Dispersion characteristics of electromagnetic excitations in a disordered one-dimensional lattice of coupled microresonators

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1. Introduction

Development of optical quantum information processing devices has created an ever-increasing demand for structures capable of “slowing down” the light [1], i.e. the effective reduction of group velocity of polaritons. This effect and similar ones occur in a variety of systems such as coupled optical resonators [2,3], solid multilayer semiconductor structures [4], bulk crystals with strong light-matter coupling (GaN, ZnO, see e.g. Refs. [5,6]) etc. There are a number of theoretical and practical problems connected with fabrication of polaritonic crystals [7,8], which present a particular type of photonic crystals [9] featured by a strong coupling between the medium quantum excitations (excitons) and the optical field. The key role in decreasing the group velocity of light is played by the peculiar properties of the so-called “dark” and “bright” polaritons, which are linear superpositions of the photonic states of external electromagnetic fields and macroscopic (coherent) perturbations of a two-level atomic medium [7].

An example of polaritonic structure can be given by a spatially periodic system formed of trapped weakly coupled two-component atomic ensembles interacting with the optical field in a tunnel-coupled cavity array [10]. A distinctive feature of such a structure is the capability of polariton confinement, which is quite analogous to light confinement in photonic crystals (see e.g. [11,12]) and exciton confinement in solid quasiperiodic structures [13–15].

An interest for optical modes in microcavity systems was originally motivated by the advent of optoelectronic devices [16,17] and has been steadily growing over the recent years. In this context defect-based resonators in photonic crystals deserve special mentioning [11]. Ref. [18] demonstrated the attainment of a tight binding between such resonators and quantum dots. Refs. [7,8] gave theoretical analysis of the formation of solitons coupled to lower-dispersion branch (LDB) polaritons in a chain of microcavities; the authors suggest that their results may be of significant importance for quantum information processing. Recent progress in fabrication of quality semiconductor microresonators with Bragg mirrors allowed to attain a Bose–Einstein condensation of LDB-polaritons in quantum wells embedded in semiconductor microcavity structures (CdTe/CdMgTe or GaAs) and to explore their superfluidity [13–15].

Based upon the previously developed concepts of ideal polaritonic structures [7,19] here we investigate the effects of varying eigenfrequencies and nearest-neighbor distances on the dispersion of exciton-like electromagnetic excitations in a one-dimensional lattice of microcavities (coupled resonators with no atomic subsystems). Next, we carry out a numerical modeling of polariton dispersion in a non-ideal chain of coupled microresonators containing impurity atomic clusters.

2. Exciton-like electromagnetic excitations in a non-ideal lattice of coupled microcavities

Unlike in Refs. [7,18,19] they devoted to coupled resonators...
with dopant atoms let us here pose a somewhat different problem. Namely, we shall examine a one-dimensional array of tunnel-coupled randomly distributed microresonators of different types at the total absence of atomic subsystem. Each resonator is assumed to possess a single optical mode. We also account for the overlap of optical fields, which enables photons to move along the chain.

Hamiltonian \( H \) of the considered system (see Ref. [7]) is written as

\[
H_{ph} = H^0_{ph} + H_{int},
\]

(1)

where

\[
H^0_{ph} = \sum_{n} E_n \Psi_n^* \Psi_n, \quad H_{int} = - \sum_{n,m} A_{nm} \Psi_n^* \Psi_m
\]

(2)

Indices \( n \) and \( m \) numerate the sites (one per each unit cell) of the one-dimensional resonator chain, \( E_n = \hbar \omega_n \), where \( \omega_n \) is the photonic mode frequency at the \( n \)th site (resonator). Quantity \( A_{nm} \) defines the overlap of optical fields of the \( n \)th and \( m \)th resonators and therefore characterizes the corresponding excitation transfer. \( \Psi_n^* \) and \( \Psi_n \) are Bosonic creation and annihilation operators of the photonic mode respectively. Hamiltonian (1) is formally identical to the excitonic one [20], hence it is natural to refer to the considered electromagnetic excitations as exciton-like.

We assume that the chain of resonators is mainly comprised by the so-called “normal” resonators with “ordinary” values of \( E_n, A_{nm} \) while containing a minor admixture of “defect” resonators whose parameters \( E_n, A_{nm} \) differ from the “ordinary” ones. Such a crystal admits at least two types of disorderliness: a compositional one (defined by distribution of different-type resonators over the sites) and a topological one (defined by varying nearest-neighbor distances between the sites). Under these circumstances Hamiltonian (1) is not translation invariant, whereas the quantities \( E_n \) and \( A_{nm} \) are configurationally dependent. More specifically \( E_n \) depends solely on composition, while \( A_{nm} \) is dependent both upon composition and resonator locations.

A general recipe for evaluation of quasiparticle spectra in non-ideal systems with randomly distributed elements consists in finding the poles of the configurationally averaged Hamiltonian resolvent [21]. The latter is translation invariant, which permits to characterize the corresponding elementary excitation spectrum by a wave vector \( \mathbf{k} \). The necessary calculation can only be carried out in the frames of a certain approximation specific to the studied system. A widespread method of computation of quasiparticle states in imperfect structures is the virtual crystal approximation (VCA), which provides an appropriate tool to clarify the spectrum transformations caused by defect concentration variations. Under the VCA the averaged resolvent is identical to the virtual crystal approximation (VCA) [21,22], which permits to invoke a wave vector \( \mathbf{k} = (k,0,0) \) for description of eigenvalues and eigenfunctions of Hamiltonian (3).

Diagonalization of Hamiltonian (3) via Bogolyubov–Tyablikov transformation [20] leads to the following expressions for excitation energies and overlap parameters of the optical fields of adjacent resonators:

\[
E(k, \{ C_{C} \}, \{ C_{T} \}) = \sum_{\nu=1} E^C_{\nu} - \sum_{\nu,\mu=1} A_{\nu\mu}(k, \{ C_{C} \}) C_{\nu} C_{\mu},
\]

(5)

\[
A_{\nu\mu}^{CT}(k, \{ C_{C} \}) = \sum_{m} A_{nm}^{CT} \exp \{ i k a_{nm} (\{ C_{T} \}) \}
\]

(6)

In (6) \( a_{nm}(\{ C_{T} \}) = a((C_{T})/(n-m)) \), where \( a((C_{T})) \) is the averaged period of the isoperiodic “virtual” one-dimensional resonator chain, \( C_{C}, C_{T} \) are the sets of types and locations of resonators. From Eq. (5) it follows that the dispersion law \( \omega(k) \) of electromagnetic excitations in the considered system is determined by the frequency characteristics of resonators as well as by the explicit form of matrix \( A^{CT}(k, \{ C_{C} \}) \).

To fix our ideas let us examine electromagnetic excitations in a binary chain consisting of two types of resonators \((s = 2)\). We assume that they are arbitrarily distributed and separated by the distances \( a_1 \) and \( a_2 \). If so, expression (5) takes the form

\[
\omega(k, \{ C_{C} \}, \{ C_{T} \}) \approx \sum_{\nu=1} E_{\nu}^{C} - \frac{1}{\hbar} \sum_{\nu,\mu=1} A_{\nu\mu}(k, \{ C_{C} \}) C_{\nu} C_{\mu},
\]

(7)

Next, the Fourier-transform of the matrix \( A^{CT}(k, \{ C_{C} \}) \) appearing in (6) can in the nearest-neighbor approximation [19] be written as:

\[
A^{CT}(k, \{ C_{C} \}) = 2 A^{CT}(a((C_{C}))) \cos ka((C_{T})).
\]

(8)

As for the period \( a((C_{T})) \) of the “virtual” 1D resonator chain it is readily found to be \( a((C_{T})) = C_{TT} a_1 + C_{CT} a_2 \), where the obvious condition \( C_{TT} + C_{CT} = 1 \) must hold. Dependence \( A^{CT}(a((C_{C}))) \), which determines the transfer probability of electromagnetic excitations between neighboring resonators can in the frames of the developed model be written as \( A^{CT}(a((C_{C}))) = A^{CT}(a_1) \exp \{ |a_1| - a((C_{C})) \} \). Quantities \( A^{CT}(a_1) \) characterize the overlap of optical fields of neighboring resonators in an ideal chain of period \( a_1 \). The latter is taken as the reference one for the subsequent variation of distances. Under these circumstances the dispersion law \( \omega(k, C_{C}, C_{T}) \) takes on the form

\[
\omega(k, C_{C}, C_{T}) = \omega_1 + (\omega_2 - \omega_1) C_{C} - A^{CT}(1 - C_{C}^2) + A^{CT}(2 + A^{CT})(1 - C_{C}) C_{T} \times \frac{2}{\hbar} \exp \left( -\frac{C_{T} |a_1 - a_2|}{a_1} \right) \cos (a_1 + C_{T} (a_2 - a_1))
\]

(9)

where notations are adjusted as \( C_{2C} \equiv C_{C}, C_{2T} \equiv C_{T} \). Numerical evaluation of Eq. (9) requires the assignment of modeling frequencies of resonance photonic modes pertaining to the first and the second types of resonators; these we take to be \( \omega_1 = 2 \pi \times 25.0 \text{ THz} \approx 157 \times 10^{12} \text{ Hz} \) and...
Special interest lies in tracing manifestations of spectrum specifics in the quasiparticle density of states \( g(\omega, C_T, C_T) \). As applied to an ideal one-dimensional resonator system function \( g(\omega, C_T, C_T) \) has the form:

\[
 g(\omega, C_T, C_T) = \frac{A(C_T)}{2\pi} \int \delta(\omega(k, C_T, C_T) - \omega)dk
\]

Integration in (10) is carried out for various wave vectors \( k(C_T) \) falling within the first Brillouin zone. Fig. 3 illustrates the concentration dependence of the density of states \( g(\omega, C_T, C_C) \) of electromagnetic excitations for \( C_T = 0.1 \) (case 1) and 0.9 (case 2). It is worthwhile noticing that the definitional domain of function \( g(\omega, C_T, C_C) \) along the \( \omega \)-axis is defined by concentration \( C_T \) (owing to the appearance of \( C_T \) in the expression for the “virtual” crystal lattice period \( a([C_C]) \) and henceforth for the Brillouin zone boundaries). This fact is illustrated by Fig. 3a and b. Quite obviously, the function \( g(\omega, C_T, C_C) \) has singularities only at the ends of the frequency interval \( \omega(k(C_C)) < \omega < \omega(k(C_C)) \), which is fully analogous to the case of phonon spectrum in one-dimensional structures [24].

3. Polaritonic crystal with an atomic subsystem and vacancies

Polaritonic crystal can be created by trapping of two-level atoms in a photonic crystal consisting of tunnel-coupled microcavities. The resulting structure is known as a coupled-resonator optical waveguide (CROW) [4]. Similarly to [25,26] in this section we study a one-dimensional chain of microcavities, each possessing a single optical mode and interacting only with its nearest neighbors. In addition we assume that every resonator contains a macroscopic cluster of one-type ultracold two-level atoms (possessing levels \( |\psi_1 \rangle \) and \( |\psi_2 \rangle \)) and interacting with the quantized electromagnetic field directed normally to the chain (Fig. 4). Optical fields and atomic wave functions are allowed to overlap so that there is a possibility of photon tunneling along the resonator chain. Hamiltonian \( H \) of the considered system reads:

\[
 H = H_{\text{at}} + H_{\text{ph}} + H_{\text{int}}
\]

Here \( H_{\text{at}} \) corresponds to an ensemble of resonator-trapped two-level atoms (quantum dots), \( H_{\text{ph}} \) corresponds to propagation of light field and \( H_{\text{int}} \) describes the atomic–optical interaction in cavities. Based on the concepts developed e.g. in Ref. [8], the above Hamiltonian components of the ideal photonic structure can be written in the form:
Let us consider a non-ideal system of the described type – a polaritonic structure with atomic subsystem and impurity atomic clusters. As above the spatial distribution of resonator traps is translation invariant (with lattice parameter L). The atomic subsystem is however allowed to contain randomly distributed foreign (relative to an ideal system) quantum dots (with one atomic complex of certain type per cavity). If so, the atomic subsystem-related parameters of the problem are configurationally dependent. Numerical simulation of such a system can be performed in the frames of the virtual crystal approximation, which essentially consists in replacement of configurationally dependent Hamiltonian parameters in their configurationally-averaged values. In our case the corresponding quantities are \( \omega_{\alpha \beta} \), \( \gamma_{\alpha \beta} \), \( g_{\alpha \beta} \), and being configurationally averaged they can be written as

\[
\langle \omega_{\alpha \beta} \rangle = \sum \omega_{\alpha \beta}, \quad \langle \gamma_{\alpha \beta} \rangle = \sum \gamma_{\alpha \beta} \quad \langle g_{\alpha \beta} \rangle = \sum g_{\alpha \beta} \gamma_{\alpha \beta}
\]

where \( C^\alpha \) are concentrations of atomic clusters (quantum dots) of different types (numbered by \( \nu \)), which are subject to the constraint \( \sum C^\alpha = 1 \). \( \omega_{\alpha \beta}, \gamma_{\alpha \beta}, g_{\alpha \beta} \) are parameters related to the \( \nu \)-th type atomic components. Configurational averaging leads to “restoration” (cf. Ref. [19]) of the translation invariance of Hamiltonian and hence allows employing calculation methods described in Refs. [7,19]. Bogolyubov transformation of Hamiltonian describing light and dark polaritons [6] yields the following diagonal form:

\[
H = \hbar \sum_k \Omega_1(k, \{C^\nu\}) \Xi_1^k \Xi_1^* k + \hbar \sum_k \Omega_2(k, \{C^\nu\}) \Xi_2^k \Xi_2^* k
\]

Annihilation operators \( \Xi_1^k \) and \( \Xi_2^k \) in Eq. (16) characterize the two types of quasiparticles resulting from the atom-field optical interaction in (14) are identical \( g = g_1 = g_2 = \ldots = g_M \).

### References


**Fig. 3.** Density of states of exciton-like electromagnetic excitations \( g(\omega, C_T, C_r) \): (a) surfaces \( g(\omega, C_T) \) plotted for \( C_r = 0.1 \) (case 1) and 0.9 (case 2); (b) surfaces \( g(C_T, C_r) \) plotted for frequencies \( \omega = 1.58 \times 10^{14} \) Hz, \( 1.59 \times 10^{14} \) Hz and \( 1.60 \times 10^{14} \) Hz in cases (1), (2) and (3) respectively.

**Fig. 4.** Schematic [7,19] of a polariton crystal: a lattice of microresonators comprised by a macroscopic ensemble of two-level atoms interacting with resonator electromagnetic modes.
interaction, namely the upper- and lower-branch polaritons respectively. The said quasiparticles propagate along the chain of coupled microresonators containing impurity atomic clusters. Characteristic frequencies $\Omega_{1,2}$ in (16) define the dispersion relations as well as polaritonic band structure of the crystal.

To be specific let us consider a non-ideal polaritonic system containing just one type of atoms and vacancies whose concentrations are $C_1$ and $C_2$ respectively. The two concentrations are related as $C_1 + C_2 = 1$. For e.g. the lower-branch polaritons we have then

$$\Omega_2(k, C_i) = \frac{1}{2} [\omega_{at}(k, C_i) + \omega_{ph}(k) - \omega_R(k, C_i)]$$

(17)

Dispersion relations of atomic and photonic subsystems, which enter this equation can fairly accurately be written as

$$\omega_{at}(k, C_i) \approx (1 - C_i) \left[ \omega_{ba} + \gamma k^2 \right]$$

$$\omega_{at} = \omega_{at}(C_i) \approx \omega_{at}(0) - \Delta I(k)$$

$$\omega_{ph}(k) = \omega_{ph} + \alpha v k^2$$

while the Rabi frequency and the atom-field detuning are equal to

$$\omega_R(k, C_i) = \sqrt{4g^2(1 - C_i)^2 + \delta^2}$$

$$= \sqrt{\delta(k, C_i)}$$

(19)

$$= \omega_{ph}(k) - \omega_{at}(k, C_i)$$

(20)

The term $C_i \omega_{ba}$ appearing in (18) is extremely large. Given the average transition frequency of the rubidium $D$-line $\omega_{ba} = 2 \times 382$ THz the mentioned term can amount to several terahertz even for negligible vacancy concentrations ($C_i \sim 10^{-4}$). For comparison, parameter $\alpha$ characterizing the photon tunneling ranges from hundreds of gigahertz to several terahertz, while the field coupling parameter does so from tens to hundreds of gigahertz. (And it is precisely these parameters $\alpha$ and $\beta$, which define the dispersion curve at the absence of vacancies).

The expression for mass of lower-branch polaritons has the form

$$m_2(C_i) = \frac{\hbar}{4 \pi} \frac{\partial^2 \Omega_2(k, C_i)}{dk^2} \bigg|_{k=0}^{-1}$$

$$\approx \frac{2m_{at}(C_i) m_{ph}\omega_R(C_i)}{\left( m_{at}(C_i) + m_{ph} \right) \omega_R(C_i) - \left( m_{at}(C_i) - m_{ph} \right) \Delta I(C_i)}$$

(21)

where

$$\omega_R(k, C_i) \equiv \omega_{ph}(k, C_i) \bigg|_{k=0} = \sqrt{\Delta I(C_i)^2 + 4g^2(1 - C_i)^2}$$

(22)

In formulas (21) and (22) $\Delta I(C_i) \equiv \delta(k, C_i) \bigg|_{k=0} = \Delta + C_i \omega_{ba}$, $m_{ph} = \hbar / 2 v k^2$, $m_{at}(C_i) = \hbar / 2 v (1 - C_i)^2 = M_{at} / (1 - C_i)$.

Concentration dependence of the group velocity for lower-branch polaritons $V_g(k, \{C\})$ is easily obtained from the expressions (17) and (21):

$$V_g(k, \{C\}) \equiv \frac{\partial \Omega_2(k, \{C\})}{\partial k} = \frac{\hbar \sin (kI)}{2m_{ph}}$$

$$\left[ 1 + \frac{m_{ph}}{m_{at}(\{C\})} - \left( 1 - \frac{m_{ph}}{m_{at}(\{C\})} \right) \frac{\omega_{ph}(k) - \omega_{at}(k, \{C\})}{\omega_R(k, \{C\})} \right]$$

(23)

Fig. 5 shows the dependence of polariton mass on vacancy concentration $m_2(C_i)$ evaluated from Eq. (21). Calculation was performed for the following numerical values of parameters: the size of resonators $l = 3 \mu m$, the effective mass of atoms in the lattice at the absence of vacancies $M_{at} = 1.44 \times 10^{-25} \text{kg}$, the effective mass of photons $m_{ph} = 2.8 \times 10^{-36} \text{kg}$, the atom-field detuning (irrespectively of the wave vector) $\Delta = 0$, the average frequency of rubidium $D$-line $\omega_{ba} = 2 \times 382$ THz, and the atom-field coupling parameter $g = 2 \times 12$ GHz. If the vacancies are absent polariton mass equals to $m_2 \approx 2m_{ph} \approx 5.6 \times 10^{-30} \text{kg}$. It is readily seen that even a minute presence of vacancies (one per $10^4$ of resonators) increases the mass of polaritons by an order, which is an illustration of the crucial role of vacancies in reducing the effective excitation velocity in chains of microcavities.

4. Conclusion

Recent experiments and theoretical investigations display an intense interest in microresonator systems whose functional properties show a promise of solution to certain engineering problems such as construction of optical clockworks of unsurpassed accuracy [28–30] as well as the creation of sources of coherent radiation. These endeavors involve the necessity of development of novel polaritonic structures comprised by spatially periodic arrays of coupled resonators [8].

In the present work we use the virtual crystal approximation to calculate the spectrum of exciton-like electromagnetic excitations in a non-ideal binary chain of coupled microcavities (cf. Ref. [31]). The model accounts for the effects of varying lattice composition (fractions of resonators with particular eigenfrequencies) as well as the nearest-neighbor distances. It also permits to elucidate the specifics of concentration dependence of the density of states of the resulting quasiparticles.

Having laid this basis we proceed to study an array of resonators containing an atomic subsystem and investigate the role of vacancies therein. The obtained relations of dispersion of electromagnetic excitations prove noticeably more complex than those of primitive lattices. This complexity is due to a non-ideality of the structure as well as to the presence of two sublattices. It has multiple manifestations in experimentally observable integral characteristics of optical processes.

Computation of electromagnetic waves in more complex resonator systems requires the use of more sophisticated techniques. Depending on particular problems such can be the (one- or
multiple-node) coherent potential method [21], the averaged T-matrix method [23] along with their various modifications. Our work contributes to the numerical modeling of functional materials designed for implementation of controllable propagation of electromagnetic excitations.

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References