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LONG-WAVE HIGH-FREQUENCY OSCILLATIONS IN IONIC CRYSTALS WITH TWO ATOMS IN ELEMENTARY CELL

Long-wave high-frequency electromagnetic oscillations in an ionic crystal with two atoms in an elementary cell have been considered in the framework of a self-consistent model for free point charges in the electromagnetic field in a dielectric medium. The frequency of longitudinal phonons is shown to equal the ionic plasma frequency divided by the square root of the high-frequency dielectric permittivity. The standard dispersion law for the upper phonon-polariton branch is obtained.
Keywords: long-wave oscillations, phonon-polariton, ion plasma frequency.

As was shown in work [1] (see also work [2]), when studying long-wave acoustic vibrations in solids, it is of importance to take the electromagnetic interaction into account. Optical vibrations also arise with the participation of the electromagnetic interaction. Let us consider long-wave vibrations in an ionic crystal with two atoms in an elementary cell. It is known [3] that both acoustic and optical vibrations are possible in such an insulator, and the transverse optical vibrations can generate polaritons due to the interaction with an electromagnetic field. Optical vibrations are high-frequency for ions, because the characteristic frequency for the latter is the plasma ion frequency, so that they may be considered as free charges. The elastic forces are proportional to the gradients of displacements, and this factor can be neglected in the long-wave approximation. It is the more so for the thermal motion of ions, because the velocity of their thermal motion is lower than the speed of acoustic waves. The vibration damping is also neglected. Since small ionic vibrations in a non-magnetic medium are studied, the nonlinear magnetic part of the Lorentz force can also be omitted. In the formulated model, the linearized equation of motion for ions looks like [4]

$$\partial \mathbf{v}_+/\partial t = Ze\mathbf{E}/M_+, \tag{1}$$

$$\partial \mathbf{v}_-/\partial t = -Ze\mathbf{E}/M_-. \tag{2}$$

Here, the subscript + or − corresponds to the charge sign, $M_\pm$ are the masses of positively and negatively charged ions, and Ze is the charge. After the linearization, the total time derivative coincides with the partial one. The self-consistent electromagnetic field should satisfy the Maxwell equations in an insulator,

$$\partial \mathbf{D}/\partial t = c\,\mathrm{rot}\,\mathbf{B} - 4\pi\mathbf{j}, \tag{3}$$

$$\partial \mathbf{B}/\partial t = -c\,\mathrm{rot}\,\mathbf{E}. \tag{4}$$

Here, the dielectric induction [5]

$$D_\alpha = \varepsilon_{\alpha\beta}E_\beta \tag{5}$$

was introduced, which is connected linearly with the electric field strength E in the approximation of small oscillations. For simplicity, let us consider an isotropic dispersionless insulator. Then the dielectric permittivity tensor $\varepsilon_{\alpha\beta}$ is reduced to a scalar. In the used approximation, the current density of ions with a definite sign is expressed in terms of the average velocities as follows:

$$\mathbf{j}_\pm = \pm Zen_0\mathbf{v}_\pm, \tag{6}$$

where n_0 is the equilibrium concentration of ions. While studying high-frequency field oscillations, it is natural to use the high-frequency dielectric permittivity ε_∞, which describes the electron polarization. Then the Maxwell equations for the self-consistent electromagnetic field described by Eqs. (3) and (4) look like

$$\partial \varepsilon_\infty \mathbf{E}/\partial t = c\,\mathrm{rot}\,\mathbf{B} - 4\pi Zen_0\,(\mathbf{v}_+ - \mathbf{v}_-), \tag{7}$$

$$\partial \mathbf{B}/\partial t = -c\,\mathrm{rot}\,\mathbf{E}. \tag{8}$$

We obtained a closed system of equations (1), (2), (7), and (8) for the coupled high-frequency long-wave ionic lattice vibrations and self-consistent electromagnetic field oscillations. Now, we should differentiate Eq. (7) with respect to the time and substitute the time derivatives from Eqs. (1), (2) and (8) to obtain

$$\partial^2 \varepsilon_\infty \mathbf{E}/\partial t^2 = -c^2\,\mathrm{rotrot}\,\mathbf{E} - 4\pi Z^2 e^2 n_0 \mathbf{E}/M, \tag{9}$$

where the reduced mass of a crystal cell $M = \frac{M_+ M_-}{M_+ + M_-}$ was introduced. Equation (9) is the wave equation for the electric field strength. It is convenient to change in it to Fourier components following the rule

$$\mathbf{E}(\mathbf{x}, t) = \int d^3 k d\omega \mathbf{E}(\mathbf{k}, \omega)\, e^{i\mathbf{kx} - i\omega t}/(2\pi)^4. \tag{10}$$

Let us divide the field into the potential and vortex parts. Then, from Eq. (9), we obtain the following linear homogeneous algebraic equations:

$$-\omega^2 \varepsilon_\infty \mathbf{E}^\perp = -c^2 k^2 \mathbf{E}^\perp - 4\pi Z^2 e^2 n_0 \mathbf{E}^\perp/M, \tag{11}$$

$$-\omega^2 \varepsilon_\infty \mathbf{E}^\parallel = -4\pi Z^2 e^2 n_0 \mathbf{E}^\parallel/M. \tag{12}$$

From Eq. (11), we obtain the dispersion law for high-frequency phonon-polaritons,

$$\omega^2 = c^2 k^2/\varepsilon_\infty + 4\pi Z^2 e^2 n_0/\varepsilon_\infty M. \tag{13}$$

This expression transforms into the photon branch at large k. This solution coincides with the well-known one (see, e.g., [3, Eq. (12.8)]). Low-frequency phonon-polaritons go beyond the scope of our approximation. Equation (12) gives us the frequency of longitudinal oscillations,

$$\omega_L^2 = 4\pi Z^2 e^2 n_0/\varepsilon_\infty M, \tag{14}$$

which are related to longitudinal phonons. To compare the obtained result with the tabulated value ω_L^{tabl} for the frequency, it is convenient to change in expression (14) from the concentration of ions of the same sign to the crystal density ρ by the formula $\frac{n_0}{M} = \frac{\rho}{M_+ M_-}$. Then, we can write down that

$$\omega_L = 1.70156\, Z \sqrt{\frac{\rho}{\varepsilon_\infty M_+ M_-}}\; 10^{-9}\ \mathrm{s}^{-1}. \tag{15}$$

Longitudinal optical frequencies of some ionic crystals

Crystal	ρ, g·cm^{-3}	ε_∞	ω_L^{tabl}, 10^{13} s^{-1}	ω_L, 10^{13} s^{-1}
LiH	0.78	3.6	21	18.1
LiF	2.64	1.9	12	10.5
LiCl	2.07	2.7	7.5	5.72
NaF	2.79	1.7	7.8	6.28
MgO	3.58	2.95	14	11.5

For comparison, let us use the data from Table 5.1 of book [6] for the dielectric permittivity at optical frequencies, ε_∞, and the value of longitudinal vibration frequency, ω_L^{tabl}. The densities of relevant ionic crystals were taken from work [7]. One can see from Table that the values obtained by formula (15) are in good agreement with the known data [6]. Certainly, for ions with large radii, the model of point charges is not so good.

Hence, we have shown that the upper branches of phonon-polaritons and longitudinal phonons are plasma oscillations [4, 8] in a medium.

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ВИСОКОЧАСТОТНІ ДОВГОХВИЛЬОВІ КОЛИВАННЯ В ІОННИХ КРИСТАЛАХ З ДВОМА АТОМАМИ В ЕЛЕМЕНТАРНІЙ КОМІРЦІ

Р е з ю м е

Розглянуто довгохвильові високочастотні електромагнітні коливання в іонному кристалі з двома атомами в елементарній комірці. Використано модель вільних точкових зарядів у самоузгодженому електромагнітному полі у діелектричному середовищі. Показано шляхом порівняння з табличними даними, що частота поздовжніх фононів є відношенням іонної плазмової частоти до кореня з високочастотної діелектричної проникності. Також отримано стандартний закон дисперсії верхньої гілки фонон-поляритонів.