doi: 10.15407/ujpe60.06.0528

A.A. STUPKA
Oles Honchar National University of Dnipropetrovsk
(72, Gagarin Ave., Dnipropetrovsk 49050, Ukraine; e-mail: antonstupka@mail.ru)

PACS 63.20. e, 71.36.+c, 72.30.+q

LONG-WAVE OPTICAL VIBRATIONS IN DIATOMIC IONIC CRYSTALS

Long-wave phonon-polaritons and longitudinal optical phonons have been considered as eigenwaves of the electromagnetic field in ionic crystals with two atoms per unit cell. The Kun Huang model is used to describe the sublattices of point charges vibrating with the frequency ω_0. The dispersion laws for optical vibrations in crystals are generalized, by considering the thermal motion of charges. An additional longitudinal phonon with the frequency $2\omega_0$ and two upper phonon-polaritons are found in the second-order approximation with respect to the ratio between the standard deviation and the wavelength.

Keywords: ionic crystal, electromagnetic field; long-wave vibrations, phonon-polaritons, longitudinal optical phonons, harmonics.

1. Introduction

While considering optical phonons, a spatial inhomogeneity is usually made allowance for if confined objects are studied [1, 2] or if a superlattice is available [3]. When optical vibration modes in infinite crystals are determined, the standard theory involving only the frequency dispersion of the dielectric permittivity is applied [4, 5]. The corresponding theory of long-wave, in comparison with the lattice constant, optical vibrations in ionic crystals with regard for the electromagnetic interaction was developed by K. Huang [6, 7]. In the framework of this theory, the relative vibrations of positively and negatively charged ionic sublattices are considered in the long-wave limit, the vibration frequency of transverse optical phonons is considered to be constant, and the spatial dispersion and the thermal motion are neglected.

However, the consideration of the thermal motion of charges results, e.g., in the emergence of cyclotron waves in the magnetized plasma [8]. Let us consider the same problem for charges in a solid. In the recent work [9], optical vibrations in ionic crystals with two atoms in an elementary cell were analyzed on the basis of Kun Huang's theory. The thermal motion of charges was also neglected, and, in contrast to the widely known Szigeti model [10], effective charges were not introduced. Our further consideration consists in a generalization of the results of work [9] by involving the thermal motion of sublattices and the related spatial dispersion of the crystal dielectric permittivity.

2. Dispersion Law for an Electromagnetic Field Weakly Interacting with the Medium

Let us consider the optical vibrations in a diatomic ionic crystal in the harmonic approximation. Their damping, as a manifestation of anharmonicity, is neglected. Following the ideas of Kun Huang, we assume the sublattices of positively and negatively charged ions to be infinitely rigid. Let us consider only the relative vibrations of those sublattices with a given constant frequency ω_0. The Lagrange function can be written in the form [11, Eq. (13.3)]

$$L_m = N(\dot{\mathbf{r}}^2 - \omega_0^2 \mathbf{r}^2) m/2, \quad (1)$$

where N is the number of ionic pairs (crystal cells), $\mathbf{r} = \mathbf{r}_+ - \mathbf{r}_-$ is the relative shift of sublattices, the sign + or − corresponds to that of the charge, and $m = \frac{m_+ m_-}{m_+ + m_-}$ is the reduced mass of the pair.

Since the considered frequencies are "slow" for electrons, the motion of electron shells (the electron polarizability) can be taken into account by introducing the high-frequency dielectric permittivity ε_∞ taken to be constant [12, Eq. (13.1)]. The Hamiltonian of the system can be presented as a sum of the Hamiltonian of only charges, $\hat{H}_{\mathrm{m}}$, and the terms describing the electromagnetic field:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_f + \hat{H}_m,$$

$$\hat{H}_1 \equiv -\int d^3x \frac{\hat{A}_\alpha(x)\hat{\jmath}_\alpha(x)}{c},\ \hat{H}_2 \equiv \int d^3x \frac{\hat{\Omega}^2(x)\hat{A}(x)^2}{8\pi c^2},$$

$$\hat{H}_f = \frac{1}{8\pi}\int d^3x[\varepsilon_\infty \hat{\mathbf{E}}^2 + (\mathrm{rot}\,\hat{\mathbf{A}})^2]. \quad (2)$$

Here, the notation

$$\Omega^2 = 4\pi e^2 n/m \quad (3)$$

is introduced for the operator of plasma frequency of ions with charges $\pm e$, as well as the nonrelativistic operator of electric current density in the absence of electromagnetic field, $\hat{\jmath}_\alpha(x)$ (see, e.g., work [13, §5.3.2]).

From the mathematical viewpoint, phonon-polaritons and longitudinal optical phonons are solutions of the Maxwell equations in an ionic crystal. Therefore, let us write the operator equations of motion for the electromagnetic field in the Heisenberg representation. For this purpose, we should take the derivatives of the field strength $\hat{E}_\alpha(x,t) = e^{it\,H/\hbar}\hat{E}_\alpha(x)\,e^{-it\,H/\hbar}$ and the vector potential $\hat{A}_\alpha(x,t) = e^{it\,H/\hbar}\hat{A}_\alpha(x)\,e^{-it\,H/\hbar}$ and calculate the commutators. The generalized momentum, which is conjugate to the vector potential, is defined by the expression $\mathbf{P} = \frac{\varepsilon_\infty}{4\pi c^2}\dot{\mathbf{A}}$ [12, Eq. (13.5)]. The operator equations for the electromagnetic field read

$$\begin{aligned}&\partial_t \hat{A}_\alpha(x,t) = -c\hat{E}_\alpha(x,t),\\ &\varepsilon_\infty \partial_t \hat{E}_\alpha(x,t) = c\,\mathrm{rot}_\alpha \mathrm{rot}\hat{\mathbf{A}}(x,t) - 4\pi\hat{J}_\alpha(x,t),\end{aligned} \quad (4)$$

where

$$\hat{J}_n(x) = \hat{\jmath}_n(x) - \frac{1}{4\pi c}\hat{A}_n(x)\,\hat{\Omega}^2(x)$$

is the operator of electric current density. Now, we should average Eq. (4) with the statistical operator for the crystal + electromagnetic field system. To find an explicit form for the average current in the ionic crystal, let us single out the weak interaction with the field created by the charge subsystem. Further calculations will be carried out with the use of general notations. Following work [13, § 4.1.1], we have free charge subsystems with the equilibrium Gibbs statistical operator w_m and a certain statistical operator ρ_f for the electromagnetic field at the initial time moment t_0. According to the correlation attenuation principle, the initial condition can be written in the form

$$\rho(t_0) = \rho_f(t_0)\,w_m(t_0), \quad \mathrm{Sp}\rho = 1. \quad (5)$$

Owing to the weak interaction between the subsystems,

$$\hat{H}_{fm} = \hat{H} - \hat{H}_0, \quad (6)$$

the statistical operator (5) is changed for a long time and becomes real. In Eq. (6), the term

$$\hat{H}_0 = \frac{1}{8\pi}\int d^3x\hat{\mathbf{E}}(x)^2 + \frac{1}{8\pi c^2}\int d^3x \times \\ \times \int d^3x'\hat{A}_\alpha(x)\omega_\alpha^2(x-x')\hat{A}_\alpha(x') + \hat{H}_m, \quad (7)$$

where the frequency $\omega_\alpha(x)$ is an unknown dispersion law, makes the main contribution to the Hamiltonian. In the interaction representation, the statistical operator looks like

$$\rho(t) = \exp(itH_0/\hbar)\times \\ \times \exp(-itH/\hbar)\,\rho\exp(itH/\hbar)\exp(-itH_0/\hbar). \quad (8)$$

Let us expand expression (8) in a series according to the thermodynamic perturbation theory [13, §3.1.2], bearing in mind that the operator $S(\lambda) = \exp(\lambda H_0)\exp(-\lambda H)$ satisfies the equation

$$S(\lambda) = 1 - \int\limits_0^\lambda d\lambda'\hat{H}_{fm}(\lambda')\,S(\lambda') \quad (9)$$

where the notation $\hat{H}_{fm}(\lambda) = \exp(\lambda\hat{H}_0)\hat{H}_{fm}\times \exp(-\lambda\hat{H}_0)$ is used. Hence, the operator $T(\lambda) = \exp(\lambda H)\exp(-\lambda H_0)$ satisfies the equation

$$T(\lambda) = 1 + \int\limits_0^\lambda d\lambda' T(\lambda')\,\hat{H}_{fm}(\lambda'). \quad (10)$$

Therefore, the statistical operator (8) can be rewritten in the form

$$\rho(t) = S(it/\hbar)\,\rho T(it/\hbar). \quad (11)$$

For simplicity, let us take the current time moment as the initial one, $t = 0$, and let us use initial condition

(5). Then, for t_0 large enough by the absolute value ($t_0 < 0$, because the evolution started in the past),

$$\rho\,(t=0) = S\,(it_0/\hbar)\, w_m \rho_f T\,(it_0/\hbar). \tag{12}$$

Expanding Eq. (12) in a perturbation series up to the first-order terms and substituting Eqs. (9) and (10), we obtain

$$\rho\,(t=0) = \left(1 - \int\limits_0^{it_0/\hbar} d\lambda' \hat{H}_{fm}\,(\lambda')\, S\,(\lambda')\right) \times$$
$$\times\, w_m \rho_f \left(1 + \int\limits_0^{it_0/\hbar} d\lambda' T\,(\lambda')\, \hat{H}_{fm}\,(\lambda')\right). \tag{13}$$

Taking into account that $S_0\,(it/\hbar) = T_0\,(it/\hbar) = 1$ in the zeroth approximation order, we obtain

$$\rho\,(t=0) \approx w_m \rho_f - \int\limits_0^{it_0/\hbar} d\lambda' \left[\hat{H}_{fm}\,(\lambda')\,, w_m \rho_f\right] \tag{14}$$

or, changing the integration variable, $\lambda' = i\tau/\hbar$,

$$\rho\,(t=0) \approx w_m \rho_f - \frac{i}{\hbar} \int\limits_0^{t_0} d\tau \left[\hat{H}_{fm}\,(\tau)\,, w_m \rho_f\right], \tag{15}$$

where the ordinary notation $\hat{O}\,(\tau) \equiv e^{i\tau \hat{H}_0/\hbar} \hat{O} \times$ $\times\, e^{-i\tau \hat{H}_0/\hbar}$ for the interaction representation of an arbitrary operator is introduced. Hence, the main and first orders of the statistical operator look like

$$\rho_0 \approx w_m \rho_f,\ \rho_1 \approx -\frac{i}{\hbar} \int\limits_0^{t_0} d\tau \left[\hat{H}_{fm}\,(\tau)\,, w_m \rho_f\right]. \tag{16}$$

Now, taking into account that the Heisenberg and interaction representations coincide at $t = 0$, the operator Maxwell equations (4) have to be averaged. For simplification, the averages of the field operators will be designated as $E_\alpha(x) = \mathrm{Sp}\, \hat{E}_\alpha(x)\rho$. Moreover, when averaging the field with small multipliers in $\hat{J}_\alpha(x)$, the main order of perturbation will be sufficient: $E_\alpha(x) \approx \mathrm{Sp}\, \hat{E}_\alpha(x)\rho_0$. Note that, in this approach (unlike the method of brief descripion used in work [13, §4.2.]), $E_\alpha(x) \neq \mathrm{Sp}\hat{E}_\alpha(x)\rho_0$ in the general case. From Eq. (4), we have

$$\partial_t A_\alpha(x,t) = -cE_\alpha(x,t), \tag{17}$$

$$\varepsilon_\infty \partial_t E_\alpha(x,t) = c\, \mathrm{rot}_\alpha \mathrm{rot}\mathbf{A}(x,t) - 4\pi J_\alpha(x,t). \tag{18}$$

The next step consists in the averaging of $\hat{J}_\alpha(x)$ with the statistical operator (15). The smallness of terms will be conventionally determined by the powers of the electromagnetic field strength. Then

$$\rho_1 = -\frac{i}{\hbar} \int\limits_0^{t_0} d\tau \left[- \int d^3x \hat{A}_\alpha(\tau,x) \hat{\jmath}_\alpha(\tau,x)/c, w_m \rho_f\right]. \tag{19}$$

The generalized momentum, which is conjugate with the vector potential, is now determined in accordance with Eq. (7) by the expression $\mathbf{P} = \frac{1}{4\pi c^2}\dot{\mathbf{A}}$. It is easy to verify that, after the spatial Fourier transformation, we obtain

$$\hat{A}_{\alpha k}(\tau) = \hat{A}_{\alpha k} \cos\left(\omega_\alpha(k)\tau\right) -$$
$$-\, c\hat{E}_{\alpha k} \sin\left(\omega_\alpha(k)\tau\right)/\omega_\alpha(k). \tag{20}$$

Hence, the electric current in Eq. (18) looks like

$$J_n(x,t) = \mathrm{Sp}\left(w_m \rho_f - \frac{i}{\hbar}\int\limits_0^{t_0} d\tau \left[\hat{H}_{fm}\,(\tau)\,, w_m \rho_f\right]\right) \times$$
$$\times\, \hat{\jmath}_n(x) - \mathrm{Sp} w_m \rho_f \frac{1}{4\pi c} \hat{A}_n(x) \hat{\Omega}^2(x). \tag{21}$$

Since the current is absent in equilibrium, $\mathrm{Sp}\, w_m \hat{\jmath}_n\,(x) = 0$, Eq. (21) can be rewritten in the form

$$\hat{A}_{\alpha k}(\tau) = \hat{A}_{\alpha k} \cos\left(\omega_\alpha(k)\tau\right) -$$
$$-\, c\hat{E}_{\alpha k} \sin\left(\omega_\alpha(k)\tau\right)/\omega_\alpha(k). \tag{22}$$

Hence, at the average field, we have the coefficient $\mathrm{Sp}\, [\hat{\jmath}_\alpha(\tau, x'), \hat{\jmath}_n\,(x)]\, w_m$, which should quickly fall down in time. Therefore, let us apply a trick that is usually made in electrodynamics: let us pass to the limit $t_0 \to -\infty$. As a result,

$$J_n(x,t=0) = \frac{i}{c\hbar} \int\limits_{-\infty}^{0} d\tau \int d^3x' A_\alpha(\tau,x') \times$$
$$\times\, \mathrm{Sp}\left[\hat{\jmath}_\alpha(\tau, x'-x), \hat{\jmath}_n\,(0)\right] w_m - \frac{1}{4\pi c} A_n\,(x,t=0)\,\Omega^2. \tag{23}$$

ISSN 2071-0194. Ukr. J. Phys. 2015. Vol. 60, No. 6

The further procedure of solution of system (17)–(18) is standard: we make the Fourier transformation with respect to the coordinate, take a derivative with respect to the time, and substitute $A_{k\alpha}$ from Eq. (17) into Eq. (18). Then, Eq. (18) looks like

$$\varepsilon_\infty \partial_t E_{kn} = -c\left[\mathbf{k}\times[\mathbf{k}\times\mathbf{A}_k]\right]_n + \frac{1}{c}A_{kn}\Omega^2 + $$
$$+ 4\pi\frac{i}{c\hbar}\int\limits_{-\infty}^{0} d\tau (A_{\alpha k}\cos(\omega_\alpha(k)\tau) - $$
$$- cE_{\alpha k}\sin(\omega_\alpha(k)\tau)/\omega_\alpha(k))\mathrm{Sp}\left[\hat{j}_\alpha(\tau,k),\hat{j}_n(0)\right]w_m. \quad (24)$$

Now, let us take a derivative. In view of Eq. (17), we have

$$\varepsilon_\infty \partial_t^2 E_{kn} = c^2\left[\mathbf{k}\times[\mathbf{k}\times\mathbf{E}_k]\right]_n - E_{kn}\Omega^2 - 4\pi i/\hbar\times$$
$$\times\int\limits_{-\infty}^{0} d\tau (E_{\alpha k}\cos(\omega_\alpha(k)\tau) + \partial_t E_{\alpha k}\times$$
$$\times\sin(\omega_\alpha(k)\tau)/\omega_\alpha(k))\mathrm{Sp}\left[\hat{j}_\alpha(\tau,k),\hat{j}_n(0)\right]w_m. \quad (25)$$

This is a homogeneous differential equation of the second order. The solution is sought in the form $E_{kn}(t) = E_{kn}\exp(-it\omega_\alpha(k))$, because just this frequency appears in H_0 as the frequency of field oscillators. Then, we obtain the equation

$$-\omega_\alpha(k)^2\varepsilon_\infty E_{kn} = c^2\left[\mathbf{k}\times[\mathbf{k}\times\mathbf{E}_k]\right]_n - E_{kn}\Omega^2 - $$
$$- 4\pi\frac{i}{\hbar}\int\limits_{-\infty}^{0} d\tau\mathrm{Sp}\left[\hat{j}_\alpha(\tau,k),\hat{j}_n(0)\right]w_m\times$$
$$\times(E_{\alpha k}\cos(\omega_\alpha(k)\tau) - i\omega_\alpha(k)E_{\alpha k}\sin(\omega_\alpha(k)\tau)/\omega_\alpha(k)). \quad (26)$$

The expression in the last parentheses can be simplified, by using the Euler formula

$$\cos(\omega_\alpha(k)\tau) - i\sin(\omega_\alpha(k)\tau) = \exp(-i\omega_\alpha(k)\tau),$$
$$-\omega_\alpha(k)^2\varepsilon_\infty E_{kn} = c^2\left[\mathbf{k}\times[\mathbf{k}\times\mathbf{E}_k]\right]_n - E_{kn}\Omega^2 - $$
$$- 4\pi\frac{i}{\hbar}E_{\alpha k}\int\limits_{-\infty}^{\infty} d\tau\exp(-i\omega_\alpha(k)\tau)\,\theta(-\tau)\times$$
$$\times\mathrm{Sp}\left[\hat{j}_\alpha(\tau,k),\hat{j}_n(0)\right]w_m. \quad (27)$$

Now, it is convenient to introduce Green's function [13, p. 169]

$$G^{(+)}_{n\alpha}(\tau,k) = i\theta(-\tau)\,Sp\left[\hat{j}_\alpha(\tau,k),\hat{j}_n(0)\right]w_m/\hbar. \quad (28)$$

Equation (27) contains its Fourier transform

$$-\omega_\alpha(k)^2\varepsilon_\infty E_{kn} = c^2\left[\mathbf{k}\times[\mathbf{k}\times\mathbf{E}_k]\right]_n - E_{kn}\Omega^2 - $$
$$- \frac{4\pi}{\hbar}E_{\alpha k}G^{(+)}_{n\alpha}(\omega_\alpha(k),k). \quad (29)$$

Equation (29) produces the well-known dispersion equation for the electromagnetic field in a medium (see, e.g., work [14, Eq. (16)]),

$$c^2\left(\delta_{n\alpha}k^2 - k_n k_\alpha\right) + \delta_{n\alpha}\Omega^2 + $$
$$+ 4\pi G^{(+)}_{n\alpha}(\omega_\alpha(k),k) - \omega_\alpha(k)^2\varepsilon_\infty\delta_{n\alpha} = 0. \quad (30)$$

In a homogeneous isotropic medium, Green's function of currents can be divided into the longitudinal and transverse parts,

$$G^{(+)}_{ml}(\omega_\alpha(k),k) = G^{(+)}(\omega_\alpha(k),k)^{\perp}\left(\delta_{ml} - \hat{k}_m\hat{k}_l\right) + $$
$$+ G^{(+)}(\omega_\alpha(k),k)^{\parallel}\hat{k}_m\hat{k}_l, \quad (31)$$

where

$$G^{(+)}(\omega_\alpha(k),k)^{\perp} = \left(\delta_{ml} - \hat{k}_m\hat{k}_l\right)G^{(+)}_{ml}(\omega_\alpha(k),k)/2,$$
$$G^{(+)}(\omega_\alpha(k),k)^{\parallel} = G^{(+)}_{ml}(\omega_\alpha(k),k)\hat{k}_m\hat{k}_l,$$

and $\hat{k}_m = k_m/k$.

Let us calculate Green's function (28) for the equilibrium medium with the temperature $T = 1/\beta$. In this case, instead of the commutator, we have (see works [15, Eq. (1.49)] and [13, Eq. (4.1.22)])

$$G^{(+)}_{n\alpha}(\omega,k) = \frac{1}{2\pi\hbar}\int\limits_{-\infty}^{\infty} d\varpi\,(1 - \exp(\hbar\varpi\beta))\times$$
$$\times\frac{\mathrm{Sp}\hat{j}_\alpha(\varpi,k)\hat{j}_n(0)\,w_m}{\varpi - \omega - i0}. \quad (32)$$

In the classical case, the difference in the parentheses in Eq. (32) can be substituted by the multiplier $\beta\hbar\varpi$, so that

$$G^{(+)}_{n\alpha}(\omega,k) = \frac{1}{2\pi T}\int\limits_{-\infty}^{\infty} d\varpi\mathrm{Sp}\hat{j}_\alpha(\varpi,k)\hat{j}_n(0)w_m\times$$
$$\times\left(-1 - \frac{\omega}{\varpi - \omega - i0}\right). \quad (33)$$

To simplify the notation, the current correlation will be denoted below as

$$\mathrm{Sp}\hat{j}_\alpha(\varpi,k)\hat{j}_n(0)\,w_m = \langle\hat{j}_\alpha(\varpi,k)\hat{j}_n(0)\rangle.$$

3. Kun Huang's Approximation for an Insulator

Now, let us detail the form of the current Green's function in the interaction representation in the case of optical phonons. For this purpose, let us consider the motion of charges without their interaction with the field. We should change to the coordinate of the center of mass $\mathbf{R} = (m_+\mathbf{r}_+ + m_-\mathbf{r}_-)/M$, where $M = m_+ + m_-$, and to the coordinate difference. Now, the random variables are the amplitude and the phase of harmonic vibrations, i.e. the relative coordinate and velocity. Let us use Kun Huang's approximation of independent one-dimensional vibrations. The velocity of the center of mass is put equal to zero. The procedure is the same as in the case of a single degree of freedom. Free vibrations are described by the following time dependences of the radius vector and the velocity (see works [11, Eq. (21.7)] and [16, Eq. (5.1.1)]):

$$\begin{aligned} r_{an}(t) &= r_{an}\cos(\omega_0 t) + v_{an}\sin(\omega_0 t)/\omega_0, \\ v_{an}(t) &= v_{an}\cos(\omega_0 t) - r_{an}\sin(\omega_0 t)\,\omega_0. \end{aligned} \tag{34}$$

Let us write down the distribution function for an oscillator. The normalization will be carried out with respect to the number of pairs in the volume, i.e.

$$N = \int d^3v d^3r_a d^3V d^3R\,\delta(\mathbf{V}) f(v, r_a).$$

Since the theory is macroscopic, the centers of mass are "scattered" randomly owing to the homogeneity and the isotropy, i.e. the crystal structure is not important. However, the centers of mass are fixed, and vibrations occur only in every pair. Let the velocity and the coordinate of an oscillator have a normal distribution

$$f(v, r) = \frac{n}{(2\pi)^3 v_s^3 r_s^3}\exp\left(-\left(v^2/2v_s^2 + r^2/2r_s^2\right)\right), \tag{35}$$

where $v_s = 1/\sqrt{m\beta}$ and $r_s = 1/\sqrt{m\beta}\omega_0$ are the standard deviations of the oscillator velocity and coordinate, respectively. Different kinds of particles reveal themselves only in the reduced mass m.

The operator of the current created by the pair looks like [16, (2.3.4)]

$$\hat{\jmath}_m(r,t) = ev_m\left(m_-/M\delta(\mathbf{r} - \mathbf{R} - m_-\mathbf{r}_a(t)/M) + \right.$$
$$\left. + m_+/M\delta(\mathbf{r} - \mathbf{R} + m_+\mathbf{r}_a(t)/M)\right).$$

The current is a sum of components created by the positively and negatively charged ions. Hence, the correlation function of currents, which is required in Eq. (33), can be written in the form

$$\begin{aligned} &\left\langle \hat{\jmath}_m(r,t)\,\hat{\jmath}_l(0)\right\rangle = e^2\int d^3r_a d^3v d^3R v_m(t)\, v_l f(v, r_a)\times \\ &\times(m_-/M\delta(\mathbf{r} - \mathbf{R} - m_-\mathbf{r}_a(t)/M) + \\ &+ m_+/M\delta(\mathbf{r} - \mathbf{R} + m_+\mathbf{r}_a(t)/M))\times \\ &\times(m_-/M\delta(\mathbf{R} + m_-\mathbf{r}_{0a}/M) + \\ &+ m_+/M\delta(m_+\mathbf{r}_{0a}/M - \mathbf{R})). \end{aligned} \tag{36}$$

The integration over the coordinate of the center of mass is trivial and gives four terms:

$$\begin{aligned} &\left\langle \hat{\jmath}_m(r,t)\,\hat{\jmath}_l(0)\right\rangle = e^2\int d^3r_a d^3v v_m(t)\, v_l f(v, r_a)\times \\ &\times(m_-^2\delta(\mathbf{r} + m_-\mathbf{r}_{0a}/M - m_-\mathbf{r}_a(t)/M) + \\ &+ m_-m_+\delta(\mathbf{r} - m_+\mathbf{r}_{0a}/M - m_-\mathbf{r}_a(t)/M) + \\ &+ m_-m_+\delta(\mathbf{r} + m_-\mathbf{r}_{0a}/M + m_+\mathbf{r}_a(t)/M) + \\ &+ m_+^2\delta(\mathbf{r} - m_+\mathbf{r}_{0a}/M + m_+\mathbf{r}_a(t)/M))/M^2. \end{aligned} \tag{37}$$

It is convenient to change to Fourier transforms in the obtained expressions, by following the rule

$$O(\mathbf{x}, t) = \textstyle\int d^3k d\omega O(\mathbf{k}, \omega)\, e^{i\mathbf{kx} - i\omega t}/(2\pi)^4. \tag{38}$$

Then the Fourier transform of the correlation function (37) with respect to the coordinate difference and the time looks like

$$\begin{aligned} &\left\langle \hat{\jmath}_m(k,\omega)\,\hat{\jmath}_l(0)\right\rangle = e^2\int d^3v d^3r\int_{-\infty}^{\infty} dt\exp(-it\omega)\times \\ &\times(m_-^2\exp(i\mathbf{k}(\mathbf{r}(\cos(\omega_0 t) - 1) + \\ &+ \mathbf{v}\sin(\omega_0 t)/\omega_0)m_-/M) + \\ &+ m_-m_+\exp(i\mathbf{k}(\mathbf{r}(\cos(\omega_0 t) + m_+/m_-) + \\ &+ \mathbf{v}\sin(\omega_0 t)/\omega_0)m_-/M)) + \\ &+ m_+m_-\exp(-i\mathbf{k}(\mathbf{r}(\cos(\omega_0 t) + m_-/m_+) + \\ &+ \mathbf{v}\sin(\omega_0 t)/\omega_0)m_+/M)) + \\ &+ m_+^2\exp(-i\mathbf{k}(\mathbf{r}(\cos(\omega_0 t) - 1) + \\ &+ \mathbf{v}\sin(\omega_0 t)/\omega_0)m_+/M))\times \\ &\times v_m(v_l\cos(\omega_0 t) - r_l\sin(\omega_0 t)\,\omega_0)f(v, r)/M^2. \end{aligned} \tag{39}$$

The exponential functions in this expression can be expanded in a series of Bessel functions (see works [8, p. 104] and [17, Eq. (39)]), as is usually done in the case of magnetized plasmas, following the rule

$$e^{i\mathbf{kv}\sin(\omega_0 t)/\omega_0} = \sum_{n=-\infty}^{\infty} J_n\left(\mathbf{kv}/\omega_0\right)\exp\left(in\omega_0 t\right). \quad (40)$$

In the framework of Kun Huang's long-wave macroscopic theory, the estimate $\mathbf{kv}/\omega_0 \ll 1$ is valid. Therefore, owing to a non-zero (by a characteristic distance $r_s = 1/\sqrt{\beta m}\omega_0 \sim 10^{-9}$ cm) thermally induced root-mean-square deviation from the equilibrium position, there emerge the vibration modes similar to the Bernstein ones [17]. However, it is easier to expand the exponential function in a power series of its small argument and to take the first three terms:

$$e^{\pm i\mathbf{kO}} \approx 1 \pm i\mathbf{kO} - (\mathbf{kO})^2/2. \quad (41)$$

The term with odd power exponents disappears after the averaging with function (35) over an interval with symmetric limits.

Let us consider the first term in expansion (41). It corresponds to the well-studied limit $k = 0$ (see, e.g., works [9, 12]). Then M^2 disappears from Eq. (39), and we obtain

$$\left\langle \hat{j}_m\left(k=0,\omega\right)\hat{j}_l\left(0\right)\right\rangle = e^2\int d^3v d^3r \int_{-\infty}^{\infty} dt e^{-it\omega} \times$$
$$\times v_m(v_l\cos\left(\omega_0 t\right) - r_l\sin\left(\omega_0 t\right)\omega_0) f\left(v,r\right). \quad (42)$$

The integral containing the product $v_m r_l$ equals zero as an integral of an odd function. So, we have

$$\left\langle \hat{j}_m\left(k=0,\omega\right)\hat{j}_l\left(0\right)\right\rangle =$$
$$= e^2\pi\left(\delta\left(\omega-\omega_0\right)+\delta\left(\omega+\omega_0\right)\right)\int d^3v d^3r v_m v_l f\left(v,r\right). \quad (43)$$

Now, Green's function from Eq. (33) can be written in the form

$$G^{(+)}_{n\alpha}(\omega, k=0) = \frac{1}{2\pi T}\int_{-\infty}^{\infty} d\varpi \delta_{n\alpha}\left(m\beta\right)^{-1} e^2 n\pi \times$$
$$\times\left(\delta\left(\varpi-\omega_0\right)+\delta\left(\varpi+\omega_0\right)\right)\left(-1-\frac{\omega}{\varpi-\omega-i0}\right). \quad (44)$$

After the trivial integration with the delta-function, we obtain

$$G^{(+)}_{n\alpha}(\omega, k=0) = \frac{1}{4\pi}\delta_{n\alpha}\Omega^2\left(-1-\frac{\omega^2}{\omega_0^2-\omega^2}\right). \quad (45)$$

Here, notation (3) is used. Substituting formula (45) into the dispersion equation (30), we have

$$c^2\left(\delta_{n\alpha}k^2 - k_n k_\alpha\right) - \frac{\omega_\alpha(k)^2}{\omega_0^2-\omega_\alpha(k)^2}\delta_{n\alpha}\Omega^2 -$$
$$-\varepsilon_\infty\omega_\alpha(k)^2\delta_{n\alpha} = 0. \quad (46)$$

The dispersion equation 46) coincides with the well-known one (see, e.g., work [9, (17)–(18)]); i.e. it gives standard solutions for phonon-polaritons.

In the same approximation, let us determine the frequency ω_0. For this purpose, we should compare the Maxwell equation in the quasistationary limit $\omega \to 0$ with the use of the static dielectric permittivity ε_0. Substituting Green's function (45) into Eq. (29), we obtain

$$-\omega_\alpha(k)^2\varepsilon_\infty E_{kn} = c^2\left[\mathbf{k}\times\left[\mathbf{k}\times\mathbf{E}_k\right]\right]_n - E_{kn}\Omega^2 -$$
$$-\frac{4\pi}{\hbar}E_{\alpha k}G^{(+)}_{n\alpha}(\omega_\alpha(k), k=0). \quad (47)$$

On the other hand, the quasistationary approximation for the Maxwell equations gives

$$-\omega_\alpha(k)^2\varepsilon_0 E_{kn} = c^2\left[\mathbf{k}\times\left[\mathbf{k}\times\mathbf{E}_k\right]\right]_n,$$

which results in

$$\omega_\alpha(k)^2\varepsilon_0 E_{kn} = \omega_\alpha(k)^2\varepsilon_\infty E_{kn} - E_{kn}\Omega^2 -$$
$$-\frac{4\pi}{\hbar}E_{\alpha k}G^{(+)}_{n\alpha}(\omega_\alpha(k), k=0). \quad (48)$$

Then, using expression (45) for Green's function, we obtain

$$\omega_\alpha(k)^2\varepsilon_0 = \omega_\alpha(k)^2\varepsilon_\infty + \frac{\omega_\alpha(k)^2}{\omega_0^2-\omega_\alpha(k)^2}\Omega^2. \quad (49)$$

Hence, as $\omega_\alpha(k) \to 0$, we have the Lyddane–Sachs–Teller relation [18]

$$\varepsilon_0 = \varepsilon_\infty + \frac{\Omega^2}{\omega_0^2}, \quad (50)$$

which determines ω_0 in the standard way [9].

Now, let us take the thermal motion into account. Let us consider the second-order term in the expansion of expression (39),

$$\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2 = -e^2\int d^3v d^3r \int\limits_{-\infty}^{\infty} dt\exp(-it\omega)\times$$

$$\times\,(m_-^2(i\mathbf{k}(\mathbf{r}(\cos(\omega_0 t)-1)+\mathbf{v}\sin(\omega_0 t)/\omega_0)m_-/M)^2+$$

$$+\,m_-m_+(i\mathbf{k}(\mathbf{r}(\cos(\omega_0 t)+m_+/m_-)+$$

$$+\,\mathbf{v}\sin(\omega_0 t)/\omega_0)m_-/M)^2+$$

$$+\,m_-m_+(-i\mathbf{k}(\mathbf{r}(\cos(\omega_0 t)+m_-/m_+)+$$

$$+\,\mathbf{v}\sin(\omega_0 t)/\omega_0)m_+/M)^2+$$

$$+\,m_+^2(-i\mathbf{k}(\mathbf{r}(\cos(\omega_0 t)-1)+\mathbf{v}\sin(\omega_0 t)/\omega_0)m_+/M)^2)\times$$

$$\times\,v_m(v_l\cos(\omega_0 t)-r_l\sin(\omega_0 t)\,\omega_0)f(v,r)/2M^2. \quad (51)$$

Introducing the notations $a = (m_-^2 - m_-m_+ + m_+^2)/2M^2$ and $b = (m_-^2 - m_+^2)^2/M^4$, and taking the evenness of the integrand into account, we obtain three terms:

$$\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^1 = -e^2\int d^3v d^3r \int\limits_{-\infty}^{\infty} dt\exp(-it\omega)\times$$

$$\times\,(\mathbf{kr})^2 a v_m v_l\cos(\omega_0 t)\,f(v,r), \quad (52)$$

$$\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^2 = -e^2\int d^3v d^3r \int\limits_{-\infty}^{\infty} dt\exp(-it\omega)\times$$

$$\times\,(((\mathbf{kr})^2\cos^2(\omega_0 t)+(\mathbf{kv})^2\sin^2(\omega_0 t)/\omega_0^2)\times$$

$$\times\,v_m v_l\cos(\omega_0 t)-2v_m r_l\sin^2(\omega_0 t)\,(\mathbf{kr})(\mathbf{kv})\times$$

$$\times\,\cos(\omega_0 t))af(v,r), \quad (53)$$

$$\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^3 = -e^2\int d^3v d^3r \int\limits_{-\infty}^{\infty} dt\exp(-it\omega)\times$$

$$\times((\mathbf{kr})^2 v_m v_l\cos^2(\omega_0 t)-(\mathbf{kr})(\mathbf{kv})v_m r_l\sin^2(\omega_0 t))\times$$

$$\times\,(-1)bf(v,r). \quad (54)$$

The Poisson integrals with the Maxwellian distribution are easily calculated. Let us write down them for the velocity (for the coordinate or the symmetric velocity projections, the values will be the same). Let the third axis (z) of the coordinate systems be directed along the wave vector. Then

$$\int\limits_{-\infty}^{\infty} dv_z v_z^2 \int\limits_{-\infty}^{\infty} dv_x v_x^2 \int\limits_{-\infty}^{\infty} dv_y f\left(v_z^2+v_x^2+v_y^2\right) =$$

$$= n\,(m\beta)^{-2} = nv_s^4, \quad (55)$$

$$\int\limits_{-\infty}^{\infty} dv_z v_z^4 \int\limits_{-\infty}^{\infty} dv_x \int\limits_{-\infty}^{\infty} dv_y f\left(v_z^2+v_x^2+v_y^2\right) =$$

$$= 3n\,(m\beta)^{-2} = 3nv_s^4. \quad (56)$$

Therefore, Eqs. (52)–(54) yield

$$k_m k_l\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^3 = k^4 n\,(v_s r_s)^2 e^2\times$$

$$\times\int\limits_{-\infty}^{\infty} dt\exp(-it\omega)(\cos^2(\omega_0 t)-\sin^2(\omega_0 t))b, \quad (57)$$

$$(\delta_{ml}k^2 - k_m k_l)\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^3 = 2k^4 n\,(v_s r_s)^2 e^2\times$$

$$\times\int\limits_{-\infty}^{\infty} dt\exp(-it\omega)\cos^2(\omega_0 t)\,b, \quad (58)$$

$$k_m k_l\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^1 =$$

$$= (\delta_{ml}k^2 - k_m k_l)\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^1/2 =$$

$$= -k^4 n\,(v_s r_s)^{-2} e^2\int\limits_{-\infty}^{\infty} dt\exp(-it\omega)\cos(\omega_0 t)\,a, \quad (59)$$

where

$$k_m k_l\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^1 = k_m k_l\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^2 =$$

$$= (\delta_{ml}k^2 - k_m k_l)\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^2/2, \quad (60)$$

since $\cos^2(\omega_0 t)+\sin^2(\omega_0 t) = 1$. Hence, the third harmonic is absent in this approximation. In addition, if the masses of ions in the pair are identical, the coefficient $b = 0$, and the second harmonic is also absent. However, the latter variant is improbable for real chemical compounds.

Introducing the delta-function by the rule

$$\delta(\omega) = 2\pi\int\limits_{-\infty}^{\infty} dt\exp(-it\omega),$$

we have from Eqs. (57)–(59) that

$$k_m k_l \left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^1 = (\delta_{ml}k^2 - k_m k_l)\times$$
$$\times \left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^1/2 = -k^4\pi n\,(v_s r_s)^{-2}\,e^2\times$$
$$\times(\delta(\omega-\omega_0)+\delta(\omega+\omega_0))a, \qquad (61)$$

$$k_m k_l \left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^3 = k^4\pi n\,(v_s r_s)^2\,e^2\times$$
$$\times(\delta(\omega-2\omega_0)+\delta(\omega+2\omega_0))b, \qquad (62)$$

$$(\delta_{ml}k^2 - k_m k_l)\left\langle \hat{j}_m(k,\omega)\,\hat{j}_l(0)\right\rangle_2^3 = 2k^4\pi n\,(v_s r_s)^2\,e^2\times$$
$$\times(2\delta(\omega)+\delta(\omega-2\omega_0)+\delta(\omega+2\omega_0))\,b/2. \qquad (63)$$

Now, we can return to sum (41), which gives, after the summation, the longitudinal and transverse Green's functions.

4. Dispersion Laws for Optical Vibrations

The transverse part of Green's function can be obtained by substituting the correlation function of currents, which consists of terms (43), (61), (60), and (63), into Eq. (33):

$$2G^{(+)}(\omega_\alpha(k),k)^{\perp} = \left(\delta_{n\alpha}-\hat{k}_n\hat{k}_\alpha\right)G^{(+)}_{n\alpha}(\omega,k) =$$
$$= \frac{1}{2\pi T}\int_{-\infty}^{\infty} d\varpi e^2 n\pi v_s^2\times$$
$$\times((\delta(\varpi-\omega_0)+\delta(\varpi+\omega_0)) - 2k^2r_s^2\times$$
$$\times(\delta(\varpi-\omega_0)+\delta(\varpi+\omega_0))\,2a + k^2r_s^2\times$$
$$\times(\delta(\varpi-2\omega_0)+\delta(\varpi+2\omega_0)+2\delta(\varpi))\,b)\times$$
$$\times\left(-1-\frac{\omega}{\varpi-\omega-i0}\right). \qquad (64)$$

It is seen after the integration that the imaginary part is equal to zero:

$$G^{(+)}(\omega_\alpha(k),k)^{\perp} = \frac{\Omega^2}{4\pi}\left(\left(-1-\frac{\omega^2}{\omega_0^2-\omega^2}\right) - 2ak^2r_s^2\times\right.$$
$$\left.\times\left(-1-\frac{\omega^2}{\omega_0^2-\omega^2}\right) + bk^2r_s^2\left(-2-\frac{\omega^2}{4\omega_0^2-\omega^2}\right)/2\right). \qquad (65)$$

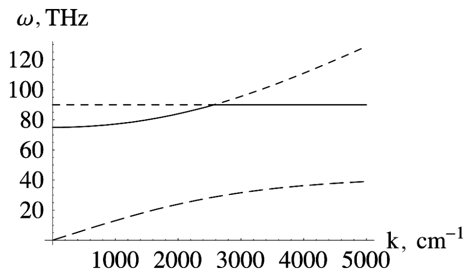

Fig. 1. Low-frequency transverse modes for NaF

Substituting formula (65) into the transverse part of dispersion equation (30), we obtain

$$c^2k^2 + \Omega^2k^2r_s^2\times$$
$$\times\left(2a\frac{\omega_0^2}{\omega_0^2-\omega_\perp(k)^2} - b/2 - b/2\frac{4\omega_0^2}{4\omega_0^2-\omega_\perp(k)^2}\right) -$$
$$-\frac{\omega_\perp(k)^2}{\omega_0^2-\omega_\perp(k)^2}\Omega^2 - \varepsilon_\infty\omega_\perp(k)^2 = 0. \qquad (66)$$

For Kun Huang's continual theory to be applicable, the inequality $k^2r_s^2 \ll 1$ must be satisfied. However, it is the condition $k^2r_s^2 \neq 0$, under which a new phonon-polariton mode arises.

The most typical representatives of diatomic ionic crystals are halides of alkaline metals. For lithium compounds, the second-harmonic phonon does not interact with a photon, because $2\omega_0 < \omega_L$, although it may probably merge with the upper phonon-polariton. But, e.g. for NaF, an additional phonon-polariton branch is obtained. For sodium fluoride, we have $\varepsilon_\infty = 1.7$, $\omega_0 = 45$ THz (see Table 5.1 in work [19]), and $\Omega/\sqrt{\varepsilon_\infty} = 63$ THz (see Table 1 in work [20]). The introduced mass-dependent constants are $a \approx 0.13$ and $b \approx 0.01$. In addition, we put $r_s \sim 10^{-9}$ cm^{-1}.

The plot for the upper phonon-polariton intersects all possible resonances; i.e. we obtain a series of phonon-polaritons following in the sequence "phonon–photon–next phonon" and not crossing one another. For sodium fluoride (see Fig. 1), within the considered accuracy, the phonon-polariton transforms into the second harmonic of a transverse phonon, as the wave number increases (the solid curve). At the same time, the second harmonic of a transverse phonon becomes a phonon-polariton (the short-dashed curve). The lower phonon-polariton branch remains standard (the long-dashed curve). Figure 2 exhibits a scaled-up section of Fig. 1, where the upper phonon-polariton branches in NaF approach each

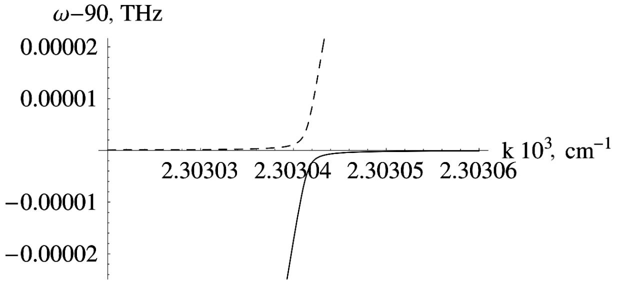

Fig. 2. Mutual approach of upper phonon-polaritons in NaF

other. It testifies to the absence of intersection between those branches.

Similarly to Fig. 1, the cyclotron resonances in a magnetized plasma are intersected by an extraordinary wave [21, p. 247] following the same rule. In other words, the presented plot is similar to the plot of the Bernstein modes. The transverse phonon-polaritons on a piezoelectric superlattice are also characterized by a similar plot [3].

The longitudinal part of Green's function consists of parts (43), (61), (60), and (62): (61), (60) та (62)

$$G^{(+)}(\omega,k)^{\|} = \hat{k}_n\hat{k}_\alpha G^{(+)}_{n\alpha}(\omega,k) = \frac{1}{2\pi T}\int\limits_{-\infty}^{\infty} d\varpi e^2 n\pi v_s^2 \times \times (((\delta(\varpi-\omega_0)+\delta(\varpi+\omega_0)) - k^2r_s^2 \times \times (\delta(\omega-\omega_0)+\delta(\omega+\omega_0))2a + k^2r_s^2 \times \times (\delta(\omega-2\omega_0)+\delta(\omega+2\omega_0))b)\left(-1-\frac{\omega}{\varpi-\omega-i0}\right). \quad (67)$$

After the integration over the frequency ϖ, we obtain the expression

$$G^{(+)}(\omega,k)^{\|} = \frac{\Omega^2}{4\pi}\left(\left(-1-\frac{\omega^2}{\omega_0^2-\omega^2}\right) - 2ak^2r_s^2 \times \times \left(-1-\frac{\omega^2}{\omega_0^2-\omega^2}\right) + bk^2r_s^2\left(-1-\frac{\omega^2}{4\omega_0^2-\omega^2}\right)\right), \quad (68)$$

which gives rise to the dispersion equation

$$k^2\Omega^2r_s^2\left(2a\left(\frac{\omega_0^2}{\omega_0^2-\omega_\|(k)^2}\right) - b\left(\frac{4\omega_0^2}{4\omega_0^2-\omega_\|(k)^2}\right)\right) - - \frac{\omega_\|(k)^2}{\omega_0^2-\omega_\|(k)^2}\Omega^2 - \varepsilon_\infty\omega_\|(k)^2 = 0. \quad (69)$$

The solution of Eq. (69) has three branches:

$$\omega_{\|1}(k)=0,\ \omega_{\|2}(k)=\pm\sqrt{\omega_0^2+\Omega^2},\ \omega_{\|3}(k)=\pm 2\omega_0. \quad (70)$$

The main result of Eqs. (70) consists in that, besides a standard long-wave longitudinal phonon with $\omega_{\|2}(k)=\sqrt{\omega_0^2+\Omega^2}$, there appears an infinite series of harmonics (if all terms in sum (40) are taken into account) with the frequencies starting from twice the lattice frequency, $\omega_{\|3}(k)=2\omega_0$.

We should separately emphasize that the new modes are similar to the second harmonic, i.e. to a nonlinear effect, which usually follows from nonlinear equations of motion. However, Eq. (26) is linear.

In the limiting case where the period of lattice vibrations considerably exceeds the characteristic time of the analyzed process, i.e. $\omega_0 \ll \omega$, the trigonometrical functions in dependences (34) should be expanded to obtain

$$r_{an}(t) = r_{an} + v_{an}\omega_0 t/\omega_0,\ v_{an}(t) = v_{an}, \quad (71)$$

which brings us back to the well-known scenario of a Maxwellian plasma with damping [8, 22].

5. Conclusions

To summarize, the dispersion laws for phonon-polaritons and longitudinal optical phonons in the macroscopic model of diatomic ionic crystal are generalized. In particular, in the second-order approximation with respect to the standard deviation of a harmonic oscillator from the equilibrium, a new branch of longitudinal optical phonon with a frequency that coincides with the second harmonic of lattice vibrations is obtained. In the transverse case, two upper phonon-polaritons are found. The infinite series of phonon-polaritons and longitudinal optical phonons that arise similarly to the Bernstein modes in a magnetized plasma are predicted. The transverse frequency of optical lattice vibrations is determined in the main approximation from the electrostatic equilibrium condition. The presented consideration generalizes the results of work [9], where the thermal motion of the lattice was not taken into account.

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Received 25.12.14.
Translated from Ukrainian by O.I. Voitenko

А.А. Ступка

ДОВГОХВИЛЬОВІ ОПТИЧНІ
КОЛИВАННЯ У ДВОХАТОМНИХ
ІОННИХ КРИСТАЛАХ

Р е з ю м е

Розглянуто довгохвильові фонон-поляритони і поздовжні оптичні фонони як власні хвилі електромагнітного поля в іонних кристалах з двома атомами в елементарній комірці. Використано модель Хуана Куня для опису підґраток точкових зарядів, що осцилюють з частотою ω_0. Узагальнено закони дисперсії для оптичних коливань в кристалах завдяки врахуванню теплового руху зарядів. У другому порядку по відношенню середньоквадратичного відхилення до довжини хвилі знайдено додатковий поздовжній фонон з частотою $2\omega_0$ та два верхні фонон-поляритони.