Local polariton states in impure ionic crystals

V.S. Podolsky, Lev I. Deych and A.A. Lisyansky

Department of Physics, Queens College, CUNY, Flushing, NY 11367

(March 24, 2022)

Abstract

We consider the dynamics of an ionic crystal with a single impurity in the vicinity of the polariton resonance. We show that if the polariton spectrum of the host crystal allows for a gap between polariton branches, the defect gives rise to a novel kind of local states with frequencies within the gap. Despite the atomic size of the impurity we find that new local states are predominated by long-wavelength polaritons. The properties of these states are shown to be different from the properties of the well-known vibrational local states. The difference is due to the singular behavior of the density of states of polaritons near the low-frequency boundary of the polariton gap. Assuming cubic symmetry of the defect site we consider a complete set of the local states arising near the bottom of the polariton gap.
I. INTRODUCTION

An existence of local excitations caused by crystal defects is a well-known phenomenon in solid state physics [1,2]. A single point-like defect can give rise to new states localized in the vicinity of a defect with frequencies outside the bands of extended states of a host crystal. These states and their interaction with electromagnetic waves (IR absorption, Raman scattering) were extensively studied since the early forties following pioneering works by Lifshitz [3–5]. In all these studies electromagnetic field was considered as an external field, which excites vibrational states. The feedback effect of the vibrations upon electromagnetic field was neglected. However, in ionic crystals in the region of frequencies closed to the crossing point of phonon and photon dispersion curves one has to take this effect into account because the coupling between electromagnetic waves and vibrations becomes so strong that the new kind of excitations – polaritons – emerges. In this situation the analyses of local vibrations and their interaction with electromagnetic field has to be done more carefully with taking the polariton effects into account. For the first time such a consideration was carried out in Ref. [6] where a novel kind of local excitations was discovered. It was shown in Ref. [6] that if the polariton spectrum of a crystal exhibits a gap between polariton branches, where the density of states of a host material is equal to zero, a defect embedded in the crystal gives rise to local states with frequencies within the gap. These states are a mix of electromagnetic field and excitations of a host material. Their properties appeared to be quite different from those of known local phonon states. Unlike pure phonon systems, in the case of isotropic materials there is no minimum critical value of the “strength” of the impurity for local polariton states to appear. This feature was shown to be caused by a negative dispersion of optical phonons resulting in a non-monotonic dispersion of polaritons.

A general analysis made in Ref. [6] refers to arbitrary “polarization waves.” It is applicable to a variety of excitations, such as phonon-polaritons, exciton-polaritons, etc. Concerning a particular case of phonon-polaritons the model of a dipole interaction between scalar electromagnetic and polarization waves, used in Ref. [6], needs to be extended to account for a
vector nature of the excitations. Moreover, the analysis of non-isotope impurities, affecting the elastic bonds around a defect, is not consistent within the scalar model.

In the present paper we take into account the vector nature of electromagnetic waves interacting with vibrations in crystals with cubic symmetry. We assumed that an impurity atom in addition to having a different mass can locally change elastic constants. The anisotropy of the crystal is assumed to be weak and is neglected in the long wavelength limit. We obtained two series of local states which differ in parity. In agreement with results of Ref. [7], all these states appear first at the bottom of the polariton gap for infinitesimally small variations of impurity parameters. This is shown to be caused by a singularity of the density of states in the lower polariton band. This singularity also provides that the localization of transverse polaritons is most effective near the lower boundary of the gap. We show that the local polariton states, unlike usual transverse extended states are affected by the interaction with the longitudinal phonon modes. This interaction narrows the frequency range available for the local polariton states.

II. POLARITONS IN A PURE CRYSTAL: ISOTROPIC APPROXIMATION

We consider below a body centered cubic (BCC) dielectric crystal with two oppositely charged ions per each elementary cell. The interaction between ions is assumed to be a central one. Denoting masses of the positive and negative ions as \( m_+ \) and \( m_- \), respectively, and their displacements as \( \mathbf{U}_\pm(\mathbf{r}) \), where \( \mathbf{r} \) belongs to the positive or negative sublattice, we can write down the equations of stationary lattice vibrations coupled to a coherent electric field, \( \mathbf{E}(\mathbf{r}) \):

\[
m_{\pm}\omega^2\mathbf{U}_\pm(\mathbf{r}) \pm q\mathbf{E}(\mathbf{r}) = -\sum_s \left[ \sum_{\mathbf{R}_s} f(\mathbf{r} \cdot \mathbf{R}_s) + \sum_{\mathbf{R}'_s} f'(\mathbf{r} \cdot \mathbf{R}'_s) \right],
\]

where \( q \) denotes an ion charge, \( \omega \) is the frequency.

The right-hand side of Eq. (1) presents all elastic forces acting on the ion hosted at the site \( \mathbf{r} \). Vectors \( \mathbf{R}_s \) and \( \mathbf{R}'_s \) denote radius-vectors of neighboring ions in the \( s \)-shell spheres of
the original and alternative sublattice, respectively. In the case of a central interaction the elastic forces within one sublattice have a form:

\[
f(r \mathbf{R}_s) = -\frac{\beta(R_s)}{R_s^2} \mathbf{R}_s \left\{ \mathbf{R}_s \cdot \left[ U_\pm(r) - U_\pm(r + \mathbf{R}_s) \right] \right\}
\]  

(2)

and forces between ions from different sublattices are:

\[
f'(r \mathbf{R}'_s) = -\frac{\beta'(R'_s)}{R'_s^2} \mathbf{R}'_s \left\{ \mathbf{R}'_s \cdot \left[ U_\pm(r) - U_\pm(r + \mathbf{R}'_s) \right] \right\},
\]  

(2')

where elastic constants of intra- and inter-sublattice interaction, \( \beta(R) \) and \( \beta'(R') \), depend on a distance between ions only.

A coherent electric field induced by the ionic vibrations, \( \mathbf{E}(r) \), invokes an additional pair of equations:

\[
\nabla \cdot \mathbf{E}(r) = -4\pi q \sum \left[ U_+(l) \cdot \nabla \delta(r - l) - U_-(l + b) \cdot \nabla \delta(r - l - b) \right],
\]  

(3)

\[
\nabla \times [\nabla \times \mathbf{E}(r)] + \frac{\omega^2}{c^2} \mathbf{E}(r) = -4\pi q \omega^2 \sum \left[ U_+(l) \delta(r - l) - U_-(l + b) \delta(r - l - b) \right],
\]  

(4)

where vectors \( l \) denote lattice vectors, \( b \) is the basis vector and \( c \) is the speed of light.

The lattice normal modes arise as simultaneous solutions of Eqs. (1,3,4). Fourier transformation of this system gives the dynamics equations in the momentum representation:

\[
\begin{pmatrix}
\hat{D}(k) + \hat{F}(k) - \omega^2 m_+ & \hat{D}'(k) - \hat{F}(k) \\
\hat{D}'(k) - \hat{F}(k) & \hat{D}(k) + \hat{F}(k) - \omega^2 m_-
\end{pmatrix}
\begin{pmatrix}
A_+(k) \\
A_-(k)
\end{pmatrix} = 0.
\]  

(5)

Here \( A_{\pm}(k) \) denote the Fourier amplitudes of the displacements, \( \hat{D}(k) \) is the dynamical matrix of the intra-sublattice interaction:

\[
\hat{D}(k) = \sum_s \frac{\beta(R_s)}{R_s^2} \sum_{\mathbf{R}_s} \mathbf{R}_s \otimes \mathbf{R}_s \left( 1 - e^{i\mathbf{k} \cdot \mathbf{R}_s} \right) + \frac{\beta'(R'_s)}{R'_s^2} \sum_{\mathbf{R}'_s} \mathbf{R}'_s \otimes \mathbf{R}'_s
\]  

(6)

and \( \hat{D}'(k) \) is the dynamical matrix of the inter-sublattice interaction:

\[
\hat{D}'(k) = -\sum_s \frac{\beta'(R'_s)}{R'_s^2} \sum_{\mathbf{R}'_s} \mathbf{R}'_s \otimes \mathbf{R}'_s e^{i\mathbf{k} \cdot \mathbf{R}'_s},
\]  

(6')
where $R \otimes R$ denote the direct products of two vectors.

The Fourier amplitudes of the field induced by the lattice vibrations can be expressed as $E = -\hat{F} \left( A_+ - A_- \right)/q$, with operator $\hat{F}$ defined as follows:

\[
\hat{F}(k, \omega) = \frac{4\pi q^2}{a^3} \cdot \frac{\omega^2 \mathbf{I} - c^2 \mathbf{k} \otimes \mathbf{k}}{\omega^2 - c^2 k^2} = \frac{4\pi q^2}{a^3} \left( \hat{P}_\parallel + \frac{\omega^2}{\omega^2 - c^2 k^2} \hat{P}_\perp \right),
\]

where $\hat{I}$ is the unit tensor, $P_{\alpha\beta}^{\parallel} = k_\alpha k_\beta/k^2$ and $P_{\alpha\beta}^{\parallel} = \delta_{\alpha\beta} - k_\alpha k_\beta/k^2$ are the longitudinal and transverse projectors, respectively.

The dynamical matrices given by Eqs. (6,6') are of a general type and solutions of Eq. (5), in general, do not split into longitudinal and transverse modes. However, considering long-wave excitations in weakly anisotropic crystals we can make use of the isotropic approximation for the dynamical matrices:

\[
\hat{D}(k) = \gamma(k) \hat{P}_\parallel + \gamma(k) \hat{P}_\perp,
\]

\[
\hat{D}'(k) = \gamma'(k) \hat{P}_\parallel + \gamma'(k) \hat{P}_\perp,
\]

where scalar functions, $\gamma(k)$ and $\gamma'(k)$, can be expressed in terms of frequencies of longitudinal and transverse phonons. In a crystal of cubic symmetry the dynamical matrices become trivial at the center of the Brillouin zone:

\[
\hat{D}(0) = -\hat{D}'(0) = \sum_s \frac{\beta'(R'_s)_{s}}{R'_s^2} \sum_s R'_s \otimes R'_s = \frac{1}{3} \mathbf{I} \sum_s \beta'(R'_s) Z'_s,
\]

where $Z'_s$ denotes a total number of ions in $s$-shell and we make use of the identity, $\sum_{s} R'_s \otimes R'_s = \mathbf{I} Z'_s R'_s^2 / 3$, valid in crystals with cubic symmetry. Eq. (9) sets a condition for parameters in Eqs. (8), so that all $\gamma(k)$ and $-\gamma'(k)$ are equal to a positive constant $\gamma = 1/3 \sum_s \beta'(R'_s) Z'_s$.

In the isotopic approximation all normal modes of a crystal become either longitudinal or transverse, $A^{(\sigma)}_{\pm}(k) = e_{\sigma}(k) A^{(\sigma)}_{\pm}(k)$, where $e_{\sigma}(k)$ are longitudinal or transverse unit polarization vectors, $\sigma$ is a polarization index. Eqs. (5,8) give the following relation between the Fourier amplitudes of displacements in different sublattices:
\[ A_+^{(\sigma)} = \frac{f_\sigma - \gamma'_\sigma}{\gamma_\sigma + f_\sigma - \omega^2 m_+} A_-(\sigma). \]  

(10)

For longitudinal modes \( f_\parallel = 4\pi q^2 / a^3 = f \). The corresponding dispersion equation,

\[ \left( \frac{\gamma_\parallel + f_\parallel}{m_+} - \omega^2 \right) \left( \frac{\gamma_\parallel + f_\parallel}{m_-} - \omega^2 \right) - \frac{(\gamma'_\parallel - f_\parallel)^2}{m_+ m_-} = \left( \omega^2 - \omega^2_\parallel \right) \left( \omega^2 - \omega^2_\parallel \right) = 0, \]  

(11)

defines acoustic, \( \omega^2_\parallel (k) \), and optical, \( \Omega^2_\parallel (k) \), branches of longitudinal phonons. For transverse modes \( f_\perp = f \omega^2 / (\omega^2 - c^2 k^2) \), therefore, the dispersion equation,

\[ \left( \frac{\gamma_\perp + f_\perp}{m_+} - \omega^2 \right) \left( \frac{\gamma_\perp + f_\perp}{m_-} - \omega^2 \right) - \frac{(\gamma'_\perp - f_\perp)^2}{m_+ m_-} = \frac{(\omega^2 - \omega^2_\perp) (\omega^2 - \Omega^2_\perp)}{\omega^2 - c^2 k^2} = 0, \]  

(12)
gives one acoustic, \( \omega^2_\perp (k) \), and two polariton, \( \Omega^2_\perp (k) \), branches.

Neglecting the field effects and solving Eqs. (11,12) in the long wavelength limit one can obtain expressions for \( \gamma_\sigma (k) \) and \( \gamma'_\sigma (k) \) in terms of conventional parameters:

\[ \gamma_\sigma (k) \approx \gamma + \mu k^2 \left( v^2_\sigma - v'^2_\sigma \right), \]  

\[ \gamma'_\sigma (k) \approx -\gamma + \mu k^2 \left[ v'^2_\sigma + v^2_\sigma \left( \frac{M}{2\mu} - 1 \right) \right], \]  

(13)

(13')

where \( \mu \) and \( M \) are reduced and total masses of ions within the elementary cell, respectively, \( v_\sigma \) and \( v'_\sigma \) are the velocities of acoustic and optical phonons with a given polarization.

Eqs. (11,12) show that the internal field affects dispersion relations of all lattice excitations. However, the physical effects of the photon-phonon interaction are substantial in a vicinity of the polariton resonance which takes place in the long wavelength region. It is straightforward to show that the acoustic branches,

\[ \omega^2_\sigma (k) \approx 2 \frac{\gamma_\sigma + \gamma'_\sigma}{M} \approx v^2_\sigma k^2, \]  

(14)

are unaffected by the field, whereas, the interaction with the field results in the uniform up-shift of the longitudinal optical branch,

\[ \omega^2 = \Omega^2_\parallel (k) + d^2, \]  

(15)

and leads to the well-known polariton dispersion relation for optical transverse excitations. \[ \Box \]
\[
\left[\omega^2 - \Omega_\perp^2(k)\right] \left[\omega^2 - c^2k^2\right] = d^2\omega^2.
\]  
(16)

Eq. (16) describes two polariton branches, \(\Omega_\pm(k)\), with corresponding dispersion laws:

\[
\Omega_\pm^2(k) = 1/4 \left( \sqrt{\Omega_\perp(k) + ck}^2 + d^2 \pm \sqrt{\Omega_\perp(k) - ck}^2 + d^2 \right)^2,
\]  
(17)

where \(\Omega_\perp\) and \(\Omega_\parallel\) are frequencies of the transverse and longitudinal optical phonons, respectively,

\[
\Omega_\perp^2(k) \approx \frac{\gamma_\sigma}{\mu} - 2\frac{\gamma_\sigma + \gamma'_\sigma}{M} \approx \omega_0^2 - v'^2_\perp k^2,
\]  
(18)

a phonon-photon coupling parameter, \(d^2 = f/\mu = 4\pi q^2/\mu a^3\), is the ionic “plasma frequency” and \(\omega_0^2 = \gamma/\mu\) is the optical activation frequency.

Analysis of Eqs. (14,15,17) shows that the lower polariton branch, \(\Omega^-_\pm(k)\), has a zero activation frequency and extends over both acoustic bands, whereas, the longitudinal optical branch, \(\Omega^\parallel_\pm(k) + d^2\), overlaps with the top part of the polariton gap. Therefore, a truly forbidden gap, with no modes of any kind inside, may exist only between the lower boundary of the polariton gap and the bottom of the longitudinal band [Fig. 1]. When the dispersion of optical phonons is neglected, both polariton branches are monotonic and the spectral gap is between the transverse and longitudinal frequencies, \(\omega_0^2\) and \(\omega_0^2 + d^2\).

It turns out that accounting for the phonon dispersion causes a qualitative change of this picture. First, the upper boundary of the frequency gap, \(\omega_2^\perp\), is now set by the bottom of the optical longitudinal band. Second, the lower polariton branch in the case of a negative dispersion becomes non-monotonic and gains a maximum at some \(k = k_0\), close to the center of the Brillouin zone [Fig. 1]. Calculations in the long wavelength approximation give \(k_0^2 \approx 2\omega_0 d/v'_\perp c\) and a new lower boundary of the gap, \(\omega_1^2 = \Omega^-_\parallel(k_0) \approx \omega_0^2 - 2v'_\perp \omega_0 d/c\). Since \(2v'_\perp \omega_0 d/c \approx v'^2_\perp k_0^2 \ll \omega_0^2\), the result is consistent with the approximation. However, because \(c^2 k_0^2 \approx 2c\omega_0 d/v'_\perp \gg \omega_0^2\), the maximum of \(\Omega^-_\parallel(k)\) is far away from the very narrow (due to \(c \gg v'_\perp\)) polariton resonance region. Since \(\Omega^-_\parallel(k)\) reaches its maximum at the surface of a finite area inside the Brillouin zone, the density of polariton states diverges at the gap’s lower
boundary. As we show latter, it causes an absence of a lower threshold for local polariton states.

III. POLARITON LOCAL STATES

When a host ion at the site \( r = 0 \) of the positive sublattice is replaced by an impurity ion with the same charge, it causes a local deviation of the crystal density and a local change of elastic constants. To account for these facts we need to add extra forces to the right hand side of Eq. (1). For positive and negative sublattices, respectively, these forces are:

\[
\delta f^+(r) = \left\{ \omega^2 \delta m U_+(0) - \frac{\delta \beta}{n^2} \sum_n n \left[ n \cdot U_+(0) - n \cdot U_-(n) \right] \right\} \delta r_0
\]

and

\[
\delta f^-(r) = -\frac{\delta \beta}{n^2} \sum_n n \left[ n \cdot U_+(0) - n \cdot U_-(n) \right] \delta r_n,
\]

where \( \delta m \) is the difference between the masses of an impurity and a host ion, \( \delta \beta \) is a shift in the elastic constant in the impurity’s near-neighbor shell and vectors \( n \) denote radius-vectors of the impurity’s nearest neighbors.

The dynamic equation (5) is now modified:

\[
\begin{pmatrix}
\hat{D}(k) + \hat{F}(k) - \omega^2 m_+ \\
\hat{D}'(k) - \hat{F}(k)
\end{pmatrix}
\begin{pmatrix}
A_+(k) \\
A_-(k)
\end{pmatrix} = \frac{1}{N}
\begin{pmatrix}
B_+ \\
B_-
\end{pmatrix},
\]

where \( N \) is the number of ions in one sublattice and

\[
B_+ = \omega^2 \delta m U_+ - \frac{\delta \beta}{n^2} \sum_n n \left[ n \cdot U_+ - U_n \right],
\]

\[
B_- = \frac{\delta \beta}{n^2} \sum_n n \left[ n \cdot U_+ - U_n \right] e^{-ik \cdot n}.
\]

Here \( U_+ = U_+(0) \) and all \( U_-(n) \) appear only in combinations \( U_n = n \cdot U_-(n) \), because ion-ion forces are central.

Let us denote the matrix in the left-hand side of Eq. (20) as Cartesian (\( \alpha \)) and sublattice (\( \varepsilon \)) indices of the amplitudes \( A_\alpha^\varepsilon \). In the isotropic approximation this matrix can be decomposed, \( \mathbf{L} = \mathbf{L}_{||} \otimes \hat{\mathbf{P}}_{||} + \mathbf{L}_{\perp} \otimes \hat{\mathbf{P}}_{\perp} \), where \( 2 \times 2 \)-matrices \( \mathbf{L}_\sigma \), operating on sublattice indexes only, are defined as the follows:
The inverse matrix, \( \mathbf{L}^{-1} = \mathbf{L} \otimes \mathbf{P} + \mathbf{L}_{\perp} \otimes \mathbf{P}_{\perp} = \mathbf{G} = \mathbf{G} \otimes \mathbf{P} + \mathbf{G}_{\perp} \otimes \mathbf{P}_{\perp} \), where

\[
\mathbf{G}_\sigma = \begin{pmatrix}
g^+_{\sigma} & g'_{\sigma} \\
g'_{\sigma} & g_{\sigma}
\end{pmatrix}
= \frac{1}{m_+ m_-} \begin{pmatrix}
(\gamma_{\sigma} + f_{\sigma} - \omega^2 m_+ - \omega^2) & (\gamma'_{\sigma} - f_{\sigma}) \\
(\gamma'_{\sigma} - f_{\sigma}) & (\gamma_{\sigma} + f_{\sigma} - \omega^2 m_-)
\end{pmatrix}^{-1} \begin{pmatrix}
l_{\sigma}^+ & -l'_{\sigma} \\
-l'_{\sigma} & l_\sigma^+
\end{pmatrix},
\]

is the Green’s function of the system in the momentum representation. In accordance with a general property of Green’s functions, poles of its matrix elements, \( g_\sigma(\omega, k) \), coincide with eigenfrequencies of a pure crystal,

\[
g_{\parallel}(\omega) \propto \left( \omega^2 - \omega^2_\parallel \right)^{-1} \left( \omega^2 - \Omega^2 - a^2 \right)^{-1},
\]

\[
g_{\perp}(\omega) \propto \left( \omega^2 - \omega^2_\perp \right)^{-1} \left( \omega^2 - \Omega^2_\perp \right)^{-1} \left( \omega^2 - \Omega^2 \right)^{-1},
\]
as it follows from Eqs. (11,12).

Solving Eq. (20) with the help of Eqs. (22,23), one can obtain Fourier amplitudes of the ion displacements, \( \mathbf{A}_+(k) \) and \( \mathbf{A}_-(k) \), and the displacements themselves:

\[
\mathbf{U}_+(r) = \sum_{\sigma} \int_{(k)} e^{i \mathbf{k} \cdot \mathbf{r}} e_\sigma(k) \otimes e_\sigma(k) \left( g^+_{\sigma} \mathbf{B}_+ + g'_{\sigma} \mathbf{B}_{-\sigma} \right)
\]

\[
\mathbf{U}_-(r) = \sum_{\sigma} \int_{(k)} e^{i \mathbf{k} \cdot \mathbf{r}} e_\sigma(k) \otimes e_\sigma(k) \left( g'_{\sigma} \mathbf{B}_+ + g_{\sigma} \mathbf{B}_{-\sigma} \right)
\]

where a symbol \( f_{(k)} \) denotes \( (1/N) \sum_{\mathbf{k}} \approx (a/2\pi)^3 \int d\mathbf{k} \), with wave vectors taken from the first Brillouin zone only.

Substitution of \( \mathbf{B}_+ \) and \( \mathbf{B}_{-\sigma} \), given by Eqs. (21,21’), into Eqs. (24) allows one to express all displacements in terms of \( \mathbf{U}_+ \) and \( \mathbf{U}_n \) only, and then obtain a closed system of equations for these variables. In the case of an isotope impurity, considered earlier in the scalar model of Ref. [4], we set \( \delta \beta = 0 \) and this system of spectral equations reads:

\[
\mathbf{U}_+ = \omega^2 \delta m \sum_{\sigma} \int_{(k)} g^+_{\sigma} e_\sigma(k) \otimes e_\sigma(k) \mathbf{U}_+.
\]
In a cubic crystal, vector $\mathbf{U}_+$ can be arbitrary [Appendix A], whereas frequencies of excitations are defined by the equation:

$$1 = \frac{\omega^2 \delta m}{3} \int_{(k)} \left( g_{\|}^+ + 2 g_{\perp}^+ \right) = \delta m \omega^2 I(\omega^2),$$

which generalizes Eq. (10) obtained in Ref. [7].

All solutions of these equations can be divided into two classes: extended and local states. Since an impurity destroys the translational symmetry of the crystal, any state is now a superposition of all normal modes available in the first Brillouin zone. For extended states, corresponding to scattering states with well-defined wave vectors, frequencies fall into the bands of a pure crystal. Local states, dependent upon the value of the parameter $\delta m$ in Eq. (26), may arise outside of the bands. From the structure of $g_{\sigma}(\omega, \mathbf{k})$ it might seem that when a frequency is close to a particular band, the modes from it dominate in the corresponding state. However, because contributions of the near and distant bands could be weakened or strengthened by the low or high density of states in them, direct calculations are required here.

As we already mentioned, the function $\Omega_-(\mathbf{k})$ reaches its maximum value, $\omega_1^2$, at $\mathbf{k} = \mathbf{k}_0$, close to the center of the Brillouin zone. Its expansion around $\mathbf{k}_0$ does not contain a linear term:

$$\Omega_-(\mathbf{k}) = \omega_1^2 - \nu^2 a^2 (k-k_0)^2 + \mathcal{O} \left[ a^3 (k-k_0)^3 \right].$$

It immediately shows that the integral in the left-hand side of Eq. (26) diverges at $\omega = \omega_1$ due to a contribution from the lower polaritons branch. Therefore, considering $\omega$ in the frequency gap close to its lower boundary we can omit $g_{\|}^+$ from Eq. (26) and rewrite $\int_{(k)} g_{\perp}^+$ using the density of states, $\rho_-(\varepsilon)$, in the lower polaritons band:

$$I^+(\omega^2) = \int_{(k)} \frac{2 g_{\perp}^+}{3} = \left( \frac{a}{2\pi} \right)^3 \int \frac{2}{3 m_+ m_-} \frac{\left( \gamma_+ + f_+ - \omega^2 m_- \right)}{\omega^2 - \omega_+^2 \omega_2^2 \omega_1^2} d\mathbf{k} = \int_{C} \frac{F(k) \rho_-(\varepsilon) d\varepsilon}{\omega^2 - \varepsilon},$$

where $F(k)$ denotes all factors of $g_{\perp}^+$, other than $\left( \omega^2 - \Omega_1^2 \right)^{-1}$ and the last integration is performed on a complex $\varepsilon$-plane [Appendix B].
Near the bottom of the polariton band, for small \( \varepsilon \), the density of states has the usual Kohn shape, \( \rho_-(\varepsilon) \propto \sqrt{\varepsilon} \). The asymptote of \( \rho_-(\varepsilon) \) near the top of the band, for small \( z = \omega_1^2 - \varepsilon \), can be found with the help of Eq. (27):

\[
\rho_-(\varepsilon) = \left( \frac{a}{2\pi} \right)^3 \int \frac{ds}{|\nabla \Omega^2(k)|} \approx \left( \frac{a}{2\pi} \right)^3 \left( \frac{k_0 + z^{1/2}/\nu
u}{\nu z^{1/2}} \right)^2 = \frac{(ak_0)^2}{2\pi^2 \nu z^{1/2}}, \quad (29)
\]

where all omitted terms are regular at \( z = 0 \).

Since for \( \omega \to \omega_1 + 0 \) the divergent part of \( I^+(\omega^2) \) is provided by a region of small \( z \), in Eq. (28) we can replace the exact density of states with the found asymptote. Considering \( \omega^2 - \omega_1^2 \ll \omega_1^2 \) it allows us to calculate the leading part of \( I^+(\omega^2) \) and transform the spectral equation (26) into the form [Appendix B]:

\[
\frac{m_+}{\delta m} \approx -\frac{2 (ak_0)^2 \omega_0^2}{3\pi \nu \sqrt{\omega^2 - \omega_1^2}} m_-. \quad (30)
\]

Using estimates made in section. 2 and recalling that \( \nu = v'_\perp \), we obtain:

\[
\frac{\delta m}{m} = \frac{3\pi c v'_\perp \sqrt{\omega^2 - \omega_1^2}}{a^3 \omega_b^3 d}. \quad (31)
\]

This result recovers Eq. (14) of Ref. [7] obtained in the scalar model and supports the conclusion of the absence of the lower localization threshold for light isotope impurities.

In a general case of non-isotope impurity the spectral system is of the 11th rank with 11 variables, \( \mathbf{U}_+ = \mathbf{U}_+(\mathbf{0}) \), \( \mathbf{U}_n = \mathbf{n} \cdot \mathbf{U}_-(\mathbf{n}) \). The system can be further simplified with the help of the crystal symmetry. The exact point group of a cubic crystal includes the space inversion. Therefore, all excitations can be classified by their spatial parity.

For the odd states, where \( \mathbf{U}_\pm(-\mathbf{r}) = -\mathbf{U}_\pm(\mathbf{r}) \), one can see that both \( \mathbf{U}_+ \) and \( \mathbf{B}_+ \) are equal to zero and the rank of the spectral system reduces from 11 to 4. Considering displacements of four negative ions at corners of one face of the BCC-lattice elementary cell (see Fig. 2) as independent variables, from Eqs. (24) we obtain the following system:

\[
\sum_{s=1}^{4} M_{ss'} U_{s'} = -\frac{n^2}{2\delta \beta} U_s, \quad (32)
\]

where index \( s \) numerates the chosen ions, their radius-vectors are denoted as \( \mathbf{n}_s \) and \( U_s = U_{n_s} = \mathbf{n}_s \cdot \mathbf{U}_-(\mathbf{n}_s) \). The matrix \( M_{ss'} \) here is given by the equation:
\[ M_{ss'} = M(n_s, n_{s'}) = \sum_{\sigma} \int_{(k)} g_\sigma (e_\sigma \cdot n_s)(e_\sigma \cdot n_{s'}) \sin(k \cdot n_s) \sin(k \cdot n_{s'}). \]  

(33)

Using transformation properties of the integrand one can show that the matrix \( M_{ss'} \) remains invariant, \( M(\hat{Q}n, \hat{Q}n') = M(n, n') \), under any point transformation \( \hat{Q} \). Therefore, the elements of the symmetric matrix \( M_{ss'} \) are equal for equivalent pairs of ions: \( M_{11} = M_{22} = M_{33} = M_{44} \), then \( M_{12} = M_{23} = M_{34} \) and \( M_{13} = M_{24} \). After finding eigenvalues of this matrix we obtain three spectral equations:

\[ -\frac{n^2}{2\delta\beta} = \mu_0 = M_{11} - M_{13}, \]  

(34)

\[ -\frac{n^2}{2\delta\beta} = \mu_{\pm} = M_{11} + M_{11} \pm 2M_{12}. \]  

(34')

The structure of the eigenvectors shows that the states corresponding to \( \mu_{+} \) and \( \mu_{-} \) represent “rhombic” and “tetragonal” oscillations localized around the stationary impurity, whereas, the states corresponding to \( \mu_0 \) involve both types of deformations of the elementary cell [Appendix C].

Near the lower boundary of the gap the arguments used in evaluation of Eq. (26) are also applicable. Retaining the leading terms in Eq. (33) and using symmetry properties of the arising expressions [Appendix C], we obtain the following expressions:

\[ \mu_0 \approx \frac{1}{5} \left[ n^4 - (n_1 \cdot n_3)^2 \right] \int_{(k)} k^2 g_\perp, \]  

(35)

\[ \mu_{\pm} \approx \frac{1}{5} \left\{ (n_1 \cdot n_3)^2 + \frac{n^4}{3} \pm 2 \left| (n_1 \cdot n_2)^2 - \frac{n^4}{3} \right| \right\} \int_{(k)} k^2 g_\perp. \]  

(35')

From the geometry of the elementary cell it follows that \( (n_1 \cdot n_2) = -(n_1 \cdot n_3) = n^2/3 = a^2/4 \) and, therefore, \( \mu_0 = \mu_{-} = (a^4/10) \int_{(k)} k^2 g_\perp. \) It leads to the unique spectral equation for all “tetragonal” modes [Appendix B]:

\[ \frac{\delta\beta}{\gamma} \approx \frac{15\pi\nu}{4 (ak_0)^4} \left( \frac{\omega_1^2 - \omega_0^2}{\omega_0^2} \right) \left( \frac{M}{m_+} \right)^2. \]  

(36)

This result shows that the odd local states arise upon an infinitesimally small strengthening of local bonds associated with the impurity, \( \delta\beta \geq +0 \). This effect, similar to the isotope
impurity case, is due to a singularity of the density of states in the lower polariton band. Eq. (36), compared to Eq. (30), has an additional small factor, $(ak_0)^2$. Therefore, for the same relative deviations, $\delta \beta/\beta$ and $\delta m/m$, the odd states lie much closer to the gap’s boundary than the states associated with an isotope impurity. Moreover, these states are much less sensitive to variations of parameters than the isotope-induced local states. This fact reveals itself in an extreme form for “rhombic” modes corresponding to $\mu_+$. Eq. (35') gives $\mu_+ = 0$ which means that within the approximations used these states appear right at the gap’s bottom for any value of $\delta \beta$. Accounting for the higher-order terms in expansions of the sin-functions in Eq. (31) will separate these modes from the gap’s boundary but the separation, $\sqrt{\omega^2 - \omega_i^2} \propto \delta \beta (ak_0)^6$, remains the smallest among all considered local states.

For the even states, where $U_\pm(-r) = U_\pm(r)$, the spectral system contains 7 independent variables. Those are components of the impurity displacement, $U_+$, and radial projections of the displacements of four chosen neighboring ions, $U_s$. The elements of the matrix in the corresponding spectral system can be written as integrals of the Green’s function elements, similar to Eq. (33). Considering local states near the gap’s bottom, we again can retain in these integrals only transverse terms and use the power expansions of non-singular factors of the integrands. As it was shown above, $\int (ak)^2 g_\perp \ll \int (k) g_\perp$ due to the dominant contribution of the small-$k$ region in these integrals. Therefore, since the local states near the gap’s bottom are, roughly, “made” of long wavelength polaritons, we can disregard the exponential factors in the matrix elements of the spectral system $[\exp(\pm ik \cdot n) \approx 1]$ and neglect in Eqs. (21) differences between displacements of identical ions within the elementary cell, $U_- \approx U_-(n)$. These approximations lead to the following spectral system for even states:

$$\begin{pmatrix} U_+ \\ U_- \end{pmatrix} \approx \begin{pmatrix} I^+ & I' \\ I' & I^- \end{pmatrix} \begin{pmatrix} \omega^2 \delta m - 8\delta \beta/3 & 8\delta \beta/3 \\ 8\delta \beta/3 & -8\delta \beta/3 \end{pmatrix} \begin{pmatrix} U_+ \\ U_- \end{pmatrix}.$$  \hfill (37)

The corresponding spectral equation reads:

$$\frac{8\delta \beta}{3} \left( I^+ + I^- - 2I' \right) - \omega^2 \delta m I^+ + 1 = \frac{8\omega^2 \delta \beta \delta m}{3} \left( I^+ I^- - I'^2 \right).$$  \hfill (38)
where all $I$-factors are straightforward to evaluate near the gap’s bottom [Appendix B]:

$$I^\pm (\omega^2) = \frac{2}{3} \int (k) g^\pm_\perp \approx \frac{2 (ak_0)^2}{3 \pi \nu \sqrt{\omega^2 - \omega_1^2}} \frac{\mu - m_\pm}{m_+ m_-},$$  \hspace{1cm} (39)$$

$$I'(\omega^2) = \frac{2}{3} \int (k) g'_\perp \approx \frac{2 (ak_0)^2}{3 \pi \nu \sqrt{\omega^2 - \omega_1^2}} \frac{\mu}{m_+ m_-}.$$  \hspace{1cm} (39')$$

The right-hand side of Eq. (38) is proportional to a determinant of a degenerate operator, the transverse propagator, and it must be equal to zero identically. Substitution of Eqs. (39,39') into Eq. (38) shows this explicitly and transforms the spectral equation of the even states into the following one:

$$\frac{2 (ak_0)^2}{3 \pi \nu \mu \sqrt{\omega^2 - \omega_1^2}} \left[ \frac{8\delta \beta}{3} - \omega_0^2 \delta m \left( \frac{m_-}{M} \right)^2 \right] = 1.$$  \hspace{1cm} (40)$$

One can check that here ions displacements satisfy the relationship, $m_-^2 U_+ + m_+^2 U_- = 0$, corresponding to optical vibrations.

If we set $\delta \beta = 0$ in Eq. (40) it reproduces Eq. (30) obtained earlier for an isotope impurity. That equation has a solution only when $\delta m < 0$. In a general case even local states exist only if variations of parameters satisfy the inequality:

$$\delta \beta - \frac{3}{8} \omega_0^2 \delta m \left( \frac{m_-}{M} \right)^2 > 0.$$  \hspace{1cm} (41)$$

Eqs. (36,40) allow us to outline regions of the local states [Fig.3] on a plane of impurity parameters, $\delta m, \delta \beta$. Taking into account obvious physical limitations, $\delta m \geq -m_+,$ $\delta \beta \geq -\beta$, one can see that odd states appear in the right upper quadrant bounded by the lines $\delta m = -m_+, \delta \beta = 0$. The region of even states is to the right of $\delta m = -m_+$ and above the critical line, $\delta \beta = (3/8) \left( m_- / M \right)^2 \omega_0^2 \delta m$. All other areas of $(\delta m, \delta \beta)$-plane are blocked for the polariton localization.

Since we deal with local states near the gap’s bottom, our analysis is valid in a vicinity of the critical line for even states, and close to $\delta m$-axis for odd states. When the impurity parameters move outside these regions the frequencies of the corresponding local states move away from the gap’s bottom. The lines where the frequencies approach the top of the gap
establish the outer boundaries of the localization regions. Unlike the situation near the
gap’s bottom, all terms of all spectral equations remain finite when \( \omega \) tends to \( \omega_2 \), what
guarantees an existence of limited localization regions. On the other hand, this makes it
impossible to do any rigorous analytical calculations. However, using the density of states
representation of the spectral equations, analogous to Eq. (28), and utilizing some trial
functions to simulate densities of states in all bands, one can obtain qualitatively reliable
results. Our preliminary estimates show that near the upper boundary of the gap local states
are substantially composed of transverse and longitudinal phonons. The balance between
them depends on widths of the corresponding bands and the polariton gap. The contribution
of the long wavelength transverse polaritons into these states is proportional to \((v/c)^3\) and is
negligible. Roughly, it is caused by the fact that the density of states is inversely proportional
to \(v^3\) for phonons and to \(cv^2\) for long wavelength polaritons. A more detailed analysis of
states located far away from the gap’s bottom will be presented elsewhere.

**IV. DISCUSSION AND CONCLUSIONS**

We have considered local polariton states in BCC ionic crystals. It was assumed that
the crystal anisotropy is weak and can be neglected in the long wavelength limit. This
approximation was proved to be self-consistent for states located near the bottom of the
polariton gap. We found two series of local states, different in parity. The new states
appear right at the bottom of the polariton gap upon infinitesimally small variations of an
impurity parameters. This is in contrast with 3-D phonon systems where a lower threshold
for local states always exists. \[12,9\] In Ref. \[9\] the general theorem regarding the presence of
the threshold for arising local states in bandgaps of periodic systems were given. However,
the proof assumed the finite values of density of states in the entire band of pure system.
We show that the singularity in the density of states in the lower polariton band causes
the absence of this threshold. This singularity also provides that the states near the gap’s
bottom are formed mostly by the long wavelength transverse polaritons. The local states
move toward the upper boundary of the gap upon increase of impurity parameters $\delta m$ and/or $\delta \beta$.

We have outlined regions of new local polariton states on a plane of impurity parameters. In a region where both types of states coexist, the odd states precede the even ones. They appear first at the gap’s bottom and remain near it when the impurity parameters vary much longer than the even states. Local states are a mixture of transverse phonons and photons. Comparing amplitudes of the field, $E$, and the crystal polarization, $P$, one can make an estimate of the energy partitions of local polariton states. Because the characteristic momentum, $k_0$, happened to be away from the polariton resonance region, the ratio $E/P$ turns out to be of the order of $v'_\perp/c$. An account for the electronic polarization of ions renormalizes $c$ and increases this ratio. More detailed analysis of these aspects of the polariton local states will be done elsewhere. Condition (41) can help in a search for compounds where local polariton states can be observed.

The results of this paper were obtained within the harmonic approximation of crystal dynamics. Phonon-phonon interaction caused by a lattice anharmonism will affect this picture. Phonon-phonon scattering causes damping of all elementary excitations and the local states as well. It leads to a broadening of all spectral lines and it also washes out all sharp boundaries in the initial excitation spectra. However, it seems physically evident that the scale of this broadening is far below the typical width of phonon bands and cannot change the topology of the initial band structure, or close the polariton gap. If we dress up the elementary excitations and renormalize their spectra, the maximum of the density of states in the lower polariton band and the corresponding singularity will persist after the renormalization since it has a topological origin. That, in turn, guarantees the absence of a threshold for local states near the (renormalized) gap’s bottom at zero temperature. However, at non-zero temperature thermal broadening of spectral lines will set a finite threshold for local states.

Another factor that leads to a threshold is crystal anisotropy. It provides a difference between maxima of $\Omega_2^2(k)$ in different directions that causes the density of states in the lower...
polariton branch to be finite everywhere. It should be emphasized, however, that properties of the local polariton states remain quite different from the corresponding properties of purely phonon local states. Particularly, one can see from our results, that eigenfrequencies of local polaritons are much more sensible to the crystal structure of the host materials.

ACKNOWLEDGMENTS

We wish to thank I.M. Vitebsky for useful discussion. This work was supported by the NSF under grant No. DMR-9632789, by a CUNY collaborative grant and PSC-CUNY grants.

It is known that under any point transformation, \( \hat{Q} \), the frequency of any normal mode remains invariant, \( \omega^2(\hat{Q} \mathbf{k}) = \omega^2(\mathbf{k}) \), and the corresponding polarization vector transforms as the follows: \( \mathbf{e}(\hat{Q} \mathbf{k}) = \hat{Q}^{-1} \mathbf{e}(\mathbf{k}) \). Because the Brillouin zone also maps exactly into itself, one can see that

\[
\hat{T} = \int_{(k)} g[\omega^2(\mathbf{k})] \mathbf{e}(\mathbf{k}) \otimes \mathbf{e}(\mathbf{k}) = \int_{(\hat{Q} \mathbf{k})} g[\omega^2(\hat{Q} \mathbf{k})] \mathbf{e}(\hat{Q} \mathbf{k}) \otimes \mathbf{e}(\hat{Q} \mathbf{k}) = \hat{Q}^{-1} \hat{T} \hat{Q}.
\]

Therefore, any tensor of this type is an invariant of the point group of a crystal. In the cubic system any group-invariant operator must be trivial, \( \hat{T} = t \hat{I} \), since the group contains non-collinear axis of different order. Calculating the trace of the operator, one can find:

\[
\hat{T} = 1/3 \int_{(k)} g[\omega^2(\mathbf{k})] [\mathbf{e}(\mathbf{k}) \cdot \mathbf{e}(\mathbf{k})] \hat{I},
\]

where \( \hat{I} \) is the identity operator.

The density of states in the lower polariton band, \( \rho_-(\varepsilon) \), is defined at the complex \( \varepsilon \)-plane, cut from 0 to \( \omega_1^2 \). The contour of integration, \( C \), in Eq. (26) runs along the upper side of the cut (it corresponds to integration over \( k < k_0 \)), turns around its right edge and then, for the integration over \( k > k_0 \), returns along the lower side of the cut to some point, \( \omega_1'^2 \), fixed by the bottom of the optical photon band.

As it was discussed in the text, the leading part of \( I(\omega^2) \) at \( \Delta(\omega) = \omega^2 - \omega_1^2 \ll \omega_1^2 \), comes from the region close to the right edge of the cut, \( \varepsilon = \omega_1^2 \). Therefore, evaluating Eq. (26), we
can use there the asymptote of the density of states given by Eq. (27). In addition, as it follows from Eq. (25), \( k - k_0 = \mp z^{1/2}/av \) near the right edge of the cut at its upper and lower sides, respectively. Taking this into account when expanding \( F(k) \) around \( k_0 \) in Eq. (26), we obtain:

\[
I^+ (\omega^2) = \int_0^{\omega^2} 2 \left[ F_0 - F_0' \sqrt{z}/av + \cdots \right] dz + \int_{\omega^2}^{\omega^2_{\text{max}}} 2 \left[ F_0 + F_0' \sqrt{z}/av + \cdots \right] dz.
\]

(44)

A rescaling \( z \to z\Delta \) shows that contributions in \( I^+ (\omega^2) \) from all terms of expansion of \( F(k) \) tend to zero in the limit \( \Delta \to +0 \), except for the first two terms. Further elementary integration gives the singular part of the considered integral:

\[
I^+ (\omega^2) = \frac{2(ak_0)^2 F(k_0)}{3\pi \nu \Delta^{1/2}} = \frac{2(ak_0)^2}{3\pi \nu \Delta^{1/2}} \left[ \frac{\omega^2 - c^2 k_0^2}{m_+ m_- [\omega^2 - \Omega_0^2(k_0)]} \right] (\omega^2 - \omega_0^2(k_0)).
\]

This result is asymptotically exact since all omitted terms are regular at \( \Delta \to +0 \). Using estimations made in Section 2. and taking into account conditions, \( ak_0 \ll 1, \quad v_{\perp}^2 k_0^2 \ll \omega_0^2, \quad c^2 k_0^2 \gg \omega_0^2 \) and \( \omega \approx \omega_1 \approx \omega_0 \), it is straightforward to obtain:

\[
I^+ (\omega^2) \approx -\frac{2(ak_0)^2}{3\pi \nu \sqrt{\omega^2 - \omega_0^2}} \frac{m_-}{M m_+}
\]

(46)

which immediately leads to Eq. (28).

In a similar way one can obtain Eqs. (37), as well as, calculate the integral in Eqs. (33):

\[
\int (k^2) g_{\perp} = \frac{2(ak_0)^4}{3\pi \nu \Delta^{1/2}} \frac{(\omega^2 - c^2 k_0^2)}{m_+ m_- [\omega^2 - \Omega_0^2(k_0)]} \approx -\frac{2(ak_0)^4 \omega_0^2}{3\pi \nu \sqrt{\omega^2 - \omega_0^2}} \frac{m_+}{M m_-}
\]

(47)

Eq. (30) with the matrix \( M_{ss'} \) defined by Eq. (31) can be rewritten as follows:

\[
\begin{pmatrix}
M_{11} - M_{13} - \mu & 0 & 0 & 0 \\
0 & M_{11} - M_{13} - \mu & 0 & 0 \\
M_{13} & M_{12} & M_{11} + M_{13} - \mu & 2M_{12} \\
M_{12} & M_{13} & 2M_{12} & M_{11} + M_{13} - \mu
\end{pmatrix}
\begin{pmatrix}
U_1 \\
U_2 \\
U_3 - U_1 \\
U_4 - U_2
\end{pmatrix}
= 0.
\]

(48)

which has three eigenvalues given by Eqs. (32).

For \( \mu = \mu_\pm \) this equation gives \( U_1 = U_2 = 0 \) and \( U_3 = \pm U_4 \). Recalling that \( U_s = n \cdot U(n_s) \) and the states we consider here are antisymmetric, one can see that in \( \mu_+ \)-mode
the elementary cell inclosing a defect experiences “rhombic” deformations. In \(\mu_\perp\)-mode, since the ion motion is anti-phased, it produces “tetragonal” deformations. For \(\mu = \mu_0\) Eq. (C1) leaves \(U_1\) and \(U_2\) independent, whereas, \(U_3 = U_1/2\) and \(U_4 = U_2/2\). It results in combined, “tetra-rhombic” deformations of the elementary cell in these modes.

To obtain the explicit expressions of the eigenvalues, \(\mu\), we have to calculate the matrix elements \(M_{ss'}\). When the frequency of the considered states is close to \(\omega_1\) we can retain only first terms in expansions of \(\sin\)-factors in Eq. (29). This approximation is self-consistent, because the region of small wave vectors is the major contribution in Eq. (29). Carrying out the calculations, one needs to know tensors of two types: \(\int k f(k) k^\alpha k^\beta\) and \(\int k f(k) k^\alpha k^\beta k^\sigma k^\beta\), where \(f(k)\) is an arbitrary invariant function. From Appendix A it immediately follows that, \(\int k f(k) k^\alpha k^\beta = (1/3) \delta^{\alpha\beta} \int k f(k) k^2\). The second tensor is obviously totally symmetric, therefore:

\[
\int k f(k) k^\alpha k^\beta k^\sigma k^\beta = I \left( \delta^{\alpha\beta} \delta^{\sigma\beta} + \delta^{\alpha\sigma} \delta^{\beta\beta} + \delta^{\alpha\beta} \delta^{\beta\sigma} \right) \int k f(k) k^4,
\]

(49)

where summation over \(\alpha = \beta\) and \(\sigma = \beta\) defines the numerical factor, \(I = 1/15\). Using these results in \(M_{ss'}\) and retaining there the transverse terms only, we obtain:

\[
M_{ss'} \approx \frac{1}{3} \left\{ (n_s n_{s'})^2 - \frac{n^4 + 2(n_s n_{s'})^2}{5} \right\} \int (k^2 g^-),
\]

(50)

that, in turn, leads to Eqs. (33).
REFERENCES

[1] Lattice Dynamics (Benjamin, New York, 1969).

[2] A.A. Maradudin, E.W. Montroll, G.H. Weiss, and I.P. Ipatova, Theory of Lattice Dynamics in the Harmonic Approximation (Academic Press, New York, 1971).

[3] I. M. Lifshitz, Doct. Acad. Nauk S.S.S.R., 48, 83 (1945).

[4] I. M. Lifshitz, Zh. Eksp. Teor. Fiz., 17, 1017 (1947).

[5] I. M. Lifshitz, Zh. Eksp. Teor. Fiz., 18, 298 (1948).

[6] M. Born and K. Huang, Dynamical Theory of Crystal Lattices (Oxford, Clarendon Press, 1954)

[7] L.I. Deych and A.A. Lisyansky, Phys. lett. A, 1998, to be published; A.A. Lisyansky and L.I. Deych, Bull. Amer. Phys. Soc. 42, 203 (1997).

[8] C. Kittel Introduction to solid state physics (Wiely, New York, 1986).

[9] A.Figotin and A. Klein, J. Stat. Phys., 86, 165 (1997).
Figure Captions

Fig. 1. Elementary cell of a body centered cubic lattice. Here \( a \) is a lattice parameter, indexes \( s, s' \) numerate ions within the near-neighbor shell, \( \pm \mathbf{n}_s \) are radius-vectors of the ions.

Fig. 2. Phonon-polariton dispersion curves in the isotropic approximation. Here lines \( \omega = \Omega_\pm(k) \) present the lower and upper polariton branches, \( \Omega_\perp(k) \) and \( \omega_+ \parallel(k) \) are transverse and longitudinal optical phonon branches, \( \omega_\perp(k) \) and \( \omega_- \parallel(k) \) are the transverse and longitudinal acoustic phonon branches, respectively. The horizontal lines \( \omega_0 \) and \( \omega_3 \) are the upper and lower boundaries of the transverse optical phonon band, \( \sqrt{\omega_0^2 + d^2} \) and \( \omega_2 \) are the upper and lower boundaries of the longitudinal optical phonon band, respectively. The polariton gap is bounded by lines \( \omega_1 \) and \( \omega_2 \). The wave number \( k_0 \) corresponds to the maximum of the lower polariton branch.

The figure presents qualitative features of phonon-polariton spectra in the long wavelength region and does not reflect an actual scale of wave velocities.

Fig. 3. Regions of existence of local polariton states. \( \delta m \) is the difference between masses of the impurity and a host atom, \( \delta \beta \) is the impurity induced deviation of the elastic constant within the near-neighbor shell, \( m_+ \) is the mass of a host ion in the “positive” sublattice, \( \beta \) is the elastic constant of a near-neighbor interaction in a perfect crystal. Odd local polariton states exist in the region bound by the solid lines \( \delta m = -m_+ \), \( \delta \beta = 0 \). The region of even local states is to the right of the solid line \( \delta m = -m_+ \) and above the dashed line, \( \delta \beta = (3/8) (m_-/M)^2 \omega_0^2 \delta m \).
\[ (\omega_0^2 + d^2)^{1/2} \]
