s = \frac{4\pi}{\Delta} \frac{\vec{\mathcal{P}} - n^2 \mathbf{s}(\vec{\mathcal{P}}, \mathbf{s})}{n^2 - 1} + \mathbf{E}_s(i\mathbf{k}, \mathbf{u}_1, \dots, \mathbf{p}_1, \dots); \tag{3}$$

Δ is the volume of the unit cell; $n = ck/\omega$ is the refractive index (c is the speed of light in vacuum); $\vec{\mathcal{P}} = \sum_s (e_s \mathbf{u}_s + \mathbf{p}_s)$; $\mathbf{s}$ is the unit vector of $\mathbf{k}$; $\mathbf{E}_s$ is a linear function of the amplitudes.

Substitution of (2) into (1) gives equations for the amplitudes:

$$\omega^2 m_s T^j_{sx'} \delta_{j1} + \sum_{j's'y'} A^{jj'}_{ss'x'y'}(i\mathbf{k})\, T^{j'}_{s'y'} + (e_s \delta_{j1} + \delta_{j2})\, \mathcal{E}_{sx'} = 0, \tag{4}$$

$$T^j_{sx'} = \begin{cases} u_{sx'}, & j = 1, \\ p_{sx'}, & j = 2; \end{cases} \qquad x', y' = x, y, z.$$

In (4) $\mathbf{k}$ enters only with the factor i, and therefore the solution for $-\mathbf{k}$ is the complex conjugate of the solution for $\mathbf{k}$:

$$\omega^2(-\mathbf{k}) = \omega^{2*}(\mathbf{k}), \qquad T^j_s(-\mathbf{k}) = T^{j*}_s(\mathbf{k}), \qquad \vec{\mathcal{E}}_s(-\mathbf{k}) = \vec{\mathcal{E}}^*_s(\mathbf{k}). \tag{5}$$

The reality of ω^2 does not follow from (4) because of the presence of the last term, and will be obtained below. (5) makes it possible to represent the general real solution (1) in the form

$$T^{jl}_s = \sum_{\alpha\mathbf{k}} q^\alpha(\mathbf{k}, t) T^{j\alpha}_s(\mathbf{k}) \exp(i\mathbf{k}\mathbf{r}^l_s), \qquad \vec{\mathcal{E}}^{\,l}_s = \sum_{\alpha\mathbf{k}} q^\alpha(\mathbf{k}, t) \vec{\mathcal{E}}^{\,\alpha}_s(\mathbf{k}) \exp(i\mathbf{k}\mathbf{r}^l_s), \tag{6}$$

where α is the number of a branch of the vibration spectrum; $q^\alpha(\mathbf{k}, t)$ are harmonic functions of time with frequency $\omega_\alpha(\mathbf{k})$, with $q^\alpha(-\mathbf{k}) = q^{\alpha*}(\mathbf{k})$.

2. The spatial mean value of the amplitude of the electric-field strength is given by the first term of (3) ([1]). The term $\mathbf{E}_s$ is independent of the frequency, and thus contains no retardation, and therefore may be included in the potential interaction, which is assumed below. It is easy to show that the expression for $\vec{\mathcal{E}}^{\,l}_s$ from (2) is valid not only for the lattice sites, but also for any point (with the corresponding choice of $\mathbf{E}_s$). Therefore we put

$$\vec{\mathcal{E}}(\mathbf{r}, t) = \sum_{\alpha\mathbf{k}} q^\alpha(\mathbf{k}, t) \vec{\mathcal{E}}^{\,\alpha}(\mathbf{k}) \exp(i\mathbf{k}\mathbf{r}), \qquad \vec{\mathcal{E}}^{\,\alpha}(\mathbf{k}) = \frac{4\pi}{\Delta} \frac{\vec{\mathcal{P}}^{\,\alpha}(\mathbf{k}) - n^2_\alpha(\mathbf{k})\, \mathbf{s}(\vec{\mathcal{P}}^{\,\alpha}(\mathbf{k}), \mathbf{s})}{n^2_\alpha(\mathbf{k}) - 1}. \tag{7}$$

(7) can be expressed through the vector potential:

$$\vec{\mathcal{E}} = -\frac{1}{c}\frac{\partial \vec{\mathcal{A}}}{\partial t}, \qquad \vec{\mathcal{A}} = c\sum_{\alpha\mathbf{k}} \dot{q}^{\alpha}(\mathbf{k},t)\omega_{\alpha}^{-2}(\mathbf{k})\vec{\mathcal{E}}^{\,\alpha}(\mathbf{k})\exp(i\mathbf{kr}). \tag{8}$$

For the magnetic-field induction this gives

$$\vec{\mathcal{B}} = \operatorname{rot}\vec{\mathcal{A}} = ic\sum_{\alpha\mathbf{k}} \dot{q}^{\alpha}(\mathbf{k},t)[\mathbf{k},\vec{\mathcal{E}}^{\,\alpha}(\mathbf{k})]\omega_{\alpha}^{-2}(\mathbf{k})\exp(i\mathbf{kr}). \tag{9}$$

The electric-field induction is $\vec{\mathcal{D}} = \vec{\mathcal{E}} + \frac{4\pi}{\Delta}\vec{\mathcal{P}}$. In the dipole approximation used, the magnetic moment is equal to zero; therefore the magnetic-field strength $\vec{\mathcal{H}} = \vec{\mathcal{B}}$. It is easy to see that the field vectors introduced in this way satisfy Maxwell' s equations.

3. Equation (4) for the branch α has the form

$$\omega_{\alpha}^{2}(\mathbf{k})\, m_s T_{sx'}^{j\alpha}(\mathbf{k})\delta_{j1} + \sum_{j's'y'} A_{ss'x'y'}^{jj'}(i\mathbf{k})T_{s'y'}^{j'\alpha}(\mathbf{k}) + (e_s\delta_{j1}+\delta_{j2})\mathcal{E}_{x'}^{\alpha}(\mathbf{k}) = 0. \tag{10}$$

Let us replace here α by β and $\mathbf{k}$ by $-\mathbf{k}$:

$$\omega_{\beta}^{2}(-\mathbf{k})\, m_s T_{sx'}^{j\beta}(-\mathbf{k})\delta_{j1} + \sum_{j's'y'} A_{ss'x'y'}^{jj'}(i\mathbf{k})T_{s'y'}^{j'\beta}(-\mathbf{k}) +$$

$$+(e_s\delta_{j1}+\delta_{j2})\mathcal{E}_{x'}^{\beta}(-\mathbf{k}) = 0. \tag{11}$$

Multiplying (10) by $T_{sx'}^{j\beta}(-\mathbf{k})$, (11) by $T_{sx'}^{j\alpha}(\mathbf{k})$, subtracting the second equation from the first, summing over j, s, x', and taking into account the Hermiticity of the matrix $A_{ss'x'y'}^{jj'}$,

we obtain

$$[\omega_{\beta}^{2}(-\mathbf{k}) - \omega_{\alpha}^{2}(\mathbf{k})]\dot{I}_{\alpha\beta}(\mathbf{k}) = 0,$$

$$\dot{I}_{\alpha\beta}(\mathbf{k}) = \sum_s m_s u_s^{\alpha}(\mathbf{k})u_s^{\beta}(-\mathbf{k}) + \frac{4\pi}{\Delta}k^2c^2\left[(\vec{\mathcal{P}}^{\,\alpha}(\mathbf{k}),\vec{\mathcal{P}}^{\,\beta}(-\mathbf{k})) - (\vec{\mathcal{P}}^{\,\alpha}(\mathbf{k}),\mathbf{s})(\vec{\mathcal{P}}^{\,\beta}(\mathbf{k}),\mathbf{s})\right]\times \tag{12}$$

$$\times\left\{[n_{\alpha}^{2}(\mathbf{k})-1][n_{\beta}^{2}(-\mathbf{k})-1]\omega_{\alpha}^{2}(\mathbf{k})\omega_{\beta}^{2}(-\mathbf{k})\right\}^{-1};$$

i.e., the orthogonality relation for the amplitudes when retardation is taken into account. If retardation is neglected, the second term in $\dot{I}_{\alpha\beta}$ is absent [(1)].

4. Lattice energy

$$E = T + U + W_e + W_m = \frac{1}{2}\sum_{sl} m_s(\dot{u}_s^l)^2 + U + \frac{1}{8\pi}\int (\mathcal{E}^2 + \mathcal{H}^2)\, dv \geqslant 0. \quad (13)$$

Expression (13) is not self-evident, since it contains the average (and not microscopic) field strengths. The choice of E in this form is justified below. Substituting (6) into (13), we obtain

$$E = \frac{N}{2}\sum_{\alpha\beta\mathbf{k}} \dot{I}_{\alpha\beta}(\mathbf{k})\left[\dot{q}^{\alpha}(\mathbf{k})\dot{q}^{\beta}(-\mathbf{k}) + \omega_{\alpha}^2(\mathbf{k})q^{\alpha}(\mathbf{k})q^{\beta}(-\mathbf{k})\right], \quad (14)$$

where N is the number of cells in the fundamental region.

From (12), (5), and the condition that E be real and positive, it follows that $\beta = \alpha$, $\omega_{\alpha}^{*2}(\mathbf{k}) = \omega_{\alpha}^2(\mathbf{k}) \geqslant 0$. Thus the reality of the frequency has been proved. Introducing the amplitude normalization condition

$$N\dot{I}_{\alpha\alpha}(\mathbf{k}) = 1, \quad (15)$$

we obtain

$$E = \sum_{\alpha\mathbf{k}}{}' \left[\dot{q}^{\alpha}(\mathbf{k})\dot{q}^{*\alpha}(\mathbf{k}) + \omega_{\alpha}^2(\mathbf{k})q^{\alpha}(\mathbf{k})q^{*\alpha}(\mathbf{k})\right], \quad (16)$$

where the prime means that the summation is carried out over the half-space of $\mathbf{k}$.

5. The equations of motion in normal coordinates must have the form

$$\ddot{q}^{\alpha}(\mathbf{k}) + \omega_{\alpha}^2(\mathbf{k})q^{\alpha}(\mathbf{k}) = 0. \quad (17)$$

This is ensured by the following choice of the Lagrange function:

$$L = T - U + W_m - W_e = \sum_{\alpha\mathbf{k}}{}' \left[\dot{q}^{\alpha}(\mathbf{k})\dot{q}^{*\alpha}(\mathbf{k}) - \omega_{\alpha}^2(\mathbf{k})q^{\alpha}(\mathbf{k})q^{*\alpha}(\mathbf{k})\right]. \quad (18)$$

L contains no terms of the type $\frac{e}{c}(\mathbf{v}, \vec{A})$ ($\mathbf{v}$ is the velocity). This is explained by the fact that the action of the field on the particles which they produce is already contained in the term $(W_m - W_e)$, since the field is expressed through the same q-coordinates as T_s^l. The indicated term enters with the opposite sign compared with the usual one. This is connected with the fact that the electric-field strength is expressed through q, while the magnetic-field strength is expressed through $\dot{q}$, in contrast to the usual case. From (18) we find for the generalized momenta

$$p^{\alpha}(\mathbf{k}) = \dot{q}^{*\alpha}(\mathbf{k}), \qquad p^{*\alpha}(\mathbf{k}) = \dot{q}^{\alpha}(\mathbf{k}), \tag{19}$$

which gives for the Hamilton function

$$H = \sum_{\alpha\mathbf{k}}{}' \left[p^{\alpha}(\mathbf{k})p^{*\alpha}(\mathbf{k}) + \omega_{\alpha}^2(\mathbf{k})q^{\alpha}(\mathbf{k})q^{*\alpha}(\mathbf{k})\right]. \tag{20}$$

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Received
7 IV 1958

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Note: Figure translations are in progress. See original paper for figures.