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A series of phonon-polaritons in a diatomic ionic crystal

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ABSTRACT

The interaction between the harmonics of the optical phonon and the transverse wave of the electromagnetic field in ionic crystals with two atoms in the unit cell is considered. The Kun Huang model is used to describe the point charges sublattices that oscillate with a frequency ω_0. The thermal motion of charges sublattices surrounding thermostat is taken into account. The local field is taken into account as well by introducing of an effective charge. A statistical operator of the system in a perturbation theory is introduced self-consistently small interaction is constructed. The new series of long-wave phonon-polaritons as the eigenwaves of the transverse electromagnetic field is obtained. The approximation is valid for a small ratio of the standard thermal deviation to the wavelength that allows to limit only the second and the third phonon harmonics in the dispersion equation at plotting the graph. A frequency line $2\omega_0$ restricts the top of the first upper phonon-polariton graph and the bottom of the second upper phonon-polariton graph for the used example of cesium bromide crystal. The rest of the phonon-polaritons have graphs in the form of stairs with a slope, asymptotically approaching to the photon graph in this crystal, and with a height ω_0.

1. Introduction

The general phonon theory requires calculation of interatomic force constants to find the forces acting on the atom after small deviations from the equilibrium position [1–3] that allows to build a dynamic matrix and get phonon frequencies, finding the roots of the secular determinant.

However, the macroscopic approach is simplier to use in a long-wave approximation. The standard theory based only on the frequency dispersion of permittivity for infinite crystals is used while finding modes of optical vibrations [4,5]. Such a theory, taking into account electromagnetic interaction when considering the long-wave optical vibrations in ionic crystals, is built by Kun Huang [6,7]. The relative vibrations of positively and negatively charged ion sublattices are considered in this theory in the long-wave limit in comparison with the lattice constant. Moreover, the frequency of these vibrations is considered constant, spatial dispersion and thermal motion does not take into account. But the accounting of the spatial dispersion of the dielectric permittivity when considering optical phonons usually carried out in the presence of macroscopic scale: the study limited bodies [8,9] or if there the superlattice [10]. However, account of the thermal motion of charges leads, for example, to the emergence of spatial dispersion and gives cyclotron waves in a magnetized plasma spectrum even in an infinite medium [11]. Let consider for charges in a solid a similar problem.

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In a recent article [12], consideration of optical vibrations in ionic crystals with two atoms per unit cell based on the Kun Huang theory, is performed excluding thermal motion of the charges. Further consideration aims to spread the results of [12] to the case of thermal motion sublattices and related spatial dispersion.

Our paper is organized in a following way. Section II is devoted to the general kinetic theory for the electromagnetic field. The dispersion relation is derived. In Section III we build the current Green function in the Kun Huang approximation in the thermostat. In Section IV we apply obtained results to plot low-frequency transverse optical modes of diatomic ion crystal.

2. The dispersion relation for the electromagnetic field

Consider the optical vibrations in a diatomic ionic crystal in a harmonic approximation. We will not consider damping as a manifestation of the anharmonicity. Following Kun Huang's ideas, sublattices of positively and negatively charged ions consider infinitely rigid and we consider only the relative vibrations of these sublattices with a given constant frequency ω_0. It is possible to write a Hamiltonian, based on a Lagrangian (see (13.3) [13])

$$\widehat{H}_{\mathrm{m}} = N\left(\dot{\widehat{\mathbf{r}}}^2 + \omega_0^2\widehat{\mathbf{r}}^2\right)m/2, \tag{1}$$

where N is number of ion pairs (cells in the crystal), $\mathbf{r} = \mathbf{r}_+ - \mathbf{r}_-$ is relative sublattices displacement, sign $\pm$ corresponds to the charge, $m = \frac{m_+m_-}{m_+ + m_-}$ is the reduced mass of a pair.

As we consider the slow frequency for electrons the motion of the electron shells (electronic polarizability) is taken into account via the high frequency dielectric constant ε_∞, which will be assumed to be constant (see (13.1) [3]). Let be ions singly charged. To account the local field [14] elementary charge e should be multiplied by a constant factor, ie we can introduce the effective charge

$$e_\bigstar = e\sqrt{(\varepsilon_\infty + 2)/3}, \tag{2}$$

which will give the correct optical vibrations frequency according to the results [5,12], in contrast to the well-known Szigeti model [15], where the effective charge was introduced with the factor without a square root $(\varepsilon_\infty + 2)/3$. The Hamiltonian of the system can be written as the sum of the charges without electromagnetic field Hamiltonian (1), and the terms with a field.

$$\begin{aligned}
&\widehat{H} = \widehat{H}_{\mathrm{m}} + \widehat{H}_f + \widehat{H}_1 + \widehat{H}_2\\
&\widehat{H}_1 = -\int d^3x\widehat{A}_\alpha(x)\widehat{j}_\alpha(x)/c, \widehat{H}_2 = \int d^3x\widehat{\Omega}^2(x)\widehat{A}(x)^2\Big/8\pi c^2\\
&\widehat{H}_{\mathrm{f}} = \int d^3x\left(\varepsilon_\infty\widehat{\mathbf{E}}^2 + \left[\nabla\times\widehat{\mathbf{A}}\right]^2\right)\Big/8\pi.
\end{aligned} \tag{3}$$

Here, the notation for the operator of the plasma frequency ion is introduced.

$$\widehat{\Omega}^2(x) = 4\pi e_\bigstar^2(\widehat{n}_+(x)/m_+ + \widehat{n}_-(x)/m_-) \tag{4}$$

($\widehat{n}_\pm(x)$ are the charge density operators); $\widehat{j}_\alpha(x)$ is the electric current density operator in the absence of an electromagnetic field (see., eg., §5.3.2 [16]).

Phonon-polaritons are the solutions of the Maxwell equations in the ion crystal. Therefore, we write the operator equations of motion for the electromagnetic field in the Heisenberg picture. For this we take the time derivatives of the field strength $\widehat{E}_\alpha(x,t) = e^{it\,H/\hbar}\widehat{E}_\alpha(x)e^{-it\,H/\hbar}$ and its vector potential $\widehat{A}_\alpha(x,t) = e^{it\,H/\hbar}\widehat{A}_\alpha(x)e^{-it\,H/\hbar}$ and calculate received commutators (enter the magnetic induction does not suitable for a nonmagnetized medium). The generalized momentum conjugate to the vector potential is given by $\mathbf{P} = \frac{\varepsilon_\infty}{4\pi c^2}\dot{\mathbf{A}}$ (see (13.5) [3]). Operator equations for the electromagnetic field are as follows

$$\begin{aligned}
&\partial_t\widehat{A}_\alpha(x,t) = -c\widehat{E}_\alpha(x,t),\\
&\varepsilon_\infty\partial_t\widehat{E}_\alpha(x,t) = c\left[\nabla\times\left[\nabla\times\widehat{\mathbf{A}}(x,t)\right]\right]_\alpha - 4\pi\widehat{J}_\alpha(x,t).
\end{aligned} \tag{5}$$

Here we introduce the operator of electric current density $\widehat{J}_\alpha(x) = \widehat{j}_\alpha(x) - \frac{1}{4\pi c}\widehat{A}_\alpha(x)\widehat{\Omega}^2(x)$. Now it is necessary to average the equation (5) with statistical operator of the crystal and field system. We distinguish the weak interaction with the field of charges subsystem to find the explicit form of the average current in the ion crystal. Further calculations were carried out in the general notation. Following §4.1.1 [16], in the beginning of evolution (denoted time t_0) there are free subsystems with the equilibrium Gibbs statistical operator for charges w_m and some statistical operator for the electromagnetic field ρ_f. Then we have a statistical operator ρ for the whole system (this can be written due to the principle of correlation weakening)

$$\rho(t_0) = \rho_f(t_0)w_m(t_0), Sp\rho = 1 \tag{6}$$

The initial statistical operator (6) for a long time due to the interaction