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Defect-induced resonant tunneling of electromagnetic waves through a polariton gap

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Abstract. – We consider tunneling of electromagnetic waves through a polariton band gap of a 1-D chain of atoms. We analytically demonstrate that a defect embedded in the structure gives rise to the resonance transmission at the frequency of a local polariton state associated with the defect.

The optical properties of materials with band gaps in their electromagnetic spectrum have recently attracted a great deal of attention. It was suggested that fundamental electromagnetic processes such as spontaneous emission [1,2], photon-atom interaction [2,3], and optical energy transfer [4] are strongly modified at band gap frequencies. Photonic crystals, which are periodic structures with a macroscopic period [5], present one of the primary examples of systems with electromagnetic band gaps. The periodicity in photonic crystals gives rise to allowed and forbidden bands for electromagnetic waves in basically the same manner as periodicity in the arrangement of atoms causes the band structure for electrons in solids.

An important property of photonic crystals is an occurrence of local photon states with frequencies inside band gaps, when the periodic structure is locally distorted. The fact that an isolated defect in an otherwise perfect periodic crystal can give rise to local modes with frequencies in forbidden gaps of a host structure is well known in solid-state physics. Local photons are similar in many aspects to other types of local states: Their frequencies always belong to forbidden gaps; in 3-D systems they split off the continuous spectrum only if the “strength” of a defect exceeds a certain threshold [6-8]; and by changing the type of the distortion one can control the position of the states inside the gap. It is essential, however, that while all other local states appear due to microscopic (of atomic dimensions) defects, local photons require both a macroscopic host structure and its *macroscopic* distortion. This fact is obviously due to the large wavelengths of electromagnetic waves in frequency regions of interest.

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Recently it was suggested that polariton gaps in regular dielectrics with strong polar properties could generate effects similar to those attributed to photonic crystals [9-12]. For example, bounded photon-atom states originally considered in ref. [3] for photonic crystals were proposed in ref. [9] for frequencies within a polariton gap. These states are formed by an optically active impurity atom, which possesses its own dipole moment different from that of the host atoms.

There exists a different type of local photon states, that is not associated with the inner optical activity of the impurities [10]. Such local states are analogous to defect modes in photonic crystals, and similarly to them can be used to modify the spectrum of radiation of the optically active impurities. At first glance it seems impossible, since the electromagnetic waves would not interact with microscopic objects without inner optical activity. However, it was shown in ref. [10] that a regular *microscopic* defect embedded in a crystal lattice gives rise to local states with frequencies within the polariton gap, which are a mixture of the electromagnetic component with excitations of a crystal responsible for the polariton gap. The most remarkable property of the local polaritons is the absence of a threshold for localization in isotropic 3-D systems, which is due to a strong van Hove singularity in the polariton density of states at the gap edge, see details in ref. [10, 11].

In this paper we show that the local states considered in ref. [10] give rise to an interesting possibility of resonance tunneling of electromagnetic waves through a polariton band gap. We would like to emphasize that this tunneling process is remarkably different from both quantum-mechanical electron tunneling [13] and photon tunneling through photonic crystals [7]. The later processes can be characterized as the result of the interaction between excitations and defects of comparable scales (electrons and impurities, electromagnetic waves and *macroscopical distortion* of photonic crystals). The tunneling studied in our paper occurs due to the interaction between electromagnetic waves with *macroscopically* long wavelength and *microscopical* impurities. This process becomes possible owing to participation of the phonon component of polaritons, which mediate the electromagnetic-wave propagation. A similar role is played by excitons in resonance scattering of exciton-polaritons due to impurities with a short-range potential considered by Hopfield in ref. [14].

We present an exact analytical solution for the transmission coefficient of a scalar wave propagating through a 1-D chain of non-interacting atoms containing a defect. These atoms are coupled to the wave due to a dipole moment caused by their mechanical vibrations. The spectrum of the coupled excitations of the chain and the field, polaritons, have a spectral gap where the excitations can exist only in an evanescent form. We show, however, that a defect, embedded in such a structure, results in the resonance tunneling of waves with the transmission coefficient independent of the chain's length and being of the order of magnitude of one. One-dimensional models usually describe tunneling processes fairly well because, by virtue of tunneling, the propagating wave is effectively confined in the transverse directions. In our particular situation it is also important that the local polariton states (transmitting centers) occur without a threshold in 3-D systems as well as in 1-D systems [10, 11]. A similar model has been studied numerically in ref. [12], where a direct interaction between atoms of the chain (leading to the spatial dispersion of the chain's excitations) has been taken into account. The results of that paper suggest that though the spatial dispersion brings about some new features, it does not affect the existence of the resonance, justifying our neglect of the inter-atomic interaction.

The atoms in our system are represented by their vibrational polarizability β_n , where the subindex n represents the position of the atom in the chain. The polarizability is given by

$$\beta_n = \frac{\alpha}{\omega^2 - \Omega_n^2}, \quad (1)$$

where α is a coupling parameter between the dipoles and the field, and Ω_n^2 represents an atom's vibrational frequency. The defect in our model differs from the host atoms in this parameter only, so $\Omega_n^2 = \Omega_0^2$ for all sites except one occupied by the defect, where $\Omega_n^2 = \Omega_1^2$. Polaritons arise as collective excitations of dipoles (polarization waves) coupled to the electromagnetic wave $E(x_n)$ by means of a coupling parameter α . The electromagnetic subsystem is described by the following equation of motion:

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

where the right-hand side is a polarization density caused by atomic-dipole moments, and c is the speed of the wave in vacuum. The coordinate x in eq. (2) goes along the chain with the interatomic distance a .

We first derive an equation for the frequency of the local polariton state in the 1-D situation. The one-dimensional nature of the model allows us to approach the problem microscopically and to take into account short-wave components of the field, including those beyond the first Brillouin band, exactly. Passing to the long-wave limit at the last stage of the calculations we avoid non-physical divergencies and renormalization procedures of the kind used in ref. [9]. The equation for an eigenfrequency of the local mode is

$$1 = \Delta\Omega^2 \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} \frac{\cos(ak) - \cos\left(\frac{a\omega}{c}\right)}{[\omega^2 - \Omega_0^2 - 2\Phi \cos(ka)] \left[\cos(ka) - \cos\left(\frac{a\omega}{c}\right) \right] - \frac{2\pi\alpha\omega}{c} \sin\left(\frac{a\omega}{c}\right)} dk, \quad (3)$$

where $\Delta\Omega^2 = \Omega_1^2 - \Omega_0^2$. It has a real-valued solution only if the frequency falls into the gap between the upper and the lower polariton branches. The integral in eq. (3) can be calculated exactly to yield

$$\omega^2 = \Omega_1^2 - d^2 \frac{\omega a}{2c} \frac{\Delta\Omega^2}{\sqrt{(\omega^2 - \Omega_0^2)(\Omega_0^2 + d^2 - \omega^2)}}, \quad (4)$$

where we passed to the long-wave limit $\omega a/c \ll 1$, and introduced the parameter $d^2 = 4\pi\alpha/a$, which determines the width of the polariton gap between Ω_0^2 and $\Omega_0^2 + d^2$. The second term in eq. (4) is small for realistic values of the parameters, therefore, the frequency of the local mode is only slightly different from the defect frequency Ω_1^2 . As we shall see below, this fact has a deep impact upon the transmission frequency profile of the chain.

The field in the eigenmode corresponding to the frequency determined by eq. (4) exponentially decreases away from the defect site:

$$E = E_{\text{def}} \exp[-\kappa a(n - n_0)], \quad (5)$$

where κ is an inverse localization length of the state, which in the long-wavelength approximation is given by

$$\kappa = \frac{\omega}{c} \sqrt{\frac{\Omega_0^2 + d^2 - \omega^2}{\omega^2 - \Omega_0^2}}. \quad (6)$$

In order to consider transport properties of the model, one has to subject eq. (2) to the standard boundary conditions. We assume that incident and transmitted electromagnetic waves propagate in vacuum so that the transmission, t , and the reflection, r , coefficients are defined in the usual way:

$$E(0) = E_{\text{in}}(1+r); \quad \frac{dE}{dx} = ik_{\omega}E_{\text{in}}(1-r); \quad E(L) = tE_{\text{in}} \exp[ik_{\omega}L]; \quad \frac{dE}{dx} = ik_{\omega}tE_{\text{in}} \exp[ik_{\omega}L], \quad (7)$$

where $k_\omega = \omega/c$ is the wave number of the electromagnetic wave in vacuum, and L is the length of the chain. Our first goal in treating the problem of resonance tunneling is to convert the differential equation (2) into the discrete form. We can do so considering separately free propagation of electromagnetic waves between sites and 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 just after scattering at the n -th site. The electric field E remains continuous at a scattering site, while its derivative undergoes a jump, which is equal to $-4\pi k_\omega^2 P_n$. Finally, one can derive the system of difference equations that can be written with the use of the transfer matrix, T , in the form

$$v_{n+1} = T_n v_n, \quad (8)$$

where we introduce the column vector, v_n , with components E_n, D_n ($D_n = E'_n/k_\omega$). The transfer matrix, T_n , describes the propagation of the vector between adjacent sites:

$$T_n = \begin{pmatrix} \cos k_\omega a & \sin k_\omega a \\ -\sin k_\omega a + 4\pi k_\omega \beta_n \cos k_\omega a & \cos k_\omega a + 4\pi k_\omega \beta_n \sin k_\omega a \end{pmatrix}. \quad (9)$$

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: $v_N = \prod_1^N T_n v_0$. In the case of a single impurity, the matrix product is conveniently calculated in the basis, where the matrix T for a host site is diagonal. With the use of the boundary conditions given by eq. (7), one finally arrives at the following expression for the transmission coefficient, t , in the limit $\kappa L > 1$:

$$t = \frac{t_0}{(1 + \varepsilon) + i \exp[-ik_\omega L] \Gamma t_0 \cosh[\kappa a(N - 2n_0 + 1)]}, \quad (10)$$

where t_0 is the transmission coefficient in the pure system, $\Gamma = 4\pi k_\omega \varepsilon \beta / (\sin(k_\omega a) \sqrt{D})$, $D = (4\pi k_\omega \beta)^2 + 16\pi k_\omega \beta \cot(ak_\omega) - 4$, and $\varepsilon = 4\pi k_\omega (\beta_{def} - \beta) / \sqrt{D}$. The last parameter reflects the difference between host atoms and the impurity, and is equal to

$$\varepsilon = \frac{4\pi\alpha}{c\sqrt{D}} \omega \frac{(\Omega_1^2 - \Omega_0^2)}{(\omega^2 - \Omega_0^2)(\omega^2 - \Omega_1^2)}. \quad (11)$$

The transmission coefficient t_0 of the pure system is given by

$$t_0 = \frac{2e^{ik_\omega L} \exp[-\kappa L]}{1 - \frac{i}{\sqrt{D}} (2 - 4\pi k_\omega \beta \cot k_\omega a)} \quad (12)$$

and exhibits a regular exponential decay.

Equation (10) describes the resonance tunneling of the electromagnetic waves through the chain with the defect. The resonance occurs when

$$1 + \varepsilon = 0, \quad (13)$$

with the transmission becoming independent of the system size. Substituting the definition of the parameter ε from eq. (11) in eq. (13) one arrives at the equation identical to eq. (4) for the frequency of the local polariton state. Typically, for resonant tunneling, the transmission takes a maximum value when the defect is located in the middle of the chain, $N - 2n_0 + 1 = 0$, and in this case

$$|t_{\max}|^2 = \frac{1}{\Gamma^2} \leq 1. \quad (14)$$

The width of the resonance is proportional to Γt_0 and exponentially decreases with an increase of the system's size. In the long-wave limit $ak_\omega \ll 1$, eq. (14) can be rewritten in the following form:

$$|t_{\max}|^2 = 1 - \left(1 - 2 \frac{\omega_r^2 - \Omega_0^2}{d^2}\right)^2, \quad (15)$$

where ω_r is the resonance frequency satisfying eq. (13). It is interesting to note that the transmission becomes exactly equal to one if the resonance frequency corresponds exactly to the center of the polariton gap. This fact has a simple physical explanation. For $\omega_r^2 = \Omega_0^2 + d^2/2$ the inverse localization length κ becomes exactly equal to the wave number ω_r/c of the incoming radiation. Owing to this fact the field and its derivative inside the chain exactly match the field and the derivative of the incoming field as though the optical properties of the chain are identical to those in vacuum. Consequently, the field propagates through the chain without reflection.

Equations (10) and (14) demonstrate that the frequency profile of the resonance is considerably different from a corresponding Lorentzian profile for electronic and other known instances of tunneling. This occurs because the parameter ε diverges at $\omega = \Omega_1$ causing the transmission to vanish. At the same time the resonance frequency ω_r is very close to Ω_1 , as follows from eq. (4). This results in a frequency dependence of the transmission strongly skewed toward lower frequencies.

Having solved the transmission problem, we can find the magnitude of the field inside the chain in terms of the incident amplitude, E_{in} , at the resonance frequency. Matching the field in the local polariton state given by eq. (5) with the outgoing field we have for the field amplitude at the defect atom

$$E_d = E_{\text{in}} t \exp[-ikL] \exp[(N - n_0)\kappa a]. \quad (16)$$

For $|t|$ being of the order of one in the resonance, this expression describes the drastic exponential enhancement of the incident amplitude at the defect side due to the effect of the resonance tunneling. This effect is an electromagnetic analogue of charge accumulation in the case of electron tunneling [15].

Resonance tunneling is very sensitive to the presence of relaxation, which phenomenologically can be accounted for by adding $2i\gamma\omega$ to the denominator of the polarizability β . This will make the parameter ϵ complex valued, and the resonance condition $\text{Re}(\epsilon) = -1$ may only be fulfilled if the relaxation is as small as $\gamma < (ad^2)/(4c)$. This inequality has a simple physical meaning: it ensures that the distance between the resonance frequency and Ω_1 , where the transmission goes to zero, is greater than the relaxation parameter γ . This is a strict condition that can only be satisfied for high-frequency oscillations with large oscillator strength in molecular crystals with large molecules in an elementary cell, and, respectively, large values of the interatomic spacing a . Another interesting opportunity can arise in the so-called atomic optical lattices, where atoms, trapped by a laser beam, form a lattice with spacing practically equal to the wavelength of the trapping field [16]. However, taking into account the spatial dispersion can lead to a more favorable situation for the tunneling resonance in our model. Numerical results of ref. [12] show that the spatial dispersion does not change the transmission properties significantly. Therefore, one can rely upon eq. (10) to estimate the effect of the dissipation in the presence of the spatial dispersion, assuming that it only modifies the parameter ϵ . The eigenfrequency of the local mode in the presence of the direct inter-atomic interaction is calculated exactly. The interaction moves the resonance frequency farther away from Ω_1 undermining the influence of the damping. Adjusting ϵ correspondingly one can arrive at the following new condition for the resonance to survive the relaxation:

$(\gamma\Omega_1)/\Phi < 1$, where Φ is the parameter of the inter-atomic interaction; it can be estimated as a bandwidth of the polarization waves (in terms of squared frequencies). This condition can be fulfilled, even for phonons with a relatively small negative spatial dispersion, and becomes even less restrictive in the case of Frenkel excitons in molecular crystals. The imaginary part of ε will prevent the exponential factor t_0 in eq. (10) from canceling out at the resonance. This restricts the length of the system in which the resonance can occur. The requirement that $\text{Im}(\varepsilon)$ be much smaller than t_0 leads to the following condition: $L \ll 1/(\kappa |\ln[\text{Im}(\varepsilon)]|)$, with $\text{Im}(\varepsilon)$ being again of the order of $\min[(4\gamma c)/(ad^2), (\gamma\Omega_1)/\Phi]$.

Concluding, we showed that a regular defect atom without internal degrees of freedom and an optical activity results in resonance tunneling of electromagnetic waves through a polariton gap. Though we considered the one-dimensional model, one can expect that the existence of the effect does not depend upon dimensionality because tunneling transport is virtually one-dimensional, and the polariton local states are present in the system of any dimension.

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