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Resonance tunneling of polaritons in 1D chain with a single defect

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Abstract

We consider propagation of coupled waves (polaritons) formed by a scalar electromagnetic wave and excitations of a finite one-dimensional chain of dipoles. It is shown that a microscopic defect (an impurity dipole) embedded in the chain causes resonance tunneling of the electromagnetic wave with a macroscopic wavelength through the forbidden band between two polariton branches. We demonstrate that the resonance tunneling occurs due to local polariton states caused by the defect. © 1998 Published by Elsevier Science B.V.

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In this Letter we demonstrate that a dipole-active defect (impurity atom without internal degrees of freedom) embedded in an otherwise ideal structure causes resonance tunneling of electromagnetic waves through the stop-band between different polariton branches of the host crystal. Though resonance tunneling of electromagnetic waves has been discussed in different situations (see, for example, Ref. [1]) it always required a "transmitter" of a size comparable with electromagnetic wavelengths, λ (assuming that it does not have internal degrees of freedom). In our Letter we discuss a principally new situation, when tunneling resonance occurs at *wavelengths much greater than the characteristic scale of the defect.* This result seems to be in contradiction with well-known facts that scattering of electromagnetic waves is ineffective if the size of scatterers is small comparing to electromagnetic wavelength and that individual atoms do not have enough polarizability to cause strong scattering. The resolution of this contradiction lies in the fact that the resonance in the considered situation occurs due to local polariton states discussed recently in our papers [2,3]. Local polaritons are states that occur inside the gap between different polariton branches ("restrahlen" region) when a dipole active defect is embedded in a regular ionic crystal. They are coupled states of transverse electromagnetic waves and excitations of a crystal such as phonons or excitons with both components localized in the vicinity of the defect. It is important that, though local polaritons are induced by a single defect, they are collective excitations, and electromagnetic radiation actually interacts with macroscopic amount of atoms. The efficiency of this interaction is determined by the polarizability of the entire mode rather than that of a single atom. In

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the case of local phonons or excitons with frequencies within a transparent for electromagnetic radiation region this interaction results in strong absorbtion or Raman scattering of light. What is actually new in the situation considered in the present Letter is that our local states arise in a frequency region that is forbidden for light propagation. As a result not only intrinsic phonon or exciton degrees of freedom, but also transversal electromagnetic field, coupled to them, become localized. Therefore, usual optical phenomena like absorbtion or scattering cannot occur, and local polariton states manifest themselves by means of the resonant tunneling.

Local polariton states were also considered independently by Rupasov and Singh [4]. However, there is an important physical difference between states considered in Ref. [4] and in our papers [2,3]. The former authors considered states of a two-level atom coupled with elementary excitations of a medium. A two-level atom considered in Ref. [4] introduces new modes (transitions between levels of the atom), which were absent in the pure system. The local states associated with such a defect are the original states of an atom modified by the interaction with its surroundings. In our papers [2,3] we considered a defect ion with no internal degrees of freedom embedded in a regular ionic crystal. The local states arising due to this kind of defect occur because of a fundamental reconstruction of the spectrum of a pure system. As a result of such a reconstruction, a discrete eigenfrequency splits off the continuous spectrum giving rise to a local state. This phenomenon is well known in systems of phonons or excitons and was originally discovered by Lifshitz. [5] Similar effects were also found for electromagnetic waves in photonic crystals [1,8,9] due to *macroscopic* defects embedded in their structure. The important general result obtained in Refs. [2,3] is that a *microscopic* defect is able to rebuild the spectrum of electromagnetic excitations in the medium in the region of wavelengths much greater than the size of the defect. One of the unusual properties of local polaritons found in Ref. [2] is that even in 3D systems the local states arise due to the defect of an arbitrary small "strength." For all previously known local states this property was an attribute of the 1D situation. We showed in Refs. [2,3] that this peculiar behavior of local polaritons is due to the spatial dispersion of the polariton branches of a host crystal.

An important question about properties of the local polaritons that has still remained open is if the electromagnetic component of the local polaritons plays any significant role (and, therefore, if the local polaritons actually deserve their name). The question arises because the energy of the electromagnetic component of the states appears to be rather small compared to the energy of polarization component (phonons, excitons, etc.). The common wisdom based upon properties of regular propagating polaritons tells us that in such a situation the propagation of an external electromagnetic wave cannot be affected by the states in any significant way. In the case of local states the situation is different. In order to show this we consider propagation of an external electromagnetic wave through a slab containing the local polaritons. Since we deal in this case with frequencies from a stopband, the incident electromagnetic wave would exponentially decay inside the slab and could emerge from the opposite side of the slab only in the form of a weak exponential tail. The experimental significance of the electromagnetic component of the local polaritons is determined by the degree of the enhancement of the transmission coefficient due to resonance tunneling at the frequency of the local polaritons.

In order to shed light on principle aspects of the problem, we study light propagation through a one-dimensional finite chain of dipoles with the nearest neighbor interaction. We assume that this chain is placed within a single-mode waveguide so that we can consider only one mode of the electromagnetic field propagating along the chain. As we mentioned above local polariton states arise at an arbitrary small "strength" of defect in any dimension. Therefore, the results obtained from the 1D model in the case of local polaritons can be more relevant to the realistic 3D case than in other situations. On the other hand, the choice of 1D model makes it feasible to treat electromagnetic waves in the system *microscopically*. This is an important feature of a model since local polaritons arise as a superposition of modes from the entire Brillouin band. Excitations with wave numbers at the edge of the band are pure phonons and electromagnetic waves, which in general cannot be treated macroscopically within the concept of the dielectric function. Our microscopical treatment ensures that high-energy short-wavelength components of the electromagnetic field do not prevent local polaritons, and hence, resonance

tunneling, from occurring.

Polaritons in the system under consideration arise as coupled states of collective excitations of dipoles (polarization waves) and electromagnetic waves. Accounting for the interaction between dipoles at different sites leads to a spatial dispersion of the polarization waves. Taking into account the spatial dispersion makes the exact analytical consideration of the problem unfeasible even in the case of a pure system due to a cumbersome algebra. Therefore, we carry out numerical simulations by means of the transfer-matrix method. The model can be described by the following equations written in the frequency domain,

$$(\Omega_n^2 - \omega^2)P_n + \Phi(P_{n+1} + P_{n-1}) = \alpha E(x_n), \qquad (1)$$

$$\frac{\omega^2}{c^2}E(x) + \frac{\mathrm{d}^2E}{\mathrm{d}x^2} = -4\pi\frac{\omega^2}{c^2}\sum_n P_n\delta(na - x), \qquad (2)$$

where the first equation describes the dynamics of site dipole moments, P_n, and the second one is the equation for the electric field E. Here Ω_n is the diagonal part of the force matrix responsible for the short-range interaction between dipoles, and Φ is its off-diagonal component. We assume that the defect, which occupies the site n_0 affects only the diagonal part of the force matrix, so that $\Omega_n = \Omega$ for all n except for $n = n_0$, where $\Omega_{n_0} = \Omega_{\mathrm{def}}$. The coordinate x in Eq. (2) goes along the chain with the interatomic distance a, and the right-hand side of this equation is the microscopic polarization density. Parameter α is responsible for coupling between polarization and electromagnetic waves. Eqs. (1), (2) present a *microscopic* description of the transverse electromagnetic waves propagating along the chain. These equations are subject to the boundary conditions for the electromagnetic and polarization subsystems. We assume that incident and transmitted electromagnetic waves propagate in vacuum so that the boundary conditions for Eq. (2) take the usual form

$$E(0) = 1 + r, \quad \frac{\mathrm{d}E}{\mathrm{d}x} = \mathrm{i}k(1 - r), \qquad (3)$$

$$E(L) = t\exp(\mathrm{i}kL), \quad \frac{\mathrm{d}E}{\mathrm{d}x} = \mathrm{i}kt\exp(\mathrm{i}kL), \qquad (4)$$

where $k = \omega/c$ is a wave number of the electromagnetic wave in vacuum, $|t|^2$ and $|r|^2$ are transmission and reflection coefficients, respectively, and L is the length of the chain. The boundary conditions for dipole excitations can be chosen in the general form

$$\frac{P_0}{P_1} = \beta, \quad \frac{P_N}{P_{N-1}} = \gamma, \qquad (5)$$

where $N = L/a$ is the number of sites in the chain, parameters β and γ describe different states of the "surface" of the chain. For example, $\beta = 0$, $\gamma = 0$ correspond to the chain with fixed terminal points. Another set of parameters, $\beta = 1$, $\gamma = 1$, describes a "relaxed surface" where the forces on terminal sites are equal to zero. We present results of calculations with these two choices of the boundary conditions.

Our first goal is to convert the differential equation (2) into the discrete form. We can do this considering separately free propagation of electromagnetic waves between sites and its scattering due to the interaction with a dipole moment at the site. Let E_n and E_n' be the magnitude of the electromagnetic field and its derivative right after scattering at the nth site. The electric field E remains continuous at a scattering site, while its derivative undergoes the jump, which is equal to $-4\pi k^2 P_n$. Finally, one can derive the system of difference equations, that can be written with the use of the transfer matrix, T, in the form

$$v_{n+1} = T_n v_n, \qquad (6)$$

where we introduced the column vector, v_n, with components P_n, P_{n+1}, E_n, D_n ($D_n = E_n'/k$) and the transfer matrix, T_n, that describes the propagation of the vector between adjacent sites,

$$T_n = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & -\dfrac{\Omega_n^2 - \omega^2}{\Phi} & \dfrac{\alpha}{4\pi\Phi}\cos ka & \dfrac{\alpha}{4\pi\Phi}\sin ka \\ 0 & 0 & \cos ka & \sin ka \\ 0 & -4\pi k & -\sin ka & \cos ka \end{pmatrix}. \qquad (7)$$

The dynamical state of the system at the right end of the chain, which is represented by the vector v_N, can be found from the initial state at the left end, v_0, by means of the repetitive use of the transfer matrix, T,

$$v_N = \prod_1^N T_n v_0. \qquad (8)$$

Since we consider the system with a single defect, all but one T-matrices in Eq. (8) are the same. These matrices have the parameter Ω_n (the only parameter, which distinguish the defect site from the regular sites) equal to Ω. For the matrix T_{n_0}, which corresponds to the defect, $\Omega_n = \Omega_{\text{def}}$. The eigenfrequencies of the pure system, i.e. polariton dispersion laws, can be found by means of the eigenvalues of the T-matrix. There exist four eigenvalues λ, which can be grouped in pairs with the product of the members of each pair being equal to one. The eigenvalues can be found as solutions of the following dispersion equation,

$$\left(\lambda + \lambda^{-1} - 2\cos ka\right)\left(\lambda + \lambda^{-1} + \frac{\Omega^2 - \omega^2}{\Phi}\right) + \frac{\alpha k}{\Phi}\sin(ka) = 0. \tag{9}$$

In the band of propagating states, the solutions of Eq. (9) are complex valued numbers with their absolute values equal to one. In this case the expression $\lambda + \lambda^{-1}$ can be presented in the form $2\cos(Qa)$, where Q is the Bloch wave number. With this replacement the dispersion Eq. (9) takes the same form as the equation obtained from the original equations (1), (2) by means of Fourier transformation. It is important to emphasize that Eq. (9) takes into account the modes of the electromagnetic field not only from the first Brillouin band but also all short-wave components of the field. In this sense, our approach to the problem is truly microscopic. In the band gap of the polariton spectrum, the eigenvalues λ become real valued and describe evanescent modes of the system. Fig. 1 presents the frequency dependence of the absolute value of one of the eigenvalues. The band gap is clearly seen as a region in which the absolute value of λ is greater than 1.

We calculated the transmission coefficient of the electromagnetic waves applying Eq. (8) to the vector v_0, with components $\{P_0, \beta P_0, 1 + r, i(1 - r)\}$, which describes the state of electromagnetic waves and dipole subsystem at the left end of the chain in accordance with boundary conditions (3) and (5). The resulting state at the right end of the chain v_N is to be matched with the corresponding boundary conditions at $n = N$. We considered two kinds of boundary conditions corresponding to fixed, $\beta = \gamma = 0$, and relaxed, $\beta = \gamma = 1$, ends of the chain. For the numeric

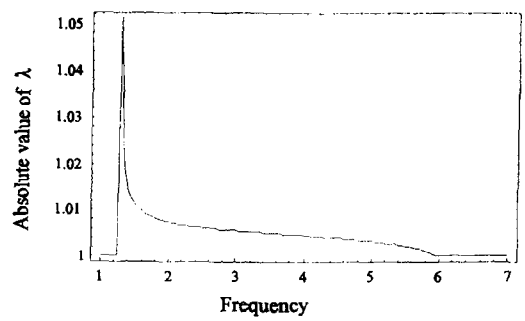

Fig. 1. Frequency dependence of the absolute value of an eigenvalue of the transfer matrix T. In the pass band, the absolute value of λ is equal to 1, in the stop band it is greater than 1.

evaluation we use the chain consisting of 30 atoms, with the defect placed at the 15th site. In order to check the computations, we calculated both transmission and reflection coefficients and verified that the equality $|t|^2 + |r|^2 = 1$ holds with sufficient accuracy.

The results of the calculations are presented in Figs. 2 and 3, which correspond to the fixed and relaxed boundary conditions, respectively. The parameter of the nearest neighbors interaction Φ was chosen to be equal to $\Phi = \Omega^2/3$, so that the maximum frequency of the polarization waves is equal to $\sqrt{5/3}\Omega$. As one can see from Fig. 1, the polariton gap has a lower boundary at a slightly lower frequency, $\simeq 1.24\Omega$. It is caused by the negative dispersion of the polariton waves assumed in the calculations. The frequency in all the figures is normalized by Ω. The wavelength of the electromagnetic waves in the region considered is much greater than the interatomic distance a, the product ka is of order of 10^{-3}, which corresponds to the position of the exciton-polariton gap in real materials. Figs. 2a and 3a present the frequency dependence of the transmission in the pure system for two types of boundary conditions. One can easily recognize the boundary between the pass and stop bands in these figures. The transmission exhibits a rich structure, corresponding to geometrical resonances due to the finite size of the system in the pass band, and monotonically increases with the frequency in the forbidden band. The increase of the transmission is due to the frequency dependence of the penetration length $l = 1/\operatorname{Im} q(\omega)$, where $q(\omega)$ is the imaginary wave number of polaritons inside the gap.

All the other plots in Figs. 2 and 3 show the transmission in a system containing the defect for differ-

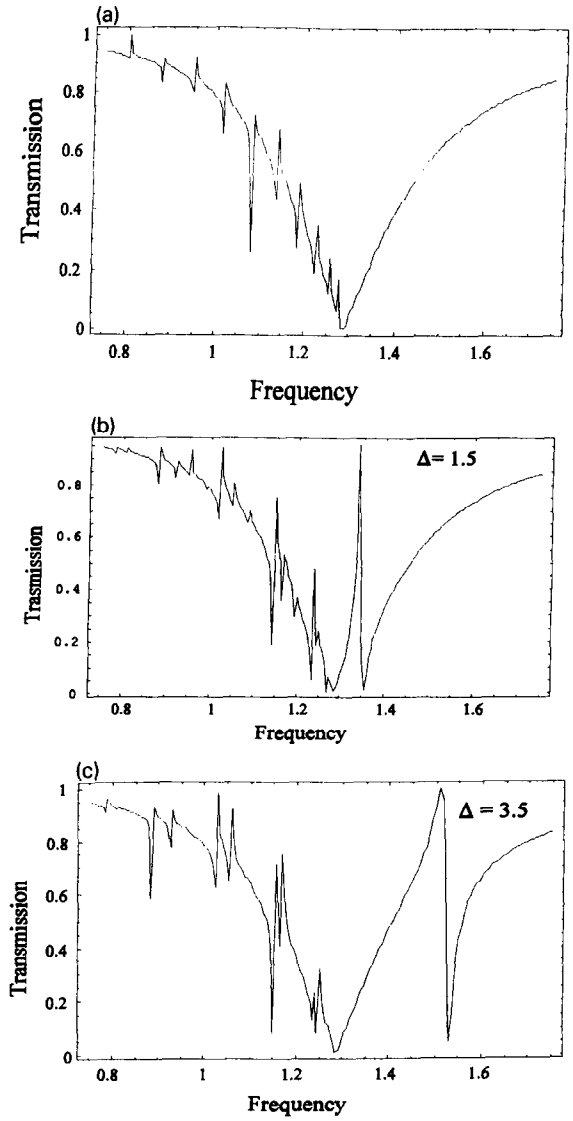

Fig. 2. Transmission through the chain with fixed ends. (a) Pure system, (b) and (c) transmission through the system with the defect for the different strength Δ.

ent values of the parameter $\Delta = (\Omega_{\text{def}}^2 - \Omega^2)/\Omega^2$, which determines the strength of the defect. One can see that the defect induces a resonant maximum at a certain value of frequency, ω_r, inside the forbidden gap. Though resonance tunneling takes place for both kinds of boundary conditions, the effect is much more prominent in the case of fixed ends. This fact is in agreement with the overall greater transmission for the latter situation than in the case of "relaxed" ends. The

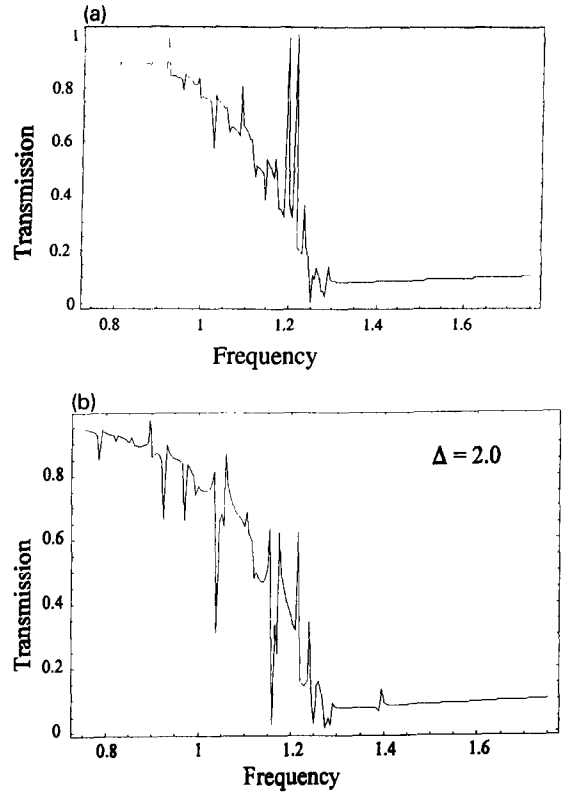

Fig. 3. Same as in Fig. 2 but for the chain with free ends.

positions of the maxima was found to be independent of the position of the defect in the chain as it should be expected. We set the defect at different sites and found just a slight modification of the shape of the maxima and their heights, but not the positions.

The value of ω_r depends upon the strength of the defect, it moves toward higher frequencies with increase of Δ. This behavior is in accordance with the results of Refs. [2,3] regarding the eigenfrequencies of local polariton states. For the model considered the frequency of the local polariton is determined by an equation similar to that obtained in Ref. [2],

$$1 = \Delta \int_{-\pi}^{\pi} \left[\left(k^2 - 1 - \frac{2\Phi}{\Omega^2} \cos x \right) [\cos(ka) - \cos x)] - \frac{\alpha k}{2} \sin(ak) \right]^{-1} [\cos(ka) - \cos x]. \qquad (10)$$

In Fig. 4 we present the dependence of the resonance frequency, ω_r, and the eigenfrequency of the local

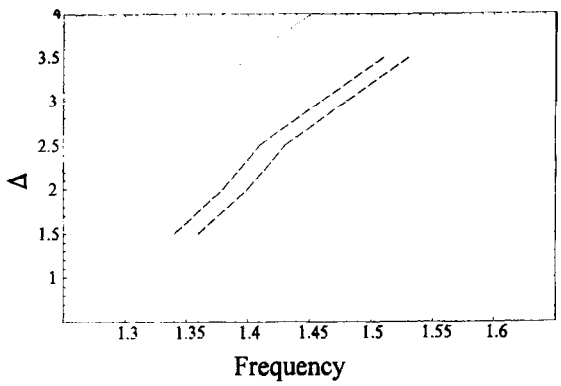

Fig. 4. Solid line: relationship between eigenfrequencies of the local polaritons and the defect parameter Δ. Dashed lines: positions of the resonance tunneling maxima for different Δ. Upper dashed line: chain with fixed ends; lower one: chain with free ends.

mode upon the defect parameter, Δ. One can see that these dependences are consistent with each other. The deviation of ω_r from the eigenfrequency is obviously due to the frequency dependence of the width of the resonance.

According to Eq. (10), local polaritons arise only for positive Δ. Indeed, when we change the sign, the resonance maximum inside the stop-band disappears (Fig. 5). At the same time, one can identify in Fig. 5a a new peak in the pass band, which arises due to the defect. Though there are no new eigenstates in the region of the continuous spectrum, the defect, nevertheless, causes resonance scattering of propagating polaritons. This effect is known as quasilocal or resonance "states," for example, in phonon physics [6,7], and was discussed for polaritons by Hopfield [10]. The defect-induced maximum observed in the pass band in Fig. 4a is caused by such "quasilocal states". Surprisingly enough, is the absence of a quasilocal resonance in Fig. 4b. This represents the transmission in the case of a "free" surface. Instead, we observe a strong dip in the transmission which was not present in the transmission of the pure chain. This situation of antiresonance scattering is interesting but requires separate consideration.

In conclusion, we have numerically shown that an electromagnetic wave with macroscopic wavelength can exhibit resonance tunneling through the forbidden polariton band ("restrahlen region") via a microscopic defect, for example, an impurity atom. The tunneling is due to the local polariton states associated with the

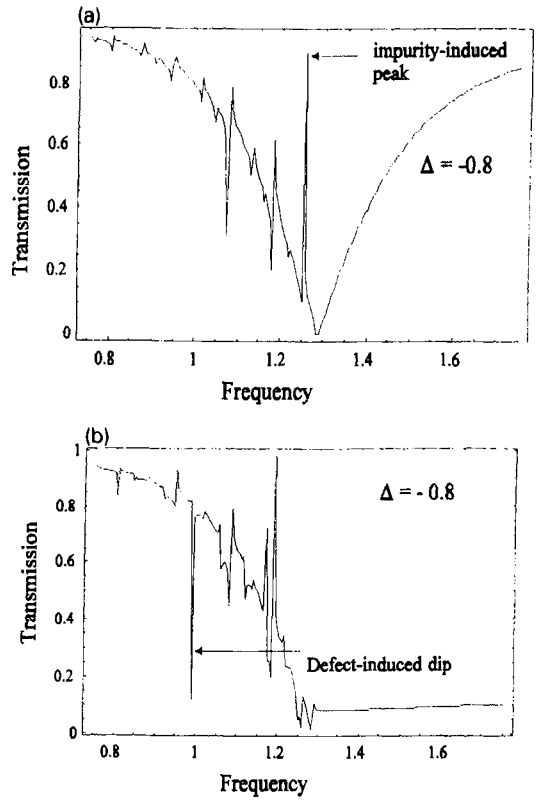

Fig. 5. Quasilocal states in the pass band for the chain with (a) fixed and (b) free ends.

defect and occurs for waves with wavelengths as much as three orders of magnitude greater than the interatomic distance. Electromagnetic waves were treated in the paper microscopically in the sense that we took into account the lattice structure of the medium and all the modes of the electromagnetic field including those with wave lengths shorter than π/a.

The results of the Letter have important implications for the physics of the local polaritons. They demonstrate that, despite the small relative contribution of the electromagnetic component, the electromagnetic field of the states plays an essential role in an interaction of the local states with external electromagnetic field.

Though we have considered the one-dimensional single-mode model, the main result obtained in the Letter – the existence of resonance tunneling of electromagnetic waves due to the local polariton states – can be expanded to more realistic situations. The one-dimensional nature of the model allowed for the microscopic treatment, which would not be feasible

otherwise. Once we have confirmed the assumption of Ref. [2] that shortwave component of electromagnetic waves do not affect the local polariton states in any significant way, one can treat the system in the framework of macroscopic methods and turn to the consideration of more realistic models. Though the resonance tunneling through a thin slab of a real 3D material will have more complicated properties, the essence of the effect will remain the same.

The most serious difference between our single-mode model of electromagnetic waves and real situations is the absence of longitudinal modes in our model. These modes could fill the gap between polariton branches and reduce the lifetime of local polaritons. It is important to emphasize, however, that unlike the above mentioned quasilocal states of propagating modes, the transverse components of the local polariton remains localized. Therefore the tunneling nature of electromagnetic wave propagation through the restrahlen region is preserved even in the presence of the longitudinal modes.

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