

Polariton Impurity Band

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Abstract. The impurity induced band arising in the gap of the polariton spectrum is studied analytically for a linear chain of dipoles. The Lyapunov exponent and the density of states of the excitations of the impurity band are calculated within the framework of the approximate microcanonical method. Analytical results are in excellent agreement with numerical simulations.

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The problem of light localization attracted a great deal of attention during the last two decades. New opportunities in this area opened up with development of the structures with periodically modulated dielectric properties, so called photonic crystals [1, 2]. Introducing isolated defects in such a structure, one can create local photon modes similar to well known defect phonon modes in regular crystals [3, 4] or electron impurity states in semiconductors [5]. The intriguing possibilities of photonic crystals initiated interest in optical effects in other types of photonic band-gaps. Such gaps exist, for example, between different polariton branches. It was shown in Refs. [6, 7] that a regular isotopic defect without any intrinsic optical activity can give rise to local states inside the polariton band-gap. These states are coupled states of the electromagnetic wave with elementary excitations of a crystal (e.g., phonons or excitons), with both components, including the electromagnetic component, being localized in the vicinity of the defect.

When the concentration of defects increases, the impurity band is formed inside the gap of the polariton spectrum. This situation was investigated numerically in Ref. [8]. In this paper we present results of an analytical study of the properties of this band.

We consider a one dimensional chain of atoms with dipole moments P_n , where n is a position of an atom in the chain. The dynamics of the dipole chain interacting with a scalar “electromagnetic field” $E(x)$ is described within the tight-binding approximation

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

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

where Φ is the parameter of the interaction between the dipoles, α is a coupling parameter, Ω_n^d represents a site energy, c is the speed of the electromagnetic wave in vacuum, and a is the lattice constant. We assume that the chain is composed of atoms of two different types which differ in their site energy $\Omega_n^d = \Omega_0^d + \Delta\Omega^d c_n$, where $\Delta\Omega^d = \Omega_1^d - \Omega_0^d$. Ω_0^d and Ω_1^d are site energies of the host atoms and the impurities, respectively, and c_n is a random variable which takes values 0 and 1 with probabilities $1-p$ and p , respectively. Eq. (1) can be interpreted in terms of both exciton-like and phonon-like excitations.

Considering the propagation of the electromagnetic wave as a sequence of scattering events separated by free propagation, one can present Eq. (2) in a discrete form. Then the system of dynamic equations (1) and (2) can be transformed into a transfer-matrix form: $v_{n+1} = \hat{r}_n v_n$, where vectors v_n represent the state of the system. In general, the matrix \hat{r}_n , which describes the field propagation between adjacent sites, is a 4×4 matrix [8, 9]. However, numerical simulations carried out in Refs. [8, 9] showed that the most of features of the impurity induced polariton band are well reproduced even in the absence of the dispersion ($\Phi = 0$) when the transfer matrix reduced to the following form:

$$\hat{r}_n = \begin{pmatrix} \cos ka & \sin ka \\ -\sin ka + \beta_n(ka) \cos ka & \cos ka + \beta_n(ka) \sin ka \end{pmatrix}, \quad (3)$$

where the parameter $\beta_n = d^2/(\omega^2 - \Omega_n^d)$, with $d^2 = 4\pi\alpha/a$, represents the vibrational polarizability of the n -th dipole.

The main object of interest in studies of one-dimensional disordered systems is the Lyapunov exponent (LE),

$$\lambda = \lim_{L \rightarrow \infty} \frac{1}{L} \ln \frac{\left\| \prod_1^N \hat{r}_n v_0 \right\|}{\|v_0\|}, \quad (4)$$

where L is the total length of the chain consisting of N atoms. LE is a self-averaging quantity characterizing the spatial extent of the envelope of system eigenstates. It also describes the typical value of the transmission coefficient, $T_{typ} \approx \exp(-\lambda L)$.

Consideration of local polariton states shows that the localization length, l_0 , of an individual local state can be so large that even in the case of a rather small concentration of impurities $(pl_0)/a \gg 1$. In this limit of the well-developed polariton impurity band the microcanonical method [10] can be successfully used for calculation of LE (4). This method enables us to calculate the density of states (DOS) as well.

Even though LE, defined by Eq. (4), has a non-random value, it is convenient to perform averaging over the random configurations of the impurities for a finite system and after that to consider the thermodynamic limit. When averaging is performed in the microcanonical ensemble, the total number of impurities is fixed and the only source of fluctuations is local arrangements of the atoms. At the same time the result of the averaging in the limit $L \rightarrow \infty$ should not depend upon the type of ensemble used by virtue of the self-averaging nature of LE. The key idea of the microcanonical method is based upon the assumption that fluctuations in the microcanonical ensemble are significantly reduced and, one can obtain reliable results when the microcanonical ensemble average of $\langle \ln(\dots) \rangle$ is replaced by $\ln(\dots)$. Such a substitution gives an exact

result in the case of commuting matrices, and leads to excellent agreement between analytical calculations and simulations in the case of 2×2 matrices with a single band spectrum [10].

When applying the microcanonical method, one introduces the matrix $\hat{D}(x) = \hat{\tau}_0 + x\hat{\tau}_1$, with $\hat{\tau}_0$ and $\hat{\tau}_1$ representing host and defect matrices, respectively. Averaging over the microcanonical ensemble is reduced to a contour integration with respect to the variable z . In the limit of large N the integration is performed by means of the saddle point method [10]. As a result, we arrive at the following expression for the complex valued LE, $\tilde{\lambda}$:

$$\tilde{\lambda} = \frac{1}{\alpha} [\ln \nu(x_0) - (1-p) \ln x_0 + p \ln p + (1-p) \ln(1-p)], \quad (5)$$

where $\nu(x)$ is the largest eigenvalue of the matrix $\hat{D}(x)$ and x_0 is the saddle point of the contour integral. The real part of $\tilde{\lambda}$ represents LE, $\lambda = \text{Re}[\tilde{\lambda}]$, while its imaginary part gives the integral DOS in the impure system, $N(\omega) \propto \text{Im}[\tilde{\lambda}]/\pi$.

Eq. (5) can be used to describe the modification of the original polariton spectrum due to defects as well as the new impurity induced polariton band, which arises within the original gap. The lower boundary of the gap, Ω_0 , is not affected by the impurities, while the upper boundary shifts toward higher frequencies with an increase of concentration, and when $p = 1$ it coincides with the upper band boundary of the new crystal, $\Omega_L^i = \sqrt{\Omega_1^2 + d^2}$. The impurity band grows asymmetrically with an increase of concentration: while its lower boundary moves towards Ω_0 , the upper edge remains fixed at Ω_1 . Such a behavior of the impurity band agrees well with the numerical results of Ref. [8]. For small concentrations the width of the impurity induced band is a linear function of p when Ω_1 is not very close to the upper boundary of the initial polariton gap Ω_L ,

$$\Delta_{\text{im}}^2 \approx pc^2(\Omega_1^2 - \Omega_0^2)/(\Omega_0^2 + d^2 - \Omega_1^2). \quad (6)$$

When Ω_1 becomes closer to Ω_L , a crossover to $\Delta_{\text{im}}^2 \approx \sqrt{d^2(\Omega_1^2 - \Omega_0^2)p}$ behavior becomes possible.

Evaluation of DOS and LE can be done in the form of an expansion in series of the parameter that measures disorder in the distribution of impurities: $\epsilon = l_{\text{def}}/l_0$, where l_{def} is a mean distance between impurities. Within allowed bands, DOS appears to be of the zeroth order in ϵ , while LE starts from the first order. For the forbidden bands, the situation is reversed: LE contains a term of the zeroth order in ϵ , while $N(\omega) = 0$. This fact allows one to interpret the zero-order of the used approximation as a description of an effective medium, while the next terms represents corrections due to fluctuation in the positions of the impurities.

The localization length, $l(\omega)$, grows significantly inside the impurity induced band with the maximum in the center, $\omega_c^2 = \Omega_1^2 - \frac{1}{2}\Delta_{\text{im}}^2$. Expansion of $l(\omega)$ in the vicinity of the maximum leads to a parabolic frequency dependence

$$l(\omega) = \lambda(\omega)^{-1} = 2l_0(p/l_0) \left[1 - 20\gamma^2(\omega) (\omega^2 - \omega_c^2)^2 / d^4 p^2 \right], \quad (7)$$

where $\gamma(\omega)$ is the longwave dielectric function of the pure chain. While the localization length grows linearly with the concentration, its maximum flattens as in proportion

$\omega \propto 1/\gamma^2$ - a fact we first observed in numerical simulations [8]. At the same region the DOS can be evaluated as

$$N(\omega) = \frac{1}{\pi l_0} \left[1 + \frac{4|\gamma|\omega_c}{pd^2} (\omega - \omega_c) + O\left(\left(\frac{\omega - \omega_c}{d}\right)^2\right) \right]. \quad (8)$$

The first term in Eq. (8) represents the total number of states in the lower half of the impurity band, which does not depend upon the concentration of impurities. The coefficient of the second term gives the differential DOS at the center and can be rewritten as $\rho(\omega_c) \simeq 2/\pi l_0 \Delta_{Im}$. This DOS is simply the average density of states uniformly distributed through the entire band over the distance of $l_0/2$. $1/\pi\rho(\omega_c)$ can also be viewed as a group velocity, v , of excitations in the center of the impurity band in the case of a uniform distribution of impurities:

$$v = pd^2/4\omega_c^2 \gamma^{3/2} \ll c, \quad (9)$$

which demonstrates that polariton excitations of the impurity band have much slower velocities even when compared to the velocities at both regular polariton branches.

The expansion developed above is not valid for frequencies close to the band boundaries. This reflects the well known fact that perturbation expansions in disordered systems usually fail in the vicinity of boundaries of the original spectrum [11]. Regularizing the expansion near these boundaries, one can obtain non-analytic corrections to their positions ($\propto (t_{def}/l_0)^{1/2}$ and $\propto (t_{def}/l_0)^{2/3}$ for the lower impurity band edge ω_L and the bottom of the upper polariton branch, respectively). The differential densities of states near the lower and upper boundaries of the impurity band have forms

$$\rho_L(\omega) = \frac{3}{\pi d} \left(\frac{\gamma}{l_0}\right)^{1/2} \frac{1}{(l_0 p)^{1/2}} \frac{\omega}{(\omega^2 - \omega_L^2)^{1/2}}, \quad \rho_U(\omega) = \frac{d\omega p^{1/2}}{\pi c (\Omega_U^2 - \omega^2)^{3/2}}. \quad (10)$$

DOS diverges much more strongly near the upper boundary, which is typical for resonance frequencies.

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