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Some aspects of polaritons and plasmons in materials

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ABSTRACT

We have studied the interaction of optical phonons with photons. So, we have calculated the coupled modes of photons and transverse optical phonons and likewise, the dielectric function. We have found an alternative relation of the splitting between the frequencies of the longitudinal optical (LO) and transverse optical (TO) phonons in crystals. Likewise, we have studied the plasmon resonance frequency. We have determined the phonon–photon and the plasmon–photon coupling constant in ionic crystals and in metals, respectively, which is very close to the elastic force constant, and we have evaluated the bulk modulus. Further we have applied these results to tetrahedrally bonded III–V semiconductors.

1. Introduction

The quantum theory of the interaction of radiation with optical phonons was first presented by Fano [1] and Hopfield [2]. Near the crossover of the dispersion relations (ω versus $\mathbf{k}$) of the uncoupled photon and optical phonon fields was obtained that a weak coupling has a drastic effects in mixing together the electromagnetic and mechanical fields. Such effects in isotropic and cubic crystals occur only for transverse optical phonons, as only these couple with an electromagnetic field, which is always transverse in isotropic materials. The mode created by the coupling of light and phonons is called a polariton. In this paper we will study this interaction by using a Hamiltonian [3] which takes into account the coupling through the flux lines. We will find an alternative relation to relation (23) for the splitting between the frequencies of LO and TO phonons. We will evaluate a coupling constant which is correlated with the cohesive energy in ionic and zinc-blende structure crystals [4]. Likewise, we will calculate the resonance frequency of plasmons and will correlate our coupling constant with the elastic constant of materials.

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2. The Hamiltonian of the system

We imagine that two phonons interact between them via electromagnetic field and likewise, two photons interact via mechanical field. In the three dimensional space the Hamiltonian density of a system of two bodies interacting via a boson field is

$$H_d = \frac{1}{2\rho}\Pi_\mu\Pi_\mu + \frac{D_lR_l}{2}\frac{\partial u_\mu}{\partial z_\mu}\frac{\partial u_l}{\partial z_l} + \frac{D_tR_l}{2}\frac{\partial u_\mu}{\partial z_l}\frac{\partial u_\mu}{\partial z_l} + \frac{D_l}{2}s_l\frac{\partial u_\mu}{\partial z_\mu}\frac{\partial u_l}{\partial z_l} + \frac{D_t}{2}s_l\frac{\partial u_\mu}{\partial z_l}\frac{\partial u_\mu}{\partial z_l} \tag{1}$$

We are to sum over repeated indices. The coordinate axes z_μ are assumed to be orthogonal. The term in D_l is the square of the trace of the strain tensor; the term in D_t is the sum of the squares of the tensor components. R_l is the distance between the two bodies, s_l is the relative displacement of the two bodies oriented along the axis connecting them,

$$\rho = \rho_o + \frac{(D_l\delta_{\mu l} + D_t)R_l}{c^2} = \rho_o + \frac{DR_l}{c^2} \tag{2}$$

The last term from the right hand side is "the density of the coupling field". Π_μ are the components of the momentum density, $u_\mu(\boldsymbol{z})$ are the displacements of the coupling field at the position $\boldsymbol{z}$

$$\begin{aligned} u_\mu(\mathbf{z}) &= \frac{\mathbf{1}}{\sqrt{NR}}\sum_{\mathbf{k}}\left(\frac{\hbar}{2\rho\omega_{\mathbf{k}\mu}}\right)^{1/2}\left(a_{\mathbf{k}\mu}e^{i\mathbf{kz}} + a^+_{\mathbf{k}\mu}e^{-i\mathbf{kz}}\right) \\ s_l(\mathbf{z}) &= \frac{1}{N}\sum_{\mathbf{q}} Q_{\mathbf{q}}e^{i\mathbf{q}.(\mathbf{z}-\mathbf{z_l})} \\ Q_{\mathbf{q}} &= \left(\frac{\hbar}{2M\Omega_{\mathbf{q}}}\right)^{1/2}\left(b_{\mathbf{q}} + b^+_{-\mathbf{q}}\right) \end{aligned} \tag{3}$$

$\omega_{\mathbf{k}\mu}$ is the classical oscillation frequency

$$\omega_{\mathbf{k}\mu} = \left(\frac{D_l\delta_{\mu l} + D_t}{\rho}\right)^{1/2}k = \left(\frac{D}{\rho}\right)^{1/2}k \tag{4}$$

where l denotes longitudinal boson and other two choices of μ denote transverse bosons. The Hamiltonian of interaction (1) becomes

$$H_I = \frac{D_l}{2}\int\sum_l s_l\frac{\partial u_\mu}{\partial z_\mu}\frac{\partial u_l}{\partial z_l}d\mathbf{z} + \frac{D_t}{2}\int\sum_l s_l\frac{\partial u_\mu}{\partial z_l}\frac{\partial u_\mu}{\partial z_l}d\mathbf{z} \tag{5}$$

where we will sum over the neighbours.

The total Hamiltonian of the interacting bodies and the connecting field is

$$\begin{aligned} H &= H_o + H_I \\ H_o &= H_{o1} + H_{o2} = \sum_{\mathbf{q}}\hbar\Omega_{\mathbf{q}}b^+_{\mathbf{q}}b_{\mathbf{q}} + \sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a^+_{\mathbf{k}}a_{\mathbf{k}} \end{aligned} \tag{6}$$

where $\Omega_{\mathbf{q}}$, $\omega_{\mathbf{k}}$ are just the classical oscillation frequencies, $a^+_{\mathbf{k}}$, $a_{\mathbf{k}}$ and $b^+_{\mathbf{q}}$, $b_{\mathbf{q}}$ are boson creation and annihilation operators for the connecting filed and the interacting bodies, respectively. N is the number of the bodies, which have the same mass M and, in the equilibrium positions, lie at a distance R from one another, $\rho_oR = m_o$ is the mass associated with the interacting field, if this is a massive field [5], c is the light velocity, and D is a coupling constant [6]. It is assumed that in the approximation of the nearest neighbours, D does not depend on l.

May be written

$$H_I = \frac{D}{2}\sum_{n,\mathbf{k},\mathbf{k}',\mathbf{q}}\left(\frac{\hbar}{2m\Omega_{\mathbf{q}}}\right)^{1/2}\left(b_{\mathbf{q}} + b^+_{-\mathbf{q}}\right)e^{-i\mathbf{q}.\mathbf{z_n}} \times \frac{1}{NR}\frac{\hbar\mathbf{k}.\mathbf{k}'}{2\rho(\omega_{\mathbf{k}}\omega_{\mathbf{k}'})^{1/2}}\left(a_{\mathbf{k}} + a^+_{-\mathbf{k}}\right)\left(a_{-\mathbf{k}'} + a^+_{\mathbf{k}'}\right)\int e^{i(\mathbf{k}-\mathbf{k}'+\mathbf{q})\mathbf{z}}d\mathbf{z} \tag{7}$$

Consider the integral over $\mathbf{z}$

$$\int e^{i(\mathbf{k}-\mathbf{k}'+\mathbf{q})\mathbf{z}}d\mathbf{z} = NR\delta\left(\mathbf{k}-\mathbf{k}'+\mathbf{q}\right) \tag{8}$$

and therefore, $\mathbf{k}' = \mathbf{k} + \mathbf{q}$. We write

$$\left(a_{\mathbf{k}} + a^+_{-\mathbf{k}}\right)\left(a_{-(\mathbf{k}+\mathbf{q})} + a^+_{\mathbf{k}+\mathbf{q}}\right) = a_{\mathbf{k}}a_{-(\mathbf{k}+\mathbf{q})} + a_{\mathbf{k}}a^+_{\mathbf{k}+\mathbf{q}} + a^+_{-\mathbf{k}}a_{-(\mathbf{k}+\mathbf{q})} + a^+_{-\mathbf{k}}a^+_{\mathbf{k}+\mathbf{q}} \tag{9}$$

First, for the sake of convenience, we assume the following situation: initially, there is a boson in $\mathbf{k}$ and none in $\mathbf{k}+\mathbf{q}$; then there is one in $\mathbf{k}+\mathbf{q}$ but not in $\mathbf{k}$. Obviously, the terms with two annihilators or two creators do not contribute, so that we omit them. Further, in the case of the weak coupling, we assume